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Together, but not the same: Quantifying emergence in collective behaviour

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Submitted in part fulfilment of the requirements for the degree of
Doctor of Philosophy of Imperial College London, December 2024

"There is obviously only one alternative,

namely the unification of minds or consciousnesses.

Their multiplicity is only apparent,

in truth there is only one mind."

— Erwin Schrödinger

Abstract

Adaptive, self-organising collective behaviour, which emerges, or arises from the 'bottom-up' without any leader or central control, is found everywhere in the animal kingdom and is crucial to survival.

Although it is easy to recognise by the naked eye, we still lack a model-agnostic, quantitative measure of emergence that can detect this collective behaviour, is applicable at multiple scales across different systems, and is as robust in simulations as in experimental data sets. This is particularly important in the study of human group activities, which tend to be studied from a 'top-down' hierarchical perspective.

The contributions of this thesis are threefold: first, the $\Psi - \Gamma - \Delta$ criteria of emergence are applied in simple particle systems. We find unintuitive behaviour of emergence measures in one-dimensional Gaussian and Ornstein-Uhlenbeck random walks, and we propose a number of interpretations. However, when applied to collective motion in two dimensions in the Vicsek model, Reynolds model and schooling fish, the criteria correctly detect flocking and schooling behaviour in both simulated and experimental datasets of varying complexity, but only when taking into account the redundancy in the system via partial information decomposition.

Secondly, informed by the case studies, we devise, implement and execute a novel experiment which successfully induces collective motion in humans through solving a spatial multi-agent problem which requires optimising the Ψ measure of emergence. Moreover, we find that successful collective motion is related to individual agency and prosocial behaviour: people with more awareness of group strategies are more likely to be part of winning groups, and moreover, members of winning groups show, on average, higher connectedness to others.

Finally, we conclude with an experimental study of synchronous movement in concert audiences, as quantified by wavelet coherence measures, showing that multiscale patterns of group synchrony can be correlated with novel group experiences.

Statement of originality

This thesis presents the main results of a number of experimental case studies related to collective movement. I declare that the work presented in this thesis is my own work, with a few exceptions that have been acknowledged at the beginning of each chapter, and in the main body where relevant, according to standard referencing practices. In particular, the analysis methods used rely on developments devised by Dr Mediano and Dr Rosas in (Rosas et al., 2020a; Sas et al., 2024b) and by Dr Nozawa in (Nozawa et al., 2019). Some case studies use models of collective behaviour or experimental data provided by other researchers, who are acknoweldged where relevant. Experiments with human subjects were designed by Dr Bor (Sas et al., 2024b) and Dr Nozawa (Nozawa et al., 2023).

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Acknowledgements

I am deeply thankful to my supervisors, Henrik Jensen and William Knottenbelt, for letting me put my mind where my heart is, and for the countless times you guided me through kafkademia. I also must thank Splunk Inc. for providing me with a scholarship that has allowed me to pursue this PhD for three years.

Standing on the shoulders of giants is a quintessential example of collective intelligence: I thank my collaborators Pedro Mediano, Fernando Rosas, Hardik Rajpal, Alberto Liardi and Pedro Palhares, for adventuring with me through mysterious landscapes of bits and nats, neurons and circumvolutions, towards the synergy of discovery; Takayuki Nozawa, for teaching me the flows and ebbs of synchronisation; Max Falkenberg, for being the first to show me the marvels of complexity, and bringing me in the same room as Henrik for the first time; David Dolan and Adrian Brendel, for teaching me about the difference between music and noise; Hillary Leone, for letting her art become our science; Dan Bor, for teaching me about experimental rigour; Jeremy Pitt, for expanding my horizons; but also all students, postdocs, researchers and visitors in the Centre for Complexity Science, for the stimulating brain massages and for teaching me the gospel of emergence.

I am grateful to Chris, whose wizardry helped make it all possible, and to all old friends and new who helped with organising experiments and being test subjects: Alexa, Vanessa, Felix, Armand, Alina, Miruna, Septi, Dragoș, Konstantinos, Christina, Antigoni, Mate, Annabel, Federica, Lala and Eloise. There is no *we* without all of *you*.

A long overdue acknowledgement to my highschool teachers: Mihaela Vișinoiu, Mariana Bahrim, Cristina Homentcovschi, Dorin Arventiev, Rodica Crăciun and Aurora Bărbulescu, who shaped my young brain; and to my undergraduate professors: Tony Field, Paul Kelly, Alastair Donaldson, Murray Shanahan, Naranker Dulay and Michael Huth, who made me feel challenged down to every neuron.

I am thankful to all my friends for their ideas, support and constant intellectual stimulation. You are too many to name, but special credit should go to Ștefan, Buni, Dani, Jules, Max, Bex, Sam, Josh, Nandor, Zeme, Carlos and Yuexuan; as well as Martin for also proofreading so much of my writing. Finally, to my family: my brother Tudor, for wanting to make the world better; my Grandfather, for being the first to stir my love of wisdom; and my Parents, for their neverending support and for drilling into me since I was little that I will grow up into a scientist (and get the Nobel prize)

This thesis is dedicated to Andrei: my roots, my armour and my wings.

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Summary of Chapters

1 Introduction 1

The scientific study of emergence is a broad interdisciplinary endeavour which draws from and is applicable to a vast range of complex systems. As a result, quantitative analysis methods used in the field are very diverse, even though they are used to identify similar properties across heterogeneous phenomena. Many multi-agent systems manifest emergence as a result of self-organised collective behaviour, and in particular this thesis concerns itself with collective behaviour expressed as complex spatio-temporal patterns of movement in groups. The main objective of this thesis is to find and test measures of emergence that are in some way substrate independent and thus can describe and quantify collective movement at many scales, from microscopic particles moving together, to animal groups and human societies.

2 Foundations to complex systems 14

This thesis makes use of methods from complexity science to study collective behaviour and a variety of concepts from statistical physics, information theory, signal processing and time series analysis, and network science. This chapter lays out the basic concepts and building blocks necessary in the search for robust, substrate-independent measures of emergence, including the wavelet analysis used in Chapter 8 and the $\Psi-\Gamma-\Delta$ criteria of emergence used in Chapters 4-7.

3 Simple models of complex systems 49

Complexity theory is a scientific practice which operates on theoretical models of complex systems with the use of simulation and mathematical analysis. In order to focus on the interactions between components and the emergent properties at the system level, this process of modelling aims to represent a phenomenon in the simplest way that still preserves the relevant emergent property. This chapter presents background on how the study of simple models can reveal similarities between very heterogeneous systems and phenomena in nature, and then presents and defines mathematically two simple models with a plethora of multidisciplinary applications in the study of complex systems, namely random walkers and self-propelled particles, and outlines the simplest definitions of collective behaviour in these systems.

4 Quantifying emergence in simple models 76

Measures of complexity, synergy and emergence may characterise emergent behaviour in a complex system in different ways. In this chapter, the models introduced in the previous chapter are used as a test-bed and null case to test the $\Psi - \Gamma - \Delta$ information-theoretic emergence measures, and an unexpected behaviour of the emergence criteria is found. The aim of this chapter is to reveal and discuss concerns about the assumptions and interpretations of information-theoretic measures when analysing complex systems, using the example of mutual information-based synergy-redundancy measures.

5 Case study: schooling and flocking 116

Collective motion, as a special case of collective behaviour, is a quintessential example of emergence, present at all scales in nature, from bacteria to birds, fish and herd animals, to humans. In this chapter, efforts to quantify emergence as well as interactions in collective movement in nature are reviewed and related to results in theoretical models, alongside with motivations for and ramifications of its study. The rest of the chapter shows results from applying information-theoretic methods tested on simple models on experimental movement trajectory data from schooling fish, as well as a more complex multi-agent model of flocking, the Reynolds model.

6 Case study: social structures and collective action 132

In the absence of pre-established hierarchical authority or coercive control, resolving collective action situations through self-organisation requires a range of alternative mechanisms, including voluntary association, mutually-agreed social contracts, or 'bottom-up' emergent social structure. In this chapter, we explore the emergence of social structure in a self-organising multi-agent system called *Megabike*, where cooperation or competition are expressed through movement, and we find causal emergence and downwards causation in all surviving cooperating groups. This is significant in the context of social systems in which local interactions between individuals produce beneficial leadership structures, which have, in turn, causal power over the individuals' agency, and as such expose the society to the risk of degenerative asymmetric power structures.

7 Case study: human groups walking 150

Having used simulation as a laboratory for testing emergence measures, explored their interpretations, and used them on real-world animal data, this chapter presents a new experimenal paradigm and technology for the study of collective self-organised movement in human groups, in which group members must devise strategies to achieve collective motion as quantified by the Ψ measure of emergence, and presents results of analysing

the resulting trajectory data with similar methods to Chapters 4 and 5. Finally, we relate the results to collective intelligence and psychological aspects of the participants, showing collective motion induces higher connectedness to others and is predicted by metacognitive awareness of individual strategies.

8 Case study: Collective motion of concert audiences 172

Physical and physiological synchrony is pervasive in collective human activities, and manifests in many different forms. This chapter focuses on collective synchrony in concert audiences, presenting related work, and aims to explore the collective effects of improvisatonal performance on the audience. In this chapter, we investigate the experience of audience members during a classical music concert by analysing the audience's subjective reports and movement patterns. Our results show that performances with improvisational elements affect movement synchronisation dynamics between audience members differently at different timescales, which are predictive of changes in the subjective perception of music.

9 Conclusions 192

The study of complex systems can provide many beneficial insights to better understand human behaviour, experience and society. In this chapter, we briefly review all the findings of the thesis and relate them to collective intelligence and shared experience. Finally, we outline some philosophical interpretations and some ideas for future work.

Chapter 1

Introduction

Chapter Summary

The scientific study of emergence is a broad interdisciplinary endeavour which draws from and is applicable to a vast range of complex systems. As a result, quantitative analysis methods used in the field are very diverse, even though they are used to identify similar properties across heterogeneous phenomena. Many multi-agent systems manifest emergence as a result of self-organised collective behaviour, and in particular this thesis concerns itself with collective behaviour expressed as complex spatiotemporal patterns of movement in groups. The main objective of this thesis is to find and test measures of emergence that are in some way substrate independent and thus can describe and quantify collective movement at many scales, from microscopic particles moving together, to animal groups and human societies.

1.1 Together, but not the same

This thesis is concerned with quantifying *self-organised collective behaviour* in multi-agent systems, in particular social groups of animals and humans, through the use of measures of emergence from the interdisciplinary study of complex systems.

Collective behaviour is a prime example of how complex patterns of behaviour can *emerge* from a group of individuals, or agents, acting together (Vicsek & Zafeiris, 2012), such that they no longer appear as individuals but each contributes to a social superorganism behaving as one. This collective behaviour cannot be reduced to any single individual in the group, or even to the sum of contributions from the individuals, as it is the result of the multitude of complex relationships and interactions between them.

Collective behaviour is a rather general term, which is used in many different ways. It can refer to systems made of simple microscopic components, such as physical systems of myriads of atoms or molecules which, through their local interactions, have some collective property that is in some way irregular or contains more information than expected from the parts alone, such as the phase transition from the solid to the liquid phases of water, superconducting materials, or arrays of magnets (Anderson, 1972). The phenomenon is also present at the cellular level, as is the morphogenesis process, namely cellular division and specialisation, a behaviour studied and modelled as early as Alan Turing's work (Turing, 1952). Another most ambitious example is the theory that behaviour, cognition and even consciousness emerge as a result of the collective behaviour of neurons (Tononi & Edelman, 1998), which manifest *collective intelligence*.

In the same spirit, collective behaviour is also used to refer to synchronous or coordinated group activities between individuals: from bacterium colonies to eusocial insects to birds, fish and herd animals, which cooperate to solve problems for the benefit of the whole group. This kind of social collective behaviour in animal groups is the focus of the research field of *swarm intelligence*.

Finally, the term can also be used to describe much human behaviour, since many human activities are performed in groups and rely on direct and indirect social interactions and deep interdependencies: from smaller scales, such as sports teams and orchestras, to much larger ones, from infrastructure, cities, companies and political powers to a long history of scientific collaboration and cultural evolution. Yet historically, most human behaviour has been studied from a rigidly hierarchical perspective, endowing only a few chosen individuals with the causal powers to affect society as a collective, although that view may be changing (Jenkins, 1991). In this thesis, I am most interested in that collective human behaviour which is most similar to how self-organising swarms behave in nature.

Swarm intelligence in animal groups

In the study of swarm behaviour, understanding the individuals in isolation will likely not reveal many answers about how the group behaves. This is due to the fact that no one individual is responsible for the group phenomenon, which seems to emerge without explicit central control, pre-ordained hierarchical structures or leaders, or *a priori* planning. In these cases we may speak of *self-organisation* (Hemelrijk & Hildenbrandt, 2012). But what exactly are the mechanisms of self-organisation, and how do collective properties arise through self-organisation?

Due to its complexity, the study of swarm behaviour needs to address multiple aspects beyond the individual components or agents: what exactly are the collective patterns emergent in the system? How do the group phenomena emerge from the behaviours of individuals? And how do the individuals coordinate? These questions have puzzled scientists for millennia: a century ago biologists still speculated that the flocking of birds or the synchrony of fireflies was the result of telepathy (Satz, 2020).



Figure 1.1: **Examples of self-organising collective behaviour in social animals. (a)** A school of fish swimming in circles to confuse a predator. This behaviour occurs spontaneously by following neighbours and behavioural cascades (Múgica et al., 2022; Oscar et al., 2023; Shaw, 1978). **(b)** A swarm of fireflies synchronising their flashes, which putatively facilitates mate discovery (Moiseff & Copeland, 2010). The group synchrony arises from fireflies slowing down their flash to synchronise with a neighbour. **(c)** Army ants building transport bridges with their bodies. Each ant locally senses the amount of traffic to decide whether to reinforce the structure or leave. The emergent responsive living architecture is very efficient at detecting and adapting to traffic flows (Garnier et al., 2013; Lutz et al., 2021). **(d)** A murmuration of starlings creating complex flock shapes by coordinating with neighbours (Ballerini et al., 2008; Cavagna et al., 2010).

Excitingly, in the last few decades, the study of swarm intelligence has made great leaps using the conceptual framework of *emergence*. In 1995, (Vicsek et al., 1995) showed, using mathematical modelling and analysis tools from statistical mechanics, that bacteria and magnetised iron share similar structural collective properties in the form of *collective movement* in the same direction, which arises or *emerges* simply by the local alignment between neighbouring bacteria or molecules. The methodology of using artificial life in order to simulate the multi-agent system following very simple rules was not new (Reynolds, 1987; Von Neumann et al., 1966), but connecting it to simulations of physical systems has allowed for interdisciplinary exchange between physicists and biologists, and the evolution of a rich field of research where experimental, theoretical and simulation-based work go hand in hand in the search for the universal properties of swarming behaviour (Huth & Wissel, 1994). This exchange between biology and physics has roots in the history of computer science as well: some of the first discoveries of artificial life were based on the first simulation study of a physical problem done at Los Alamos in the 1950s in the context of modelling crystal structures (Fermi et al., 1955), which, in turn, inspired computational explorations of ideas such as morphogenesis, self-evolving algorithms (Barricelli, 1963) and self-reproducing machines (Von Neumann, 1951; Von Neumann et al., 1966).

Following this interdisciplinary methodology, more and more collective behaviours in nature were revealed to be emergent: thousands of fish can move together without leaders, achieving schooling or shoaling behaviour simply by sensing and following fish around them (Shaw, 1978) or, especially in dangerous situations, by choosing to follow a fish that has shown intiative or a novel movement (Múgica et al., 2022; Oscar et al., 2023); spectacular patterns, characterised by near-optimal information processing, are created by hundreds of thousands of starlings when they coordinate with the 6-7 birds flying nearest to them (Ballerini et al., 2008; Cavagna et al., 2010); a colony of acellular organisms known as slime mould can find solutions to a maze by exploring the space individually and coming together to exchange information (Sims & Kiverstein, 2022); ants can make consensus decisions by emitting pheromones and sensing the concentration around them (Franks et al., 2007), and many others.

Importantly, this collective behaviour is cooperative and seems crucial to survival (Shaw, 1978; Sumpter, 2006), with applications to foraging and transport (Garnier et al., 2013; Sims & Kiverstein, 2022) including the emergence of a collective memory of their previous movements and spatial configurations (Couzin et al., 2002), building colossal shelters (Heyde et al., 2021), but also avoiding predators (Cavagna et al., 2010) and mating (Moiseff & Copeland, 2010). There are many studies suggesting this behaviour has an evolutionary advantage and has great ecological importance.

Collective behaviour in humans

While some aspects of human behaviour, such as the emergence of language, culture, or markets are self-organised, most people view human history and complex social behaviour as the result of a few leading figures manifesting their causal powers, which is profoundly unlike how collective phenomena seem to arise in most other social animals.

As the complexity of the agents increases from a bacterium to a person, so does the range of interactions between individuals and the collective properties of the group expand in diversity and structure. In animal societies, the behaviour becomes more elaborate the more diversity and variability is seen in the agents' behaviours: the collective behaviour of bacteria swimming can be detected with a single, scalar order parameter measuring their alignment (Vicsek et al., 1995); but more descriptive power is needed for birds or fish, with scientists proposing a broad range of much more complex measures, even discussing the effects of social relationships on the collective behaviour (Bode, 2011).

Obviously, human collective behaviour is even more complicated. It often combines multiple nested structures that influence each other and are, in turn, influenced by each other: first, the complexity of a human as an agent, then social norms, families, social networks, settlements, ruling powers, infrastructure, states etc.

Among this broad spectrum, few behaviours are considered self-organised and have been studied as such: pedestrian dynamics, free markets, contagion and epidemics, political polarisation etc. These cases are interesting insofar as they are likely to share characteristics with collective behaviour in nature, and to be related to collective intelligence at the human level. For example, similar to animal group movement, pedestrians will create bidirectional flows simply by aiming for a desired velocity and avoiding each other while walking (Helbing & Molnár, 1995). Modelling and studying this behaviour aids our understanding of how people move collectively, and can inform new means to foster crowd cooperation and efficient transport. The applications are manifold, including matters even relevant to our own survival: for example, including insights from models and simulations of crowd behaviour in civil engineering design and the development of evacuation plans (Klupfel et al., 2004; Von Schantz & Ehtamo, 2019).

Interestingly, many self-organising group activities are also related to positive social and emotional outcomes. There is a sense of togetherness, connectedness, or social attachment felt by many spectators to ritual behaviours (Alnabulsi et al., 2018; Konvalinka et al., 2011), sports events (Baranowski-Pinto et al., 2022), concerts (Ardizzi et al., 2020; Czepiel et al., 2021; Ellamil et al., 2016) and films in the cinema (Richardson, 2019) to name a few, whose collective experiences manifest as shared attention, coordinated movements and even physiological synchrony. Moreso, co-creation and collective action, seen in activities as simple as walking together (Jackson et al., 2018; Wilson & Mansour, 2020) or being in

the same crowd (Baranowski-Pinto et al., 2022) and as diverse and complex as musical improvisation (Dolan et al., 2018), synchronised group dancing (Noy et al., 2015) and collaborative problem solving (Wiltshire et al., 2019) are associated with states of group flow (Shehata et al., 2020), feelings of shared identity and rich group experiences that may also result in novel and complex outcomes, such as innovative solutions to problems, rich cultural artefacts or collectively intelligent patterns of behaviour.

Studying human groups with a focus on self-organisation and individual local interactions is highly relevant to our times, as we find ourselves strongly connected by globalisation and techno-social systems. Scientific discoveries and technological progress are examples where the collective intelligence of humanity is engaged at a global level. The tools provided by contemporary technologies, from the Internet to sensing and imaging to artificial intelligence, allow for new means of cooperation and collaboration and facilitate self-organisation better than ever before in our history, but also pose high risks if used unsoundly, as can be seen, for example, in the political polarisation (Falkenberg et al., 2022) and social alienation that can result from the use of social media. Therefore, the study of self-organising collective behaviour, as related to positive psychosocial outcomes and collective intelligence, may reveal important insights and methods to address important global challenges, from wellbeing to economics to climate change (Bak-Coleman et al., 2021).

Brief history of emergence

Many physical phenomena in nature, from the formation of galaxies and solar systems all the way to the mysteries of life – natural or artificial – can be seen as forms of emergent collective behaviour, of many parts behaving as one and creating something at a higher level. Molecules interact, creating protein chains, which produce the mechanisms of cell organoids and cells, which then aggregate in organs; but an individual is more than an aggregation of organs, a society is more than an aggregation of individuals, and the economic and techno-social systems as well as the artificial life and intelligence a human society can create can no longer be reduced to mere images of its creators.

As long ago as 350 BCE, Aristotle muses on the nature of such phenomena and teases the causal links between the parts and the emergent whole: ‘with respect both to definitions and to numbers, what is the cause of their unity? In the case of all things which have several parts and in which the totality is not, as it were, a mere heap, but the whole is something greater than the parts, there is a cause’ (Aristotle, 2016).

Albeit present in philosophical and scientific dialogue ever since, the idea of emergence is incompatible with the *reductionism* prevalent during most of the 20th century, which holds that to understand a phenomenon, it is sufficient to know the properties of the

constituent parts. Many scientific discoveries have been possible within the framework of reductionism, yet also many emergent phenomena have remained unexplained under this paradigm.

In contrast, *emergentism* holds that many natural phenomena arise as new, autonomous properties or causal forces at the collective level from the interactions between constituent parts. To understand such phenomena, it is less important to understand its constituent parts, than the relationships and interactions between the parts, other systems, and the environment, at a multitude of hierarchical levels and spatiotemporal scales. As seen vividly in the field of swarm intelligence, an emergentist conceptual approach has been crucial to progressing our understanding of self-organising animal groups (Satz, 2020).

Of importance to the science of complex systems in general is the idea that the natural world is not composed of things or substances, but rather is the result of a collection of *interacting processes* (Jensen, 2022; Whitehead, 1978). Unlike the cartesian or aristotelian views, process philosophy is a philosophical tradition that emphasizes dynamics, or 'becoming over being' (Prigogine, 1980). Such a view is better poised to understand complex dynamical phenomena such as cosmology, evolution, stock markets, the electrical spikes between cells, communications, social behaviour, consciousness and so on. This idea is relevant to research methodologies as it makes scientists aware of the fact that isolating parts from the whole may also destroy underlying processes producing the collective force or phenomenon.

The concept of emergence has been developed and discussed individually in many different disciplines. In philosophy, processism, as well as British emergentism and non-reductionist or non-dualist accounts of philosophy of mind (Gibb & Lancaster, 2019); in physics, the study of phase transitions and criticality extended to other physical and multi-agent systems has given rise to complexity theory, which aims to produce mathematical models and theories of emergent behaviour, which have, in turn, improved our understanding of geophysics, biology, epidemiology and neuroscience (Jensen, 2022); in cybernetics, the idea of control and agency influenced the study of multi-agent systems frequently employed by complexity sciences today (Wiener, 1948); and of course in the social sciences, from Adam Smith to Friedrich Engels to Keith Sawyer, markets, social classes and other social structures are seen as more than just the sum of the actions of individuals, and moreover, the action of individuals is seen as more than just forced or influenced by social structures (Elder-Vass, 2010).

A systematic approach to the study of phenomena made of many interacting agents has been seen in the 20th century in the structuralist movement, which made claims of structural universality in various diverse social phenomena. Interestingly, while these approaches have become less popular in the second half of the century, they have had

a lasting impact on quantitative studies of largely qualitative social phenomena. For example, thousands of languages exist in the world, but the field of transformational generative grammars, which treats language as a formalism of generators and operators, is able to describe most languages (Chomsky, 1965). This theory has deeply influenced both the fields of programming languages and natural language processing. There is a plethora of cultures and behaviours adopted by humans all around the world, yet structural anthropology can describe many common patterns and building blocks of ritual behaviour (Levi-Strauss, 1971). More recently, the field of neurosciences has been using a structural and emergentist approach, by relating functional brain networks, complexity measures, or critical dynamics to behaviours or states of mind (Beggs, 2008; Carhart-Harris et al., 2014; Chialvo, 2010; Sporns, 2002). Even though beauty is 'in the eye of the beholder', the same patterns of brain activity manifest in different people experiencing different works of art they find beautiful (Ishizu & Zeki, 2011). All of these discoveries have been made, in some way, by acknowledging the processess underlying the relationships and interactions between the components of a larger whole and not just studying the components themselves – individual words, behaviours, neurons, or minds.

Complexity: the science of emergence

Today, emergence is still difficult to define systematically and still posing problems to philosophers and scientists alike (Gibb & Lancaster, 2019). Many theoretical fields, starting from complexity theory and not limited to artificial life, dynamical systems and chaos theory (Thompson & Stewart, 2002), and synergetics (Haken, 2004) seek to generally understand higher-level phenomena that cannot be explained or predicted from the lower-level parts in isolation, and may operate with a variety of concepts and operationalisations of emergence. Nonetheless, we can still speak of a *science of emergence* which reunites these many developments towards the goal of the systematic study of many-body systems manifesting emergent phenomena that are somehow 'more than the sum of its parts' (Jensen, 2022). We refer to such systems as *complex systems*.

Some thinkers consider emergent phenomena at the higher level to be impossible to understand or deduce in any way from the lower-level parts or their processes; this account, held in particular by the British emergentists and some non-reductionist philosophers of mind, is termed *strong emergence* (Chalmers, 2008). In contrast, the idea of *weak emergence* (Bedau, 1997) more frequently adopted by complexity scientists suggests the collective properties can at least be understood or explained in terms of the lower level, though they may still be unexpected. Such weak emergence has been strongly associated with artificial life and cellular automata simulations (Von Neumann, 1951; Wolfram, 1983). Albeit fascinating, the debate between the strong and weak emergentist views is not discussed any further in this thesis.

Taking a more practical approach, complexity science works by looking for the common characteristics of a large range of phenomena that show emergence empirically, and by making use of a large toolbox from many disciplines including dynamical systems, statistical mechanics, artificial life, information theory, network science, sociology, economics, bioinformatics and neuroscience. The aim is not necessarily to find universal laws of all complex systems, but more to identify common principles that allow us to recognise and understand these systems (Goldenfeld, 1999). From flocks to stocks and from brains to rain, complexity science has helped us reveal many shared characteristics among very different systems existing at various scales, and is thus perfectly poised for the investigation of self-organisation in social systems.

Complexity science abounds with measures and metrics which address different quantitative aspects or research questions in the study of emergence. Due to the large variety of interdisciplinary contributions to complexity science, one of the most important goals in the study of complex systems is devising metrics that are *substrate independent*: namely, that are applicable to different systems and different kinds of data extracted from those systems, as long as the data captures in some quantifiable way the behaviour of the parts as well as the system as a whole.

From the methodological approach of complexity science, the work in this thesis leverages modelling and simulation to isolate the necessary and sufficient conditions for emergent behaviour, and seeks to make use of analysis methods that are robust in the study of complex systems to quantify emergence in both simulated and experimental data of collective behaviour across many different scales.

1.2 Objectives and aims

While complexity science seeks to find universal principles of emergent behaviour, actually quantifying it is done differently across disciplines and different systems. This thesis is a result of a broad exploration of quantitative methods which can be applied to collective motion or generally collectively intelligent behaviour to measure if and how exactly is the whole 'greater than the sum of parts'. From bacteria, to insects, birds and fish, to human beings, an omnipresent form of collective behaviour is *collective motion*, manifesting through spatially or temporally coherent patterns that can be seen at the group level. Therefore, collective movement provides a rich and broad testbed for the measures under investigation. As such, my research objectives are:

1. To identify or, if needed, develop a novel, data-agnostic measure of emergence which can detect self-organising collective behaviour and is as robust in simulations as in real data;

2. To test the measure in null models, gain thorough insights into its interpretation, then use it in practice in both simulation-based and experimental applications to detect emergent collective movement; and
3. To test claims that self-organised emergent collective behaviour in humans can have prosocial outcomes, to relate the quantitative aspects of collective movement to qualitative aspects of collective experience, and to identify and foster conditions that aid collective intelligence in humans.

The aim of this thesis is not to present an exhaustive account of complexity science, emergent phenomena or measures of emergent behaviour, nor is it to classify or present a complete taxonomy of self-organising collective motion. The focus is rather on specific candidate measures that can be applied to time series data extracted from trajectories of simulated and real-world multi-agent systems in order to detect collective behaviour: by investigating spatially and temporally ordered patterns that emerge at the group level, such as directional or coherent spatial movement, or temporal synchronisation.

In the current zeitgeist of social alienation, climate change, loss of digital sovereignty and uneven exploitation of our collective intelligence, it seems more important than ever to turn our eyes to collective behaviour in nature and to design experiments, experiences and technologies that leverage the collective, adaptive and social advantages of our collective intelligence. To pursue this direction of inquiry, the measures used in null models, simulation studies and animal data are used to devise and build new experimental designs for the study of collective intelligence in humans through motion.

1.3 Contributions

To address these research objectives, two candidate methods of analysis are investigated: the $\Psi - \Gamma - \Delta$ information-theoretic criteria of emergence of(Rosas et al., 2020a) and the wavelet coherence measure of temporal synchronisation of (Grinsted et al., 2004). The theory of emergence in (Rosas et al., 2020a) proposes measures to quantify and criteria to assess whether some group's collective behaviour is emergent from the behaviours of individuals, using statistical measures of reduction in uncertainty applied to the system's trajectories: the Ψ measure quantifies whether the past history of a group can better predict its own future than the past of the individuals; Δ quantifies whether the group can better predict the indivduals than the individuals themselves; and Γ quantifies if the group has no predictive power over the components. Meanwhile, wavelet methods can be used to robustly assess the degree of synchrony between two time series at certain frequencies as well as time intervals in the dynamical evolution of the system.

These methods are selected due to their non-linearity and robustness in many kinds of time series, regardless of system size. In order to address the robustness of the methods at different scales, the research effort is organised in layers of increasing complexity in the three parts of the thesis.

Part I focuses on the foundations to quantifying emergence in complex systems using the $\Psi - \Gamma - \Delta$ criteria and includes the following contributions:

Studies of the $\Psi - \Gamma - \Delta$ in the null case The robustness of the measures was tested in *null cases* constructed from simple particle models in one and two dimensions: random walks and the Vicsek model, in which particles moving around with some degree of noise can align with their neighbours on a given radius, producing self-organised collective behaviour at certain parameter configurations. In the random walks, the measures unexpectedly detect statistical interdependencies in spite of having no mechanistic interactions in the model. In the Vicsek model, the measure detects the presence of flocking movement but only after a more accurate implementation of the estimators is produced.

Implementation of flocking library and improved emergence estimators Two Python packages were developed, to provide simulations and basic analysis of flocks with local interactions (Sas, 2021), and to implement and test more accurate information-theoretic estimators for the Ψ and Δ measures (Sas, 2024).

Part II presents case studies where Ψ is successfuly used to quantify collective motion in flocking data from animal motion and multi-agent systems, and includes the following contributions:

Comparison between experimental and simulated flocking Trajectory data from two case studies of collective motion were compared using the $\Psi - \Gamma - \Delta$ measures: fish schooling in a tank, and the Reynolds model, a multi-agent algorithm to simulate artificial birds in flight which supplements the alignment rule of the Vicsek model with avoidance and aggregation. We find that schooling behaviour in fish is quantitatively similar to the intermediate regime of the Reynolds simulations, where there is a balance between conflicting individual and group tendencies in agents. Importantly, results were obtained by applying a more accurate estimator for Ψ which accounts for redundant information across all agents.

Link between emergence measures and social systems We introduce the idea that motion can represent more complex underlying social behaviour in *Megabike*, a self-organising multi-agent simulation of social agents which must cooperate to survive in a hostile environment. We find Ψ is positive in all surviving groups, suggesting cooperation

is characterised by causal emergence. Moreover, we find Δ is positive as well, suggesting downwards causation. We relate these measures to causal feedback loops inherent in social structures, and suggest that measures of emergence in conjunction with the *Megabike* multi-agent system can be used to create quantitative indices of governing systems.

Part III relates the quantitative findings of the first two parts to the qualitative aspects of collective movement and group activities in humans:

Novel experimental paradigm and technology for human flocking First, we designed and implemented a new artistic experience and experimental paradigm, `Synch.Live`, which applies the Ψ criterion to induce collective movement in human groups. The design of the experimental technology and the implementation of experimental software, as well as the running of the experiment, was undertaken by the author with support from collaborators. The software is documented online (Sas, 2022).

Link between collective behaviour and collective experience Using this technology, we show that solving a multi-agent optimisation problem through collective flocking motion has a positive effect on participants' state of mind, through eliciting feelings of connectedness to others.

Link between movement synchrony and collective experience We conclude with another study relating collective motion and collective experience, where wavelet measures of synchrony are used to quantify collective motion, and we find that synchrony in different timescales is correlated to the the audience's collective experience.

1.4 Publications

This thesis presents work which was the result of large interdisciplinary collaborations and has been already been reported in a range of publications and pre-prints. This thesis presents the author's contributions and other relevant main findings of the following articles:

1. Alberto Liardi*, *Madalina I. Sas**, George Blackburne, William J. Knottenbelt, Pedro A.M. Mediano and Henrik J. Jensen. *Simple physical systems as a reference for multivariate information dynamics*. Submitted to Chaos, and cited as (Liardi et al., 2025)

2. *Madalina I. Sas*, Fernando E. Rosas, Daniel Bor, Henrik J. Jensen and Pedro A. M. Mediano. *Improved approximation of causal emergence estimators for large systems with high redundancy. In prep.* Cited as (Sas et al., 2024b)

3. Matthew Scott*, *Madalina I. Sas**, Jeremy V. Pitt. *An Information-Theoretic Analysis of Emergence and Leadership in Self-Organised Collective Action*, in the *5th International Conference on Autonomic Computing and Self-Organizing Systems (ACSOS)*, IEEE, pp. 101-110, Sep. 2024, and cited as (Scott et al., 2024b)

4. *Madalina I. Sas*, Pedro A. M. Mediano, Fernando E. Rosas, Hillary Leone, Andrei Sas, Christopher Lockwood, Henrik J. Jensen and Daniel Bor. *Synch.Live: Collective problem-solving through flocking motion induces higher connectedness to others*, submitted to Collective Intelligence, and cited as (Sas et al., 2024a). The work was also presented as a poster at the Santa Fe Insitute Collective Intelligence Symposium, Jun. 2023, and at the 26th annual conference of the Association for the Scientific Study of Consciousness (ASSC26), Jun. 2023.

5. Takayuki Nozawa*, *Madalina I. Sas**, David Dolan, Hardik Rajpal, Fernando E. Rosas, Christopher Timmermann, Pedro A. M. Mediano, Keigo Honda, Shunnichi Amano, Yoshihiro Miyake, and Henrik J. Jensen. *Swinging, Fast and Slow: Multiscale Synchronisation Dynamics Reveals the Impact of an Improvisatory Approach to Performance on Music Experience*, accepted for publication by *Scientific Reports*, and cited as (Nozawa et al., 2023)

Author's publications on related topics that are not thoroughly presented in this thesis are:

6. Hardik Rajpal*, *Madalina I. Sas**, Christopher Lockwood, Rebecca Joakim, Nicholas S. Peters and Max Falkenberg. *Interpretable XGBoost classification of 12-lead ECG applying information theory measures from neuroscience*, presented in *Computing in Cardiology*, IEEE, pp. 1-4, Sep. 2020, cited as (Rajpal et al., 2020)
7. Max Falkenberg, Alessandro Galeazzi, Maddalena Torricelli, Niccolo Di Marco, Francesca Larosa, *Madalina I. Sas*, Amin Mekacher, Warren Pearce, Fabiana Zollo, Walter Quattrociocchi and Andrea Baronchelli. *Growing climate polarisation on social media*, published in *Nature Climate Change*, 12(12), pp. 1114-21, Dec. 2022, and cited as (Falkenberg et al., 2022)
8. Asimina Mertzani, Jeremy V. Pitt, Stefan Sarkadi, *Madalina I. Sas*, Matt Scott, Ciske Smit. *Cohesion and the Explanation of Constitutional Choice in Self-Governing Systems*, presented at the *6th ALife Workshop on Agent-based Modelling of Human Behaviour*, Jul. 2024, and cited as (Mertzani et al., 2024)
9. Pedro T. Palhares, *Madalina I. Sas* and Óscar F. Gonçalves. *Music and states of consciousness: A narrative review of the broader significance of music to understanding absorption, mind wandering and creative thought*, published in *Neuroscience & Biobehavioral Reviews*, 167, article no. 105920, Dec. 2024, and cited as (Palhares et al., 2024)

Chapter 2

Foundations to complex systems

Chapter Summary

This thesis makes use of methods from complexity science to study collective behaviour, and as such a variety of concepts and methods from statistical physics, information theory, signal processing and time series analysis, and network science. This chapter lays out the basic concepts and building blocks necessary in the search for robust, substrate independent measures of emergence, including the wavelet analysis used in Chapter 8 and the $\Psi - \Gamma - \Delta$ criteria of emergence used in Chapters 4-7.

2.1 Preliminaries

A **complex system** is a dynamical, non-linear system of interacting parts, which exhibits emergent properties or behaviours at the systemic level that cannot be reduced to the features of the individual components (Holland, 2014; Mitchell, 2009).

Emergence refers to the patterns and behaviours that can arise out of complex systems, and in the context of this thesis is seen as organisation, a form of collective behaviour in which agents coordinate to achieve goals, which manifest physically through some degree of **structure** or **pattern formation** in space and/or time. This view is similar to Norbert Wiener's view of *organised complexity*. This thesis is concerned with the self-organised formation of spatiotemporal patterns in collective movement of social groups. But an enormous range of emergent behaviour appears in nature beyond these examples, and a multitude of books provide beautiful reviews of their diversity (Holland, 2014; Jensen, 2022; Mitchell, 2009).

Self-organisation refers to the ability of an open system to spontaneously behave in an organised fashion, solely as a result of the dynamics of the components, with no explicit ordering or influence, and neither preordained internally through a fixed leading agent, nor externally through some control scheme.

The study of complex systems often discusses different **scales** at different **levels of description**, in particular when discussing systems characterised by supervenience such as a human social system: emergence exists at the molecular, cellular, organ and social level, and different quantities may be evaluated based on the behaviours manifest at each level. Some relative terms are to be used to refer to the scales of the whole and the parts: the *microscopic* scale refers to the components or agents forming the system and their interaction; the *macroscopic* scale refers to the systemic behaviour that can be described by collective variables. When multiple layers of organisation are discussed together, the *mesoscopic* scale refers to levels in between 'micro' and 'macro'. What is 'macro' at one level may also be 'micro' or 'meso' at another level (Rupe & Crutchfield, 2024). When the same property pervades at multiple scales in a system, it may be referred to as *scale-free* or *scale-invariant*, since no matter how much one 'zooms in or out', the same kinds of patterns can be seen.

Emergence: order, disorder, complexity

The emerging system behaviour can manifest in many different ways, and can have different kinds of dependencies on the number of components. Emergent phenomena may manifest even in small and simple systems, such as a small school of a dozen fish, or a small chamber music ensemble – even a pair of dancers.

One way to characterise the systemic level is by thinking in terms of **order** and **disorder**. Systems that are too disordered or chaotic may be too unstable to sustain complex interactions, while those too ordered may be too inflexible to be capable of adapting (Kauffman, 1990). Many theoretical studies show systems of many identical interacting components exhibit complex collective dynamics when approaching a *chaos-order transition* (Crutchfield & Young, 2020; Grassberger, 1986). As such, the most interesting and complex behaviour is seen where disorder and order coexist, arising from the conflict between the random, disordered tendencies of the components and the order induced by their interactions, which self-organise into a near-critical collective dance with near-optimal information processing and extremely high adaptability. The canonical example of such behaviour in nature would be a flock of birds or school of fish posed against a predator.

In multi-agent systems, this can be seen also as the conflicting tendencies between the *cooperation* of agents who either couple together and behave as one, or the *competition* between agents who behave according to their intrinsic, individual drives. More general than cooperation and competition, developments in neuroscience and consciousness research have also introduced the two opposing concepts of *integration*, which refers to the extent to which the system acts as a whole, and *segregation*, which refers to the extent to which the components act independently (Tononi et al., 1994; Tononi & Edelman, 1998).

This idea can also be expressed in terms of the number of *degrees of freedom* seen in the system. A highly ordered system will show a reduced number of degrees of freedom, as the components in the system behave together and can be described with a smaller number of parameters; conversely, a highly disordered system may show as many, or more, degrees of freedom than components. In statistical mechanics, for example, an infinity of individual behaviours have a single degree of freedom in the ordered state, such as magnets aligning along the same polarity.

While both ordered and disordered emergence have been discussed in the literature, this thesis considers kinds of emergence where **complexity** or **organisation** arises somewhere between the ordered and disordered states, between regularity and randomness, between integration and segregation, as is the case of critical phase transitions and *metastability* (Hancock et al., 2023).

Historically, order and disorder have been quantified with collective variables known as **order parameters** in the field of statistical physics, which are average quantities that behave profoundly different depending on the amounts of interactions in the system. While a certain order parameter can describe many different physical systems, sadly, there is no universal scalar quantifier of organisation: a different order parameter is needed for different kinds of organised structures arising at the system level in different systems.

Yet the myriad of complex emergent behaviours seen in self-organising systems in nature makes clear that there are many phenomena these concrete measures do not capture, which have, historically, mostly focused on the narrow example of symmetry and breaking of symmetry as examples of disorder and order (Rupe & Crutchfield, 2024).

A more generalist attempt is through an understanding of the interactions in the system, for example, of how correlated the components of the systems are on average, or even further, through **measures of statistical complexity** (Feldman & Crutchfield, 1998), many of which use correlations at different scales to capture how global and local interactions relate, or rely on the use of information theory to gain insights over processes in the system. A vast number of measures of statistical complexity have been proposed and used, as due to the practical nature of many studies in complex systems in nature, these methods must balance computational challenges, theoretical assumptions, data availability and efficient estimation of relevant quantities from incomplete data.

Interactions: correlation, coupling, coordination

As previously hinted by organisation being related to strongly correlated behaviours, we revisit another important aspect of complex systems research, namely how exactly to quantify the interactions between components? The simplest such method is the use of **correlation functions**, which have historically been used in simulation studies of large ensembles of physical systems with large number of components, but have also shown promise on much smaller amounts of available data in the study of economics, flocks and brain behaviour. Moreover, correlation functions can even be computed instantaneously with insightful results, and not just on time-averaged data (Palmieri & Jensen, 2020). Nonetheless, the main disadvantage of correlations as a method of analysis is that they fail to capture non-linear relationships between components.

Especially when the components of a complex system are social individuals with a form of agency, the local interactions between agents can be seen as a form of **coordination**: the parts communicate and behave in ways that are influenced by each other in some way. The field of *coordination dynamics* is frequently concerned with how parts communicate and coordinate behaviour, including both tendencies that are spontaneous and self-organising, as well as more concrete and asymmetric forms of control, such as following a leader or centralised stimulus (Kelso, 2009). More recently, the field of *joint action* has also been exploring, from an interdisciplinary perspective, the psychological, cognitive and neurological aspects of coordinated or rhythmic behaviour in humans (Keller et al., 2014), some of which highly complex, such as group musical or dance performance. Many researchers in these fields have proposed new ways of quantifying the coupled actions of agents from time series data, and as such, measures of interaction are sometimes taken to reflect relationships of agency or causality between individuals.

This thesis is only concerned with a small number of measures of interactions which are largely data-agnostic and aim to be robust in non-linear systems. Interested readers should consult a review which lists more than 200 different measures used to quantify interactions in complex systems (Cliff et al., 2023). To then relate local interactions to system behaviour, measures of interactions are sometimes averaged per individual or across the whole group. This method can often reveal insightful average trends but may fail to capture non-linear or beyond pairwise relationships - as such, mathematical descriptions of the complex network of interactions (such as its communities) have also become a popular method of study.

Some issues from the study of complex systems with pairwise measures in general are addressed by *higher-order measures*, which aim to study interactions beyond pairwise relationships. Such measures used in this thesis are based on information theory and more specifically on the decomposition of mutual information (Rosas et al., 2020a).

Finally, the study of pairwise interactions can also be continued with the study of the overall structure or even dynamical trends in the structure of interactions through the use of complex networks. As many multi-agent complex systems of interest are social, it is important to understand whether the collective behaviour is in any way associated with certain network properties which may reveal how the information is shared in the system or which agents coordinate with others and in what way.

The work in this thesis uses two kinds of interaction measures for time series data: (i) spatiotemporal measures based on mutual information and (ii) temporal measures based on phase synchrony. These are introduced in Sections 2.3 and 2.2. The network analysis tools used to study the structure of interactions are presented in Section 2.4.

Synergy and redundancy

As a result of coordination, what may emerge is synergetic behaviour (Fuchs & Scott Kelso, 2018). **Synergy** arises in functional groupings of components or agents whose behaviour is coupled and thus are temporarily acting as a singular coherent unit in ways which depend entirely on the presence and interactions of all the components. Conversely, removing a singular contributor from the group would result in the disappearance of the collective behaviour. From the deep interconnectedness seen at all scales in nature, it is intuitive to posit the synergy hypothesis: that biological complexity arises as a result of synergetic emergent phenomena resulting from the complex multilevel processes inherent to all life (Corning, 2008).

While philosophically similar to some definitions of emergence, we consider synergy to be only one of the many possible kinds of emergent behaviour.

Redundancy, on the other hand, more specifically characterises groupings of components of agents who are acting as a singular unit by virtue of identical behaviour which shares a high amount of information. Both synergy and redundancy may characterise ordered complex systems in different ways, and have been associated in turn to behaviours showing novelty, or, respectively, robustness. An illustrative example is provided by the informational architecture of the brain: it has been suggested that perception is characterised by more redundancy, in order to provide robust information about the environment, while cognition is more often characterised by synergy (Luppi et al., 2022), which may empower adaptability, flexibility, and creativity.

Notation

Suppose the underlying processes in a complex system manifest as the observed **time series** $(\mathbf{x}_t)$: $\mathbf{x}_1$, $\mathbf{x}_2$ … $\mathbf{x}_t$ …, at time instants indexed by $t \in T$. We call each $\mathbf{x}_t$ an **observable**, where the subscript represents the temporal index. Time series are **realisations** of **random variables** $\mathbf{X}_t$ that form the **random process** $X(t)_{t\in T}$. An **ensemble** refers to the set of all the possible realisations of the random process, but the term is frequently used to refer to a large enough set of realisations to capture relevant statistical properties of the system. We use X_t to refer to a scalar random variable, and x_t to refer to one of its realisations. $\mathbf{X}_t$ and $\mathbf{x}_t$ refer to multidimensional random variables and their realisations. In the current work we focus on both discrete and continous multivariate time series measured at discrete regular intervals.

When discussing systems consisting of many components, the random variable X_t^i is associated with component i, where the superscript represents the component's identifier. Random variables without indices e.g. $\mathbf{X}$ are used to denote the combined time series of a single realisation of a complex system with multiple components unfolding over time.

Each random variable X_t at fixed time point $t \in T$ with possible outcomes $x \in \mathcal{X}_t$ has a **probability mass function** $p_{X_t}(X_t = x)$. We use the simplified notation $p(x)$ to denote this probability distribution and its statistics are given by the **expected value** or first moment (often the mean) $\mathbb{E}[X_t]$, and **variance** $\mathbb{V}[X_t] = \mathbb{E}[X_t^2] - \mathbb{E}[X_t]^2$. Alternative notations for these quantities are $\bar{X}$ or μ_X for the mean and σ_X^2 for variance.

If the same probability distribution describes all X_t^i regardless of t, we refer to this system as **stationary**, and use $p^i(x)$ to denote probabilities at any time t. In general, the models with stationary statistics employed in this thesis also use the same probability distributions for all agents i at a given time t, and there the notation $p(x)$ is used. For non-stationary systems, $p_t(x)$ and $p_t^i(x)$ are used to denote the different probability distributions at each time-step when the components x^i are, or respectively, are not, identically distributed.

When computing statistical averages over the whole system at a given time, function application notation $f(t)$ is used rather than indices, as such an average acts as a *coarse-graining function* applied to the micro scale. $\mathbf{f}(t)$ refers to a function with a multidimensional or vectorial output, while $f(t)$ is a function with a scalar output.

While many agents in complex systems are identically distributed, their local interactions heavily suggest they are not statistically independent. The notation $X \perp\!\!\!\perp Y$ is used to state X and Y are independent random variables. The term *i.i.d.* is used as an abbreviation only when the random variables are both *independent and identically distributed*.

2.2 Time and frequency domain methods

The research in this thesis makes use of **time series data** that results from the unfolding of interacting processes in complex systems. As such, many of the methods used to measure interactions or collective properties in complex systems are based on the analysis of how the statistics of time series evolve over time and reveal important properties of the processes underlying the emergent behaviours under scrutiny.

The gateway to the study of relationships between processes based on time series data is the use of correlation coefficients directly on the data, using sample statistics. But time series analysis methods are particularly useful in the study of *dynamics*, as they can capture the interdependencies between system variables at specific time points or even temporal patterns of behaviour if it repeats with certain frequencies. Non-linear and non-stationary behaviour may be better captured by metrics (often also correlations) defined on the **frequency domain**.

For a time series to be analysed in the frequency domain, a range of methods exist to **transform** the data depending on assumptions. For a stationary signal, its Fourier transform (FT) robustly describes to which extent various frequencies are present in the signal. The output of the transform is a complex-valued function of frequency, which conveys, in polar coordinates, both the amplitude and phase of each frequency, a so-called *analytical signal*. For example, the FT of a musical chord would result in a function that gives the intensity (loudness) of each of the notes (frequencies) in the chord.

The *uncertainty principle* postulates that we cannot be accurate in both time and frequency when analysing signals. Higher time resolution (i.e. smaller time windows) implies lower frequency resolution (i.e. larger frequency bins) and vice-versa. To address these tradeoffs FT can be performed over different sized time windows, as is the case of the Short-time Fourier Transform (STFT). Varying sliding windows are also used as the basis of other function transforms that are more robust in non-stationary signals. These kinds of transformations are at the basis of *spectrograms* which are very relevant in the analysis of music, a quintessential example of non-stationary and complex time series.

Function transforms are reversible by definition, so signal reconstruction from a Fourier or Wavelet transform could also result in robust noise reduction. Such applications are often used for cleaning oscillatory data such as EEG, ECG, or data from various sensors. Similar other function transforms have been defined for different purposes and underlying assumptions, which all convolve a function (the time series) with specific bases or kernels. In this thesis, Wavelet transforms are used extensively as the basis of pairwise and group measures of collective behaviour relating to temporal synchrony. The rest of this section introduces relevant mathematical tools.

2.2.1 Correlation coefficients

Correlation coefficients are a class of statistical measures that quantify the degree of *linear* dependence or association between two variables.

Pearson's Correlation coefficient is defined as the covariance normalised by the product of standard deviations. The normalisation allows the value of the correlation function to be dimensionless and thus makes it a useful measure for comparing the statistics of two processes.

$$\rho_{XY} = \frac{\mathrm{Cov}(X,Y)}{\sqrt{\mathbb{V}[X]\mathbb{V}[Y]}} = \frac{\mathbb{E}[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X\sigma_Y} = \frac{\sum_i (x_i-\mu_X)(y_i-\mu_Y)}{\sqrt{\sum_i (x_i-\mu_X)^2}\sqrt{\sum_i (y_i-\mu_Y)^2}} \quad (2.1)$$

where i ranges through all the observations in the two time series. Covariance is defined only if both second moments of X and Y are finite. The correlation coefficient is invariant under scaling and translation as well as symmetric. The coefficient is bounded by the interval $[-1, 1]$; in general, two variables are considered to be correlated when ρ_{XY} is larger than 0.7.

By computing the correlation coefficient with a time delay between two different time series, or over specific time windows, we can identify predictive patterns in the data that may be associated to how components influence each other over time. This kind of 'predictive' or statistical understanding of causal influence, which was introduced by Granger and Wiener, has yielded valuable insights in the study of complex sytsems so far, including but not limited to neural systems (Bressler & Seth, 2011).

Correlation functions are mathematical tools of analysis of complex systems which compute average correlations between pairs of components at certain distances or time intervals: *Scale-free correlations*, for example, characterised by a power law correlation function, are known to be a marker of *critical behaviour*.

Temporal and spatial correlation functions are at the core of a broad range of analysis methods which are applicable to the study of collective behaviour in nature (Grigera, 2021), with possible implications for our understanding of biological systems in general (Mora & Bialek, 2011). Not only collective motion, such as in locusts (Buhl et al., 2006) and starlings (Cavagna et al., 2010), but also cognition in the brain have been discussed in terms of criticality as measured with correlation functions (Beggs, 2008; Chialvo, 2004; Expert et al., 2010; Linkenkaer-Hansen et al., 2001).

Cross-correlation is defined as a correlation function of the time interval:

$$\rho_{XY}(m) = \frac{\mathrm{Cov}(X_t, Y_{t+m})}{\sqrt{\mathbb{V}[X]\mathbb{V}[Y]}} = \frac{\mathbb{E}[(X_t - \mu_X)(Y_{t+m} - \mu_Y)]}{\sigma_X \sigma_Y} \tag{2.2}$$

Auto-correlation is the cross-correlation of the same variable at different times:

$$\rho_{XX}(m) = \frac{\mathrm{Cov}(X_t, X_{t+m})}{\mathbb{V}[X]} = \frac{\mathbb{E}[(X_t - \mu_X)(X_{t+m} - \mu_X)]}{\sigma_X^2} \tag{2.3}$$

Circular correlation refers to the circular analog to Peasons' correlation coefficient, a statistical measure that quantifies the association between two cyclic variables (Fisher & Lee, 1983). This circular correlation coefficient of X and Y measures the similarity between two cyclic variables, in terms of the degree to which they are in phase with each other. This is done by transforming data points in X and Y with a sin function:

$$r_{XY} = \frac{\sum_i \sin(x^i - \mu_X)\sin(y^i - \mu_Y)}{\sqrt{\sum_i \sin(x^i - \mu_X)^2}\sqrt{\sum_i \sin(y^i - \mu_Y)^2}} \tag{2.4}$$

where $\mu_X = \mathrm{atan2}\left(\sum_i \sin x^i, \sum^i \cos x_i\right)$ is the circular mean of X and $\mathrm{atan2}(y, x) = \mathrm{Im}\log(x + iy)$ is an unambiguous variant of the arctan function in the interval $[-\pi; \pi]$.

2.2.2 Wavelet methods

The correlation coefficients and function transforms briefly introduced above can be used to construct various measures of pairwise synchrony, or more generally spectral measures of interaction. Of the many techniques for the study of interactions between pairs of processes currently in use, the authors of a recent review list more than 200 measures of which around half are 'spectral measures' (Cliff et al., 2023). This variety suggests that analysis in the frequency domain provides rich opportunities for understanding the relationship between structure of interactions and dynamics of collective behaviour.

Among the many existing measures, those based on wavelet transforms are robust, make few assumptions, and are very data agnostic. Importantly, the cross-wavelet transform as well as the wavelet coherence are frequently used in the analysis of human interaction (Issartel et al., 2015).

Wavelet transforms make the least assumptions regarding the shape of the data by representing signals through correlations at a given time with another function, known as kernel or **mother wavelet**. Various mother wavelets that are best suited to specific applications have been proposed across different fields of study.

Continuous wavelet transforms were discovered while studying the reaction of the human ear to sound (Zweig, 1976), and were initially known as cochlear transforms. CWT is used in a large variety of fields, from music analysis and image compression to medicine, economics and geophysics. The continuous wavelet transform represents the input signal x_t as a transformation of the mother wavelet function $\psi(\cdot)$:

$$W(t,s) = \frac{1}{\sqrt{s}} \int_{-\infty}^{\infty} x_u \bar{\psi} \left(\frac{u-t}{s} \right) du \tag{2.5}$$

where s is the wavelet **scale** which compresses or stretches the wavelet in time (i.e. refers to the width of the wavelet), u is the translation, or number of timesteps in the signal after which the wavelet is applied, and $\bar{\psi}$ is the complex conjugate of ψ.

$W(t,s)$ are also sometimes referred to as **wavelet coefficients**. The **wavelet power** is given by $|W(t,s)|^2$. The complex argument of $W(t,s)$ is interpreted as the phase.

Mother wavelets are families of continuously differentiable functions ψ which satisfy certain criteria of admissibility such as zero mean, $\int_{-\infty}^{\infty} \psi(x)dx = 0$ (Torrence & Compo, 1998). A taxonomy of wavelets has been established, based on the number, shape and direction of their pulses, showing useful applications for different kinds of data. As such, the choice of scale and mother wavelet is particularly important as it may have unexpected effects on analysis (Zhang et al., 2016).

In particular, many applications using oscillatory data make use of the Morlet wavelet, which is defined as:

$$\psi_0(t) = \pi^{-\frac{1}{4}} e^{i\omega_0 t} e^{-\frac{t^2}{2}} \tag{2.6}$$

where ω_0 and t denote frequency and time. The Morlet wavelet (with $\omega_0 = 6$) provides a good balance between localisation in time and frequency, and as such is a good choice for feature extraction (Grinsted et al., 2004).

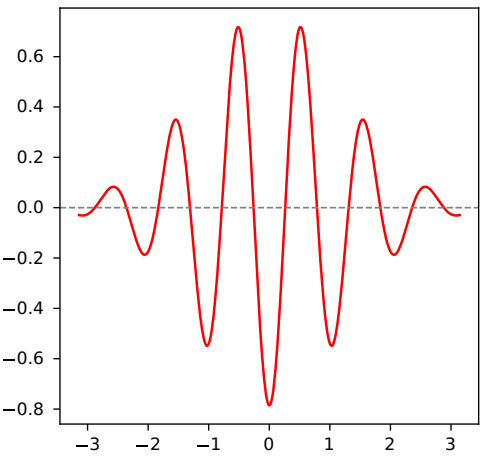


Figure 2.1: Morlet wavelet with $\omega_0 = 6$.

Cross-wavelet power between X_t and Y_t reveals areas (i.e. time translations and frequencies) where both signals have high power. It is defined as the absolute value of the **cross wavelet transform (XWT)** of X and Y, $|W^{XY}|$, defined as the product between the wavelet transform of X and the complex conjugate of Y's wavelet transform:

$$W^{XY} = W^X \bar{W}^Y \tag{2.7}$$

W^X and W^Y are the continuous wavelet transforms of X and Y. As before, the complex argument of W^{XY} refers to local phase, this time the relative phase between X_t and Y_t (Torrence & Compo, 1998).

Wavelet coherence transform (WCT) measures the phase coherence between the two signals, rather than common power. Its definition is similar to that of a correlation coefficient, owing to the fact that the wavelet coherence can be seen as a localised correlation coefficient in time-frequency space (Grinsted et al., 2004):

$$R^2(t,s) = \frac{|S(s^{-1}W^X(t,s)W^Y(t,s))|^2}{S(s^{-1}|W^X(t,s)|^2)S(s^{-1}|W^Y(t,s)|^2)} \tag{2.8}$$

where s and t refer to scale and translation, as in the continuous wavelet transform, and S is a smoothing operator usually chosen to be similar to the wavelet. Keen readers may consult (Grinsted et al., 2004; Torrence & Compo, 1998) for thorough mathematical fundamentals of these wavelet methods and further details on the smoothing operator.

A growing body of work exists using both the XWT and WCT to study interactions in complex systems, recently focusing extensively on the study of human social interactions (Issartel et al., 2015). Given previously outlined difficulties in defining interactions, a practical and empirical understanding is used, where interaction is seen as the expression of actions which occur as two or more agents have an effect upon one another (Sebanz & Knoblich, 2009). This relies on the assumption, that for a simple cause and effect relationship between the phenomena recorded in the time series we expect phase locked oscillations (Grinsted et al., 2004), or in other words, that interaction is seen as a synchronization phenomenon (Kelso, 1995).

The field of social psychology provides also plenty of examples of how data-agnostic and robust the XWT and WCT are. The WCT has been successfully applied to measure not only coupled or coordinated physical movement in humans (Nozawa et al., 2019; Walton et al., 2015; Xu et al., 2013), but even inter-brain synchrony (Nozawa et al., 2019, 2021). WCT has been used with movement data recorded with accelerators (Nozawa et al., 2019) or with cameras (Fujiwara & Daibo, 2016), and as such appears to be robust to the mode of data aquisition (Fujiwara & Yokomitsu, 2021), and it even allows computing synchrony between the body movements of people and audio, such as speech or music (Nozawa et al., 2020, 2023). Applications of the WCT to collective movement in human crowds will be presented in Chapter 8.

2.3 Information theoretic methods

The use of correlation coefficients can reveal linear relationships between different variables, and as such is very relevant to the study of complex systems. Reversely, a lack of correlation may imply *linear independence* but does not capture any *non-linear dependencies*, which is why some studies require more complex metrics. Many non-linear methods exist in the field of dynamical systems and beyond (Kantz & Schreiber, 2003), but these are beyond the scope of this thesis.

Introduced by Claude Shannon in 1948 to analyse digital signals and formalise communication protocols, what became known as information theory started as a foundational mathematical theory of communication operating on probability distributions (Shannon, 1948). Today, an information-theoretic account is one of the foremost approaches to study complex systems. The practical advantages of using Shannon-based measures are in the possibility of estimating them directly from data, and that they can capture non-linear statistical relationships between processes.

Following a cybernetic philosophy that many complex processes in nature are a result of feedback mechanisms and as such, can be described by a form of communication (Wiener, 1954), Shannon's theory has been used successfully to quantify many aspects of complex processes in nature and beyond. A large body of work relates information-theoretic properties to emergent behaviour, with applications to models of complex systems and data alike (Lizier & Zomaya, 2007). Information-theoretic methods form the basis of many measures which can be applied to multivariate probability distributions or to time series data. These measures can be used in many ways, either to assess the complexity of an agent, of a system, or relationships between microscopic components and macroscopic emergent properties within a system.

Information theory is now ubiquitous in many technical disciplines, not just complexity science, but also data science in general, machine learning and many more. Its concepts have become the basis of an intuitive, natural language to describe the world, such as the metaphor of 'brain as computer'. The profound relationship between thermodynamics, information and communication has even been used to suggest a computational approach to emergence in nature (Rosas et al., 2024).

This section introduces and defines some fundamental tools from information theory used in the current work, building up towards a state-of-the-art theory of emergence proposed by (Rosas et al., 2020a), which will be further discussed in Chapter 4, alongside its interpretations. A thorough exploration of information-theoretic concepts can be found in (Cover & Thomas, 2006).

2.3.1 Entropy and mutual information

As before, x_t and $\mathbf{x}_t$ denote univariate or multivariate observed realisations of random variables X_t and $\mathbf{X}_t$ which describe a process. We use $\mathcal{X}$ to represent the space of possible events or outcomes for x. Unless otherwise stated, all random variables in the studied systems are considered identical.

Information content $h(x)$, also called the *surprisal* of observing an event x, refers to how much information is revealed by X taking the value x, or in other words how much reduction in uncertainty results from knowing that $X = x$:

$$h(x) = -\log\left(p(x)\right) \tag{2.9}$$

It follows that less probable outcomes reveal more information than more probable ones. A sure event with $p(x) = 1$ has no uncertainty and thus a null information content. Importantly, information content measures the length of the binary length of the 'message' x in the optimal encoding of random variable X.

Shannon entropy $H(X)$ of a discrete random variable X is a measure of the average surprise, or average information:

$$H(X) = \mathbb{E}[h(x)] = \sum_{x\in\mathcal{X}} p(x)h(x) = -\sum_{x\in\mathcal{X}} p(x)\log p(x) \tag{2.10}$$

Unlike the information content which is connected to a single event, the Shannon entropy reveals a property of the underlying probability distribution of the random variable. It can generalise to two variables as:

$$\textbf{Joint entropy} \quad H(X,Y) = -\sum_{x\in\mathcal{X}}\sum_{y\in\mathcal{Y}} p(x,y)\log p(x,y) \tag{2.11}$$

$$\textbf{Conditional entropy} \quad H(X|Y) = -\sum_{x\in\mathcal{X}}\sum_{y\in\mathcal{Y}} p(x,y)\log p(x|y) \tag{2.12}$$

With the two measures being related by:

$$H(X,Y) = H(X) + H(Y|X) = H(Y) + H(X|Y) \tag{2.13}$$

An important property that can be deduced directly from the definition is that in the discrete domain, the uniform probability distribution maximises uncertainty, since all events are equally probable. The maximum entropy distribution is, intuitively, the least informative one, as it provides the least reduction in surprisal. This is rigorously stated in the Maximum Entropy Principle (Jaynes, 1957).

Shannon entropy has a number of other relevant properties:

$$\text{Positive} \quad H(X) \geq 0 \tag{2.14}$$

$$\text{Transform invariant} \quad H(\lambda X + c) = \lambda H(X) + \log|\lambda| \tag{2.15}$$

$$\text{Symmetric} \quad H(X,Y) = H(Y,X) \tag{2.16}$$

$$\text{Subadditive} \quad H(X,Y) \leq H(X) + H(Y) \tag{2.17}$$

$$\text{Additive if independent} \quad H(X,Y) = H(X) + H(Y) \iff X \perp\!\!\!\perp Y \tag{2.18}$$

We must emphasise that additivity is only valid for independent variables, while many complexity measures based on summing or subtracting entropies may be used on data even when the variables are not independent, which would give a formal result but would be difficult to interpret. More on interpretation in Chapter 4.

We should note that a direct translation of Shannon entropy to the continuous domain as $H(X) = \int_{x\in\mathcal{X}} p(x)h(x)dx = -\int_{x\in\mathcal{X}} p(x)\log p(x)dx$ is not the continuous analogue of Shannon entropy, as it does not carry the same properties – for example, it can be negative and is not invariant under continuous coordinate transformations. This quantity has come to be known as **differential entropy**. The quantities are not equivalent because when trying to derive entropy from Eq. 2.10 by binning a continuous variable in the limit of bin width Δ going to zero, one obtains the above integral plus a diverging term $\log\Delta$ which is removed to obtain this definition.

Relative entropy of a random variable X is defined as the Kullback-Leibler (K-L) divergence between the probability distribution of $P(X)$ and the corresponding maximum entropy uniform distribution $P_U(X)$ (Kullback & Leibler, 1951):

$$H(X) := \log N - D_{KL}(P(X)||P_U(X)) \tag{2.19}$$

$$= \log N - \int_{x\in\mathcal{X}} p(x)\log\frac{p(x)}{p_U(x)}dx \tag{2.20}$$

The K-L divergence quantities the dissimilarity between two probability distributions. This alternative definition does share its properties with Shannon's entropy, and is also equivalent to Jaynes' formulation of a generalisation to continuous variables (Jaynes, 1957).

When applied to time series, entropy can be taken to mean the reduction in uncertainty provided by observing one more realisation of a stochastic process. When used in this way it is referred to as **entropy rate**.

In complex systems research, entropy is used to quantify the complexity of a component's or agent's behaviour, but also that of a system as a whole. Entropy has been used

to describe biological systems, such as individual behaviour in a model of how ants build nests (Miramontes, 1995); human behaviour and health, through quantifying physiological signals such as respiration and heart rate (Rajpal et al., 2020; Rosas et al., 2023); and even profoundly qualitative phenomena, such as music (Margulis & Beatty, 2008), literary styles (Kontoyiannis, 1997), poems (Kozhemyakina et al., 2023) and archaeological findings (Diachenko & Sobkowiak-Tabaka, 2022). One of its most staggering uses is in the Entropic Brain Hypothesis, a theory of conscious states in which the complexity of EEG signals estimated by the entropy rate is an indicator of the richness of experience (Carhart-Harris et al., 2014).

Mutual information is a non-linear measure of similarity between two random variables, which was originally devised by Shannon to quantify the data loss in a message sent through a noisy channel by comparing the original lossless message with the lossy transmitted and received one. The mutual information captures how much does knowing about one variable reduce the uncertainty about the other:

$$I(X;Y) = \sum_{x\in\mathcal{X}}\sum_{y\in\mathcal{Y}} p(x,y)\log\frac{p(x,y)}{p(x)p(y)} \tag{2.21}$$

$$= H(X) - H(X|Y) = H(Y) - H(Y|X) \tag{2.22}$$

$$= H(X) + H(Y) - H(X,Y) \tag{2.23}$$

or, using the Kullback-Leibler (K-L) divergence between the joint probability and the product of the marginals, we can define a continuous analogue of mutual information which preserves the properties of the discrete definition:

$$I(X;Y) := D_{KL}(P(X,Y)||P(X)P(Y)) \tag{2.24}$$

$$= \int_{x\in\mathcal{X}}\int_{y\in\mathcal{Y}} p(x,y)\log\frac{p(x,y)}{p(x)p(y)} \tag{2.25}$$

Unlike the entropy, if a continuous random variable is binned to be used with the discrete definition in Eq. 2.21, one obtains the K-L definition in Eq. 2.24 in the limit of bin width going to 0. Moreover, both differential and relative entropy can be used in Eq. 2.23 to derive the same quantity for mutual information for continuous variables.

From the definitions of both correlations and mutual information, it follows that two independent variables X and Y, whose joint distribution $P(X,Y)$ is equal to the product of marginal distributions $P(X)P(Y)$, have both a null correlation function and a null mutual information. But that there exist cases when mutual information of two dependent variables is null, which makes it difficult to differentiate completely random from perfectly predictable events. These ideas are further explored in Chapter 4.

We will make use of the following relevant properties of mutual information, which as in the case of entropy, are crucial to interpreting the measure:

$$\text{Positive} \quad I(X;Y) \geq 0 \text{ with } I(X;Y) = 0 \Leftrightarrow X \perp\!\!\!\perp Y \tag{2.26}$$

$$\text{Symmetric} \quad I(X;Y) = I(Y;X) \tag{2.27}$$

$$\text{Transform invariant} \quad I(f(X);g(Y)) = I(X;Y) \text{ with } f, g \text{ bijective} \tag{2.28}$$

The mutual information between a variable and itself is equal to the Shannon entropy, but only in the discrete case. In continuous variables $I(X;X) = \infty$.

$$I(X;X) = H(X), \text{ if } X \in \mathbb{Z} \tag{2.29}$$

The additive and subtracted relationships between entropies and mutual information of two variables can be represented visually as seen in Fig. 2.2. Joint entropy relates to the information contained in both X and Y, while the mutual information contain only what constitutes an overlap between them. The definition in terms of conditional entropies reminds us that this measure is statistical, quantifying the reduction in uncertainty knowing one variable offers about the other.

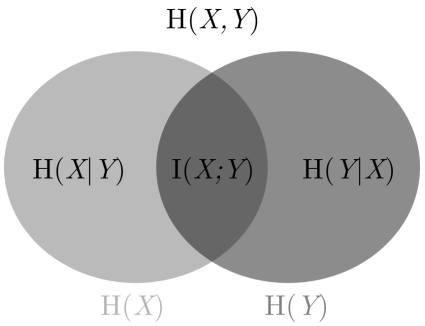


Figure 2.2: The relationship between entropy and mutual information.

An important application of the mutual information is that it can be used to detect phase transitions from random to collective behaviour using less data than phase transition analysis. Examples are in financial data (Harré & Bossomaier, 2009), in physical systems describing magnets (Matsuda et al., 1996) and, of particular relevance, in simple models of collective behaviour such as the model introduced by (Vicsek et al., 1995) presented in Chapter 3. Using this model, it has been proposed that mutual information between components peaks at the phase transition from a disordered to an ordered regime, entailing long-range correlations, and can be used to detect phase transitions even in incomplete data (Wicks et al., 2007). These findings were challenged in (Barnett et al., 2017), where the mutual information did not peak at the phase transitions, and diverged at low noise in finite systems. This is an example of how theoretical assumptions made in the thermodynamic limit do not apply in real-world data.

Mutual information is not necessarily descriptive of an information *flow* between two variables, but rather a measure of their joint co-incidence. But when introducing a temporal

delay in our study, similar to the cross-correlation measure in Eq. 2.2, the reduction of uncertainty about a future state provided by past states allows for novel interpretations.

The **time-delayed mutual information** (TDMI) $I(X_t; Y_{t+\tau})$ can track how much information is preserved in the system during its temporal evolution by applying mutual information with a fixed time delay between the two time series. When the time delay is significantly later, the quantity is called **persistent mutual information** and has been used to find emergent behaviour in chaotic dynamical systems such as the logistic map (Ball et al., 2010).

TDMI cannot distinguish between information that relates to actual interdependencies in the dynamics from shared information due to common history and input signals. We will see a clear demonstration of this when trying to compute TDMI between spatial coordinates in Chapter 4. An alternative measure is to use the **transfer entropy** where mutual information is conditioned on past history (Schreiber, 2000), or other various decompositions of the mutual information into quantities with different intepretations.

Mutual information has become an important tool to quantify interactions, and has been used to create fine-grained descriptions of non-trivial information processes between agents and groups of agents in complex systems (Lizier & Zomaya, 2007; Rosas et al., 2019). Even more so than correlation functions, information-theoretic quantities are broadly applicable to different systems and examples of usefulness of mutual information are endless. The TDMI is an integral part of the information-theoretic measures of emergence which will be used throughout the thesis.

Practically, when analysing time series, mutual information must be estimated from data. There are many different ways to do so (Cellucci & Albano, 2005). For most of this thesis, we settle on the method proposed by (Kraskov et al., 2004) for all non-parametric data. This method estimates mutual information using a kernel of varying size. For each point, bin size is determined by the distance to a point's k nearest neighbour, such that it is smaller in regions densely populated with data and larger in sparely populated ones. This helps overcome limitations of using bins of a fixed size, such as by preventing empty bins.

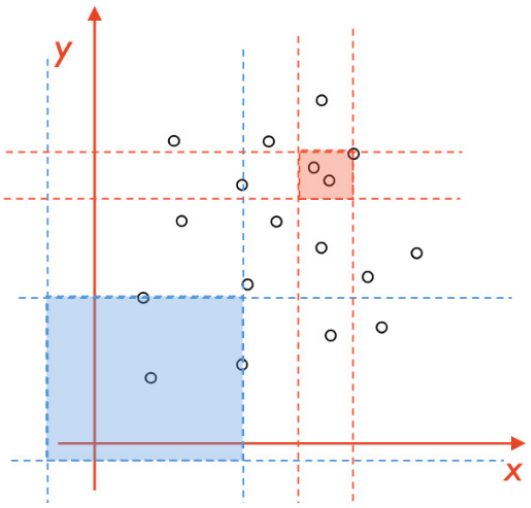


Figure 2.3: An example of the Kraskov mutual information estimator for two random variables. Reproduced from (Lizier, 2015).

2.3.2 Partial information decomposition

Mutual information quantifies how much knowing one variable reduces the uncertainty about another, but is difficult to generalise to larger numbers of variables, which is necessary in complex systems with relationships between multiple components. In other words, we require to generalise bivariate mutual information to the multivariate case, so that we can potentially quantify higher-order interdependencies between components in complex systems (Rosas et al., 2019).

Consider the simplest case of three variables, where using knowledge about two *source* variables X_1 and X_2 can be used predict a third *target* variable Y, by using the mutual information $I(X_1, X_2; Y)$. Intuitively, this term can be seen as the union of two sets: the information that X_1 provides about the target, $I(X_1; Y)$, and the one provided by X_2, $I(X_2; Y)$, with some information provided by both. This can be decomposed into pairwise and conditional mutual information using the *information chain rule*:

$$\begin{aligned} I(X_1, X_2; Y) &= I(X_1; Y) + I(X_2; Y|X_1) \\ &= I(X_2; Y) + I(X_1; Y|X_2) \end{aligned} \tag{2.30}$$

where the conditional term $I(X_2; Y|X_1)$ denotes information provided by X_2 to Y given X_1 is already known.

A fascinating case is when the target Y contains some information that is not individually provided by neither source, X_1 nor X_2, but which results from their combination. This reduction in uncertainty which only emerges from the combination can be considered *synergetic*. The simplest example of synergy can be seen in the binary `xor` function, where the result can not be predicted by or reduced to either of the operands.

The set-theoretic intuitions provided by the relationship between entropy and mutual information can be leveraged to further quantify the synergetic reduction in uncertainty by decomposing the mutual informaton of the three variables into pairwise relations. The work in this thesis uses such a non-negative decomposition inspired by set-theoretic concepts introduced by (Williams & Beer, 2010), which has come to be known as **Partial Information Decomposition (PID)**.

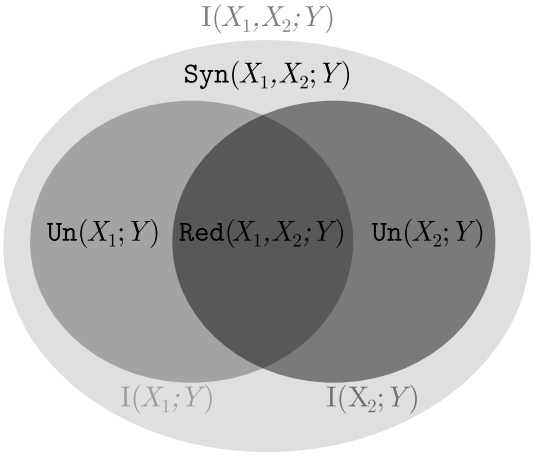


Figure 2.4: The relationship between PID information atoms.

PID proposes a decomposition of $I(X_1, X_2; Y)$ using only non-negative terms called *information atoms* (Fig. 2.4):

- **unique** information, that is contained uniquely within each source but not the other, denoted $\texttt{Un}(X_2; Y|X_1)$ and $\texttt{Un}(X_1; Y|X_2)$
- **redundant** information, that is shared between both sources and target, denoted $\texttt{Red}(X_1, X_2; Y)$
- **synergistic** information, that exists in the target, but is only predicted by both sources together, denoted $\texttt{Syn}(X_1, X_2; Y)$

These atoms can then be used to express in a more fine-grained manner the information quantities and how they are shared in this three variable system:

$$I(X_1; Y) = \texttt{Red}(X_1, X_2; Y) + \texttt{Un}(X_1; Y|X_2) \tag{2.31}$$

$$I(X_2; Y|X_1) = \texttt{Un}(X_2; Y|X_1) + \texttt{Syn}(X_1, X_2; Y) \tag{2.32}$$

which give that the mutual information between sources and target can be expressed as a sum of the unique, redundant, and synergetic information:

$$\begin{aligned} I(X_1, X_2; Y) = \texttt{Red}(X_1, X_2; Y) + \texttt{Un}(X_1; Y|X_2) \\ + \texttt{Un}(X_2; Y|X_1) + \texttt{Syn}(X_1, X_2; Y) \end{aligned} \tag{2.33}$$

Generalising to more variables requires a more elaborate mathematical formalism, which also started with work by Shannon on information lattices (Shannon, 1953). In PID, the mutual information is decomposed based on how various groupings of source variables provide information towards the target, and how this information is split in unique, redundant and synergetic atoms, based on *lattice theory*. In the order theory subdiscipline of abstract algebra, a *lattice* is a way to describe partially ordered sets that have a unique supremum (maximum element or upper bound) and a unique infimum (minimum element or lower bound). In a *partially ordered* set, the elements cannot be totally ordered, i.e. we cannot state that for every element in the set, every other element is either 'larger' or 'smaller'. The 'smaller' elements would be on a lower level in a lattice, and the 'bigger' ones higher, but at the same level, elements are uncomparable.

A possible partial ordering function that may produce a lattice is the relationship of one set being a subset of another. Applying this ordering to the decomposed information atoms produces a *redundancy lattice*, in which a higher element provides at least as much redundant information as a lower one. This lattice can be visualised in Fig. 2.5.

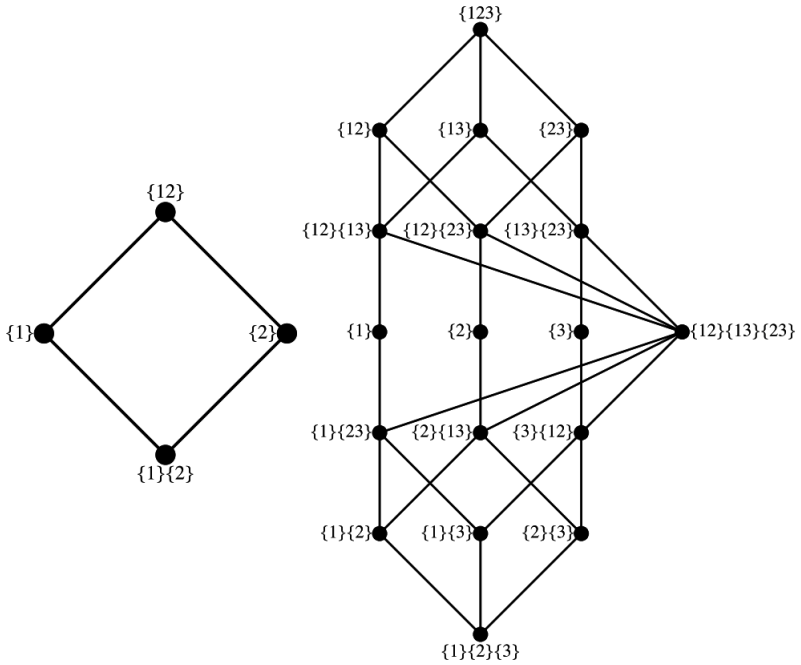


Figure 2.5: **Redundancy lattice for three and four variables**. Sets of singletons `{1}{2}` denote the information jointly provided by variables 1 and 2 to the target, or redundant information. Lone singletons `{1}` and `{2}` denote the unique information in each source variable, which both contain the redundant information `{1}{2}`. Sets of multiple elements `{12}` denote the synergetic information provided by `{1}` and `{2}` together. When generalised to more variables, the lattice captures these partially hierarchical information relationships between groups of variables of different sizes, with the synergetic information provided by all sources at the top and the redundant information common to all sources at the bottom. Reproduced from (Williams & Beer, 2010).

The decomposition of multivariate mutual information is non-unique, as the above PID depends on how redundancy or synergy are defined. Unfortunately, there is a lack of a generally agreed-upon method to quantify the information atoms.

The PID of (Williams & Beer, 2010) uses of a redundancy function defined as the minimal information $I_{\min}$. $I_{\min}$ captures the information common to all sources while taking into account sources may provide information about different outcomes.

In general, quantifying redundancy is somewhat of an arcane art. Many other redundancy functions have been proposed and are being used in the PID literature, such as bivariate redundancy based on information projections I_{proj} (Harder et al., 2013), intersection information $I_\cap$ (Griffith et al., 2014), minimum mutual information I_{MMI} (Barrett, 2015) and pointwise change in surprisal I_{CCS} (Ince, 2017), to name a few. None of these measures is perfect and each provides different advantages and disadvantages depending on the data or system under scrutiny (James et al., 2018b).

The PID presented here focuses on redundancy, but other information atoms can be used to construct the lattice, which may produce different PIDs, some of which were found to be more intuitive in null cases than the MMI-PID. Examples are information loss (Chicharro & Panzeri, 2017), unique information (James et al., 2018b), synergistic disclosure (Rosas et al., 2020b) and union information (Kolchinsky, 2022). (Rosas et al., 2020b) observe in numerical comparisons similar results between different redundancy functions or PIDs.

Finally, it should also be noted that many other information measures of synergy and/or redundancy have been proposed aside from PID. A review of the most important ones can be found in (Timme et al., 2013). PID is preferred as it supports simultaneous synergy and redundancy through the decomposition, allowing us to putatively quantify the ordering and disordering tendencies coexisting in a complex system.

The work in this thesis makes use of PID with the Minimum Mutual Information (MMI) to quantify redundancy:

$$I_{\text{MMI}} = \min_i I(X^i; Y) \tag{2.34}$$

The MMI-PID is by far the most trivial computationally, and has been shown by (Barrett, 2015) to be equivalent to other redundancy-based PIDs (Griffith & Koch, 2014; Harder et al., 2013; Williams & Beer, 2010) in Gaussian random variables.

It is important to interpretation to recall that MMI indicates the variables share a common amount of information, but not that they share the *same information*. Another drawback is that I_{MMI} assigns a zero value to at least one of the unique informations. Moreover, since the `min` function is non-linear, decompositions based on MMI may be difficult to interpret when adding and subtracting information quantities.

It has also been shown that I_{MMI} can behave in unintuitive ways in some null cases (Varley, 2024), for example, some systems paradoxically seem to become more synergistic even though they are more disintegrated, with less couplings between components.

Redundancy-based PIDs also appear, in general, to produce difficult to interpret results in Gaussian variables (Barrett, 2015), as Gaussian systems appear to exhibit net synergy even without any interactions. The latter fact will become relevant in the studies in the first part of the thesis, and more on the drawbacks of MMI-PID when applied to Gaussian null cases will be discussed in Chapter 4.

2.3.3 Information, causality and emergence

We have seen how the formalism introduced by Shannon can give us various tools that can be related to underlying non-trivial processes in complex systems: entropy, as a measure of statistical complexity to study individual component or agent complexity, or the complexity of one system or group property; mutual information, to study pairwise intedependencies; and PID, to study interdependencies between more than two components. We can use these tools to construct more temporally directed and fine-grained measures that may be able to quantify the emergent features in a complex system, and describe in detail how the conflicting tendencies between order and disorder act at the microscopic, mesoscopic, and macroscopic levels, influencing each other at the same level or across the ones above and below.

By using the measure of time-delayed mutual information (TDMI) to quantify predictive relationships between components and collective properties in complex systems, we are also indirectly making the assumption that we may quantify some mechanistic relationships or interactions between the components, whose actions have an effect upon one another. In other words, time-delayed measures such as the cross-correlation, TDMI or transfer entropy are sometimes interpreted to describe a putative cause-and-effect relationship between the phenomena recorded in the time series.

It follows that we should briefly explore the idea of causality and how it relates to systematic definitons of emergence.

Causal concepts of emergence

In the words of Wiener, who also gave us ideas of cybernetics and organised complexity, a measure of causality would allow us to 'observe how much a change in one aspect of the universe will bring out changes in others'. Wiener also suggested that 'partial information which our knowledge of one part of the system gives us about the rest of it' could be considered as a candidate measure (Wiener, 2014). This insight only appears even more ahead of its time in light of the developments in the study of causality and emergence using PID to be presented below.

A few years later, when reasoning about econometrics, Granger introduced the idea of causality as statistical predictibility: if past states of X reduce uncertainty in knowing the future of Y, then X is said to 'Granger-cause' or 'G-cause' Y (Granger, 1969).

The G-causality is not the only attempt to quantify or operationalise the causal structure of complex systems of interacting processes, but it forms the basis of important ideas that are used in the candidate measures of emergence explored in this thesis. For example Seth (Seth, 2010) proposes that a systemic level feature $\mathbf{V}_t$ of a complex system is Granger-

emergent (or G-emergent) with respect to the processes of its components $\mathbf{X}_t$ if two conditions are met: $\mathbf{V}_t$ is autonomous with respect to $\mathbf{X}_t$, i.e. its evolution is independent or cannot be predicted by $\mathbf{X}_t$, and $\mathbf{V}_t$ is G-caused by $\mathbf{X}_t$.

More specifically, we use the idea that a causally emergent *macroscopic* (or coarse-grained) property $\mathbf{V}_t$, such that it describes the system as a whole, or with much lesser granularity, would have greater causal power over the system's future than a description of the *microscopic* components it consists of $\mathbf{X}_t$. This is the basis of the idea of **causal emergence** proposed by (Hoel et al., 2013). Yet this causal emergence can use a variety of measures of causation beyond G-causality. Interestingly, while these have different properties, it appears they agree when used on data (Comolatti & Hoel, 2022).

The theory of dynamical dependence proposed by (Barnett & Seth, 2023) also considers the coarse-grainings at the meso or macro scale to describe collective behaviour. The authors propse criteria of supervenience, and dynamical independence or autonomy, based on the conditional mutual information between past and future states and transfer entropy. Unlike (Seth, 2010) and (Rosas et al., 2020a), this measure does not rely on self-predictability of macroscopic variables or the prediction power of macro over micro, and it does not use PID. This measure appears very versatile: it supports studies in both time and frequency domain, as well as deterministic systems, and is focused on the *discovery* of emergent properties rather than criteria.

Whether these measures truly quantify causality has been disputed (Dewhurst, 2021), and it is important to make the distinction, as we have previously warned, between mechanistic behaviours of the system and what can be detected by our measures based on behavioural trajectories. In general, it is known that the capacity of a variable X to predict another Y does not mean X *causes* Y. In contrast, the theory of causality and the do-calculus propososed by Judea Pearl (Pearl, 2009) makes use of structural causal models which aim to describe the causal mechanisms in a system. This approach is much more rigurous but less practical when we only have access to the behaviour of a system via observed time series, and not its true causal model to encode in do-calculus.

On the other hand, the formalism of a *statistical understanding of causation* introduced by Granger still provides practical methods of analysis that are tremendously useful in the study of complex systems (Bressler & Seth, 2011) when taken as face value and interpreted in awareness of limitations. Even Granger himself did not consider G-causality to be equivalent to *true* causality, but rather as a form of *precedence* or *forecasting*, which he specifically called *temporally related* (Granger, 1980). We should also note the deeply philosophical difficulties in the question of causality and the long history of misunderstanding causality as precedence, or the classical *post hoc ergo proper hoc* fallacy.

To return to information theory, we should briefly note that transfer entropy (Schreiber, 2000), the directed information measure based on conditional mutual information mentioned earlier in this chapter, is a generalisation of G-causality, and equivalent to G-causality on Gaussians (Barnett et al., 2009). The ideas of autonomy and G-emergence in (Seth, 2010) can also be expressed in terms of the conditional mutual information: autonomy as $I(\mathbf{V}_t; \mathbf{V}_{t'}|\mathbf{X}_t) > 0$ while the G-causal relationship could also be described by $I(\mathbf{X}_t; \mathbf{V}'_t|\mathbf{V}_t) > 0)$.

Inspired by G-emergence and PID, the work in (Rosas et al., 2020a) leverages some limitations of the previous work, is data agnostic, does not require constructing causal models, and can capture different aspects of emergence with respect to the relationships between the whole and parts, as we will see shortly. A review of many more causal emergence measures is in (Yuan et al., 2024).

Reconciling emergences

One of the most important goals in the study of complex systems is to provide means to describe and identify different kinds of emergence. For example, we may wish to make a distinction between collective properties or forces which arise from or are caused by the components, which philosophers have called *causal emergence*, and collective properties or forces which affect the parts in turn, also called *downwards causation*.

Using the theory introduced by (Rosas et al., 2020a; @ Mediano et al., 2022), the work in this thesis makes use of three information criteria for different types of emergent behaviour and their associated measures. The measures use the TDMI to estimate how much the behaviour of a component can predict that of another or that of the system, but also how much is component behaviour influenced, in turn, by the system as a whole.

We consider a system of n individuals or parts, described by trajectories $\mathbf{X}$, and two time points in its evolution $t < t'$. Individuals can be grouped in sets α, so that $\mathbf{X}^\alpha$ represents the group of random variables corresponding to the parts in α. The corresponding dynamics are encoded in the transition probability $p_{\mathbf{X}_{t'}|\mathbf{X}_t}$

Our goal is to study the emergence of a robust *collective* systemic property $\mathbf{V}_t$ that can describe the evolution of a system better than any of the individual trajectories or groups of trajectories corresponding to the parts. We consider features $V_t \in \mathcal{V}$ with $p_{V_t|\mathbf{X}_t}$ that are *supervenient* on the underlying system: a change in V_t would imply a change in X_t. We formalise this condition for stochastic processes by requiring V_t to be statistically independent of $\mathbf{X}_{t'}$ when $\mathbf{X}_t$ is given for all $t' > t$, i.e. $V_t - \mathbf{X}_t - \mathbf{X}_{t'}$ form a Markov chain. This includes as deterministic functions $\mathcal{F} : \prod_{j=1}^{n} \mathcal{X}_j \to \mathcal{V}$ such that $\mathbf{V}_t = \mathcal{F}(\mathbf{X}_t)$, as well as aggregate properties affected by observational noise.

Having systematically defined this collective property or *coarse-graining* of a complex system's trajectories, which we consider to be a candidate description for collective behaviour said system, we can test whether this it is emergent with respect to the properties of the individuals (if $k = 1$) or groups of individuals α of size $|\alpha| = k$ and in what way:

Causal emergence, quantified by Ψ, refers to the property of a system feature to be irreducible to the sum contributions of its components. In this theory, causal emergence is defined by a synergy-redundancy index, by subtracting the sum contributions of the parts from the synergetic information in the whole.

$$\Psi^{(k)}_{t,t'}(V) := I(V_t; V_{t'}) - \sum_{|\alpha|=k} I(X^\alpha_t; V_{t'}) \tag{2.35}$$

Ψ is equivalent to the synergy-redundancy index, which was first used to study information in the monkey brain (Gat & Tishby, 1999).

Downwards causation, quantified by Δ, refers to a system where a macro feature has a causal effect over one or more particular agents, but this effect cannot be attributed to any other individual component or group

$$\Delta^{(k)}_{t,t'}(V) := \max_{|\alpha|=k} \left(I(V_t; X^\alpha_{t'}) - \sum_{|\beta|=k} I(X^\beta_t; X^\alpha_{t'}) \right) \tag{2.36}$$

Causal decoupling, quantified by Γ, refers to a system where a macro feature can predict its own evolution, but no component or group of components may predict the evolution of any other

$$\Gamma^{(k)}_{t,t'}(V) := \max_{|\alpha|=k} I(V_t; X^\alpha_{t'}) \tag{2.37}$$

The associated criteria for emergence are given by the following propositions

(1) $\Psi^{(k)}_{t,t'}(V) > 0$ is sufficient for V to be causally emergent.

(2) $\Delta^{(k)}_{t,t'}(V) > 0$ is sufficient for downward causation.

(3) $\Psi^{(k)}_{t,t'}(V) > 0$ and $\Gamma^{(1)}_{t,t'}(V) = 0$ is sufficient for causal decoupling.

Information decomposition and redundancy

The $\Psi-\Gamma-\Delta$ theory outlined above provides practical criteria to detect causal emergence in experimental or simulated data. Yet, these are *sufficient* and not necessary conditions: e.g. it is possible that an emergent system may have a negative Ψ.

Both Ψ and Δ are defined as 'whole-minus-sum' or 'synergy-minus-redundancy' estimators, similar to the interaction information (Williams & Beer, 2010) and the Ω-information (Rosas et al., 2019), which aim to quantify the balance between synergy and redundancy and capture the fine balance between conflicting collective and individual tendencies, or ordered and disordered tendencies, which create the most spectacular kinds of complex emergent behaviour.

Unfortunately, Ψ, Δ, and other such estimators based on the mutual information are affected by the non-additive property of the mutual information. In the case of Ψ, for example, we are adding all the marginal mutual informations $I(X_t^i; V_{t'})$ in Eq. (2.35) to represent the sum contributions of the components towards the emergent property of the system. But each of those terms, for example, contains the redundant information provided by all components X^i. For systems of n variables, this redundant information ends up being subtracted 'double-counted' $n-1$ times in excess from $I(V_t; V_{t'})$.

Not only is there redundant information shared by all variables, but there is likely also redundancy in every group of $n-1$, $n-2$ variables and so on down to pairs. PID provides an answer to quantifying this redundancy through its redundancy lattice. Rosas and Mediano (Sas et al., 2024b) propose a technique of *lattice expansion* to identify which atoms of redundant information are being included multiple times when going up the lattice. This allows outlining a new family of measures $\Psi^{(k,q)}$, where $q \in \{0, \dots n-1\}$ for systems of n variables is the approximation order, such that $\Psi^{(k,0)} = \Psi^{(k)}$, and in which the redundancy across groups of information atoms of size $n-q+1$ and larger is accounted for in the synergy-redundancy index.

The Ψ approximation of order q, $\Psi^{(k,q)}$, is formally defined as:

$$\Psi^{(k,q)} = \Psi^{(k)} + \sum_{r=n-q+1}^{n} \sum_{\substack{\alpha \in \mathcal{M}^n \\ |\alpha|=r}} C_{q,r}^n I_\cap^\alpha(\mathbf{X}_t; V_{t'}) \ , \tag{2.38}$$

where α denotes a set of singleton information atoms, $\mathcal{M}^n$ represents all the subsets of the lattice consisting of *uncomparable* singleton elements, $I_\cap^\alpha$ is the redundancy (or intersection information) shared by atoms in α and the coefficients $C_{q,r}^n$ are defined recursively:

$$C_{q,r}^n = r - 1 - \sum_{s=n-q+1}^{r-1} C_{q,s}^n \binom{r}{s} \tag{2.39}$$

$$C_{q,n-q+1}^n = n - q \tag{2.40}$$

$$C_{1,n}^n = n - 1 \tag{2.41}$$

where n is the system size, $q \in \{1, \ldots, n-1\}$ is the order of the expansion, and $r \in \{n-q+1, \ldots, n\}$ the cardinality of the set of sources being considered, with $q, n \in \mathbb{N}$. Atoms in $\alpha \in \mathcal{M}^n$ are computed as all the combinations of all n singleton elements in groups of size r. The number of evaluations of $I_\cap^\alpha$ grows with q as $\mathcal{O}\left(\binom{n}{q-1}\right)$.

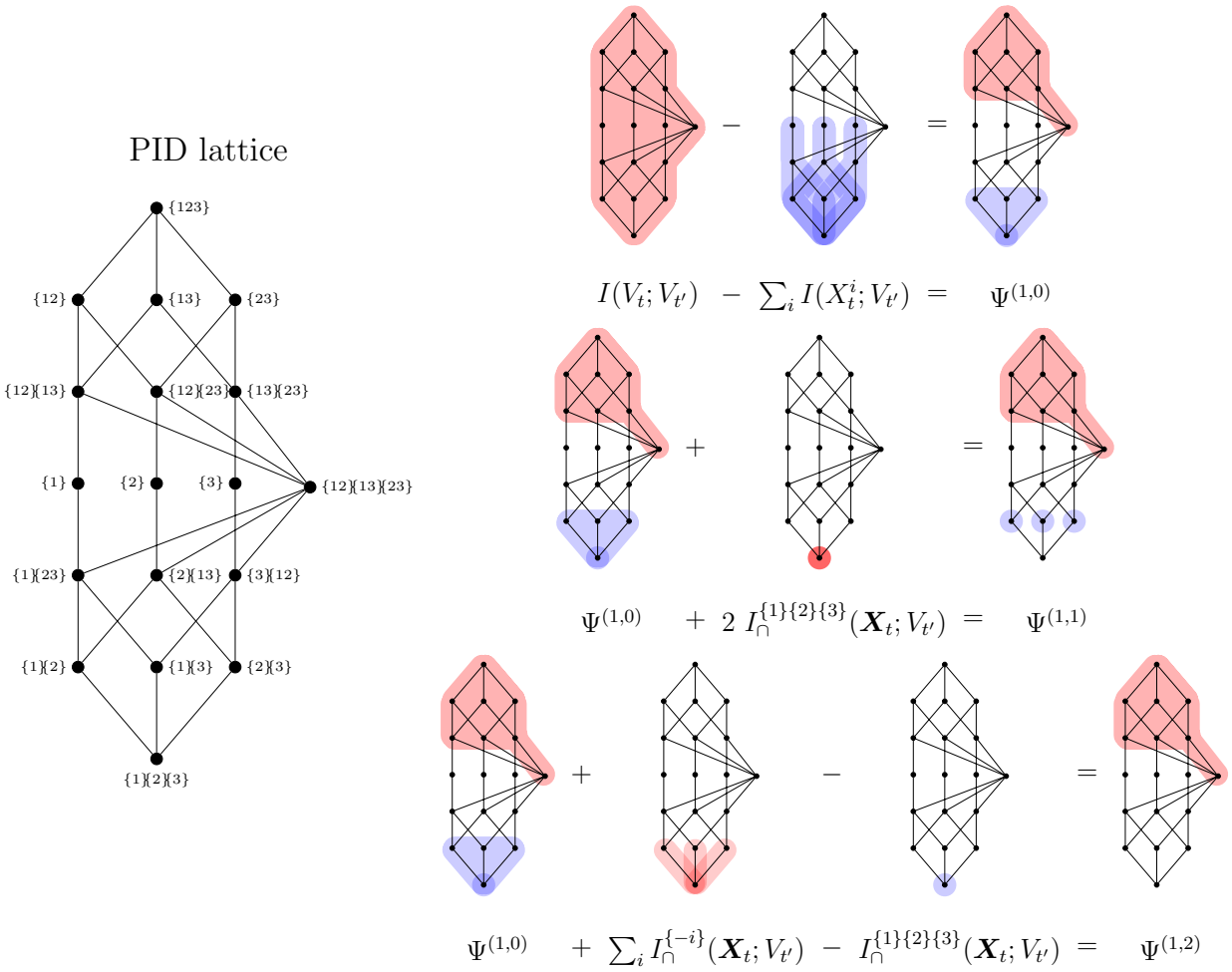


Figure 2.6: **The PID redundancy lattice and lattice expansion method for 3 source variables**. To compute $\Psi^{(1)}$ the sum of parts term would subtract the bottom atom (representing the redundancy across all $N = 3$ variables) three times, instead of only once, and the atoms one level up (representing the redundancy across groups of $N - 1 = 2$ variables) twice, as opposed to once. The improved estimator with approximation order $q = 1$ corrects for the intersection information of all $n-q+1 = 3$ variables, which is found at the bottom of the lattice, while the $q = 2$ approximation corrects for atoms sets of $n - q + 1 = 2$ variables, which is found at the second level. As this system is only composed of 3 sources, these are all the possible combinations of atom sets. With more sources, the number of combinations grows factorially.

For a given n, q, we begin by correcting the highest level in the lattice (i.e. the level with the lowest r). Intuitively, nodes with r singletons need to be corrected by a factor $r-1$; and thus the coefficient for the lowest r in the expansion satisfies $C^n_{q,n-q+1} = n-q$. After atoms with cardinality c have been corrected, we can consider the set of atoms in $\mathcal{M}^n$ with cardinality $c+1$. In general, an atom with cardinality r will precede $\binom{r}{s}$ atoms

with cardinality $s < r$, which need to be accounted for in the expansion – and thus the recursive expression for $C^n_{q,r}$. The quantity $\Psi^{(k,q)}$ (Eq. (2.38)) being greater than 0 is a valid criterion for emergence, and it is always greater than $\Psi^{(k)}$. Please see (Sas et al., 2024b) for detailed proofs of the criteria.

As an example, the first- and second-order lattice expansions yield a corrected Ψ:

$$\Psi^{(k,1)} = \Psi^{(k,0)} + (n-1) I_\cap^{\{1\}\ldots\{n\}}(\mathbf{X}_t; V_{t'}) \tag{2.42}$$

$$\begin{aligned}\Psi^{(k,2)} = \Psi^{(k,0)} &+ (n-2) \sum_{i=1}^{n} I_\cap^{\{-i\}}(\mathbf{X}_t; V_{t'}) \\ &+ (n-1-n(n-2))\, I_\cap^{\{1\}\ldots\{n\}}(\mathbf{X}_t; V_{t'})\end{aligned} \tag{2.43}$$

where $I_\cap^{\{-1\}}$ denotes the redundant information shared by the set of all singleton atoms apart from `{i}`.

This lattice expansion method can also be extended to the $I(X^i_t; X^j_{t'})$ terms, so that $\Delta_{t,t'}$ also provides a more accurate estimation of the downwards causation term.

This lattice expansion allows us to bridge between whole-minus-sum measures (Rosas et al., 2019), which are fast but coarse, and the full PID lattice, which is precise but computationally demanding. Additionally, it is worth noting that since all the redundancies only involve singleton sources, these terms are also easy to estimate empirically.

Nonethess, the estimation of the criteria for either large k or large q requires the traversal of all the possible combinations of atom sets. For a fixed number of sources this the number of operations grows factorially with the size of the atom sets. For 10 sources, more than a thousand atom combinations are possible. If we wanted to compute the most fine-grained estimator, the criteria soon become untractable, requiring the order $\mathcal{O}(2^n)$ computations for a system of n parts only to traverse all the atom sets.

Notably, using the lattice expansion does involve choosing a particular PID from the multiple options available (see the previous Section 2.3.2). However, so far in practical comparative analyses many of these tend to yield qualitatively similar results in null models (Rosas et al., 2020b).

A note on interpretation

Having introduced both PID and synergy-redundancy indexes, it is important to re-emphasise the difference between the underlying mechanisms that define the agent interactions, and the emergent patterns of behaviour that we can observe (Benhamou, 2007; Rosas et al., 2022). This distinction is often made, more specifically, between statistical dependencies, as can be calculated by various measures which aim to quantify the emer-

gent patterns of behaviour captured by time series, and the underlying processes that produce that behaviour, such as the distinction between G-causality and *true* causality.

The language used to refer to information atoms often does not distinguish mechanism from behaviour and may create misleading interpretations. The definitions only deal with reductions in uncertainty as robustly quantified by the conditional entropy and conditional mutual information, but terms like *synergy*, *redundancy*, *causality*, *information flow* and *information transfer* also have 'natural interpretations' which could suggest a mechanistic or causal aspect that may not be present in the underlying dynamics.

Since information-theoretic quantities like entropy and mutual information are not conserved due to non-additivity in dependent random variables, interpreting measures which rely on summing or subtracting them should be made with utmost care. The PID aims to mitigate this issue by splitting the mutual information into atomic terms that can be added and subtracted, but the information decomposition can be performed in multiple ways, may incur computational difficulties, and can become untractable in large systems.

Finally, while the research community generally agrees on bivariate information measures, there is a great diversity of multivariate measures in use today which differ in subtle, yet significant ways, but which we may risk to interpret in the same way. A review of some of these similarities and differences is in (Timme et al., 2013), while some of the shortcomings of the redundancy function MMI-PID used throughout the thesis are outlined in (Barrett, 2015) and (Varley, 2024).

As mentioned before, most different PIDs appear to agree on some kinds of systems but disagree on others. However, there are conceptual issues with some measures in how information from different sources is conflated. For example, in MMI-PID, all source variables having some mutual information with the target is not necessarily a sign of redundancy, but we often do interpret it as such. Moreover, Gaussian variables, for example, show net synergy even when there is no coupling or collective behaviour *per se* amongst them, making the measure more difficult to interpret.

For all of these reasons, the exciting prospects of the $\Psi - \Gamma - \Delta$ criteria and the lattice expansion method make it all the more important to explore some of these ideas and to test the correspondence between mechanism and measure first. In the spirit of complexity science, we will employ simulations of known theoretical models that can manifest emergent behaviour as a *null case* to test the criteria in Chapter 4, before proceeding to use it on data from multi-agent system simulations and real experiments in Chapters 5-7.

2.4 Network science methods

Dependencies between two or more time series can be investigated using a broad range of linear and non-linear measures. In order to obtain even finer descriptions of the complex systems producing those time series, measures can be computed and assembled into networks that model the fine-grained structure of the system's interdependencies. Networks themselves can then be analysed and quantified with measures of complexity. These methods are frequently used in neuroscience, and an extensive review can be found in (Sarasso et al., 2021), but they are relevant to all studies of complex systems.

A **network** or graph $\mathcal{G}(n, m)$ is a set of n **nodes** or vertices $\mathcal{N} = (1, 2, ...n)$, which usually represent components in the system, connected together by a set of m **links** or edges $L = \{(i, j) : (i, j) \in \mathcal{N} \times \mathcal{N}\}$ which represent their interactions or relationships. A **weighted network** associates a weight w_{ij} to every link (i, j). Networks can be represented as **adjacency matrices** $(\mathbf{A}_{ij})$ where $a_{ij} = 1$ (or w_{ij}) if $(i, j) \in \mathcal{L}$ and 0 otherwise.

For example, in a structural brain network, the nodes refer to various brain regions, links to physiological pathways of axons between brain areas, while weights can represent the amount of white matter found in the pathways. Or, the links can be used to represent functional connections, in which nodes representing brain regions are connected if said regions are active simultaneously during an activity or a stimulus.

Networks can be **undirected**, in which case $(i, j) \in \mathcal{L} iff (j, i) \in \mathcal{L}$, or **directed**, where the former does not hold. Undirected networks can be used to characterise some mutual, bi-directional relationships between agents, such as describing that two devices are physically connected over the internet, whilst directed networks can capture asymmetric relationships, such as a webpage containing a hyperlink to another. A **simple network** does not allow self-links or multiple links between nodes. A **multi-network** allows multiple links between the same nodes.

The **neigbourhood** N_i of a node i is defined as the set of its immediately connected neighbours $N_i = \{j : (i, j) \in \mathcal{L} \vee (j, i) \in \mathcal{L}\}$. The **degree** of a node refers to the number of edges connected to that node, $k_i = |N_i| = \sum_i a_{ij}$. In directed networks, we may differentiate between edges going in and out of a node.

A **path** between two nodes is a sequence of edges which joins the two nodes. If the network is directed, then a directed path has the added requirement that all the edges are directed the same way. In a simple network, the **shortest path length** λ_{ij} is given by the number of edges in the shortest path from node i to j. If the network is weighted, then the path length is the sum of all the weights of the edges.

2.4.1 Network properties

When studying complex nextworks it is useful to observe how they are similar in terms of the distribution of node importance, the density of links, how fast information reaches all nodes, the number of communities and many more. Such means of characterising networks reveal there are similarities between social networks, brain networks, the internet, or ecological networks.

A **complete network** $\mathcal{G}_n$ has links between every pair of nodes. It is the densest possible network with n nodes and , where $a_{ij} = 1$ for all $i \neq j$. The number of links in this network is given by all the possible pairs of nodes $\binom{n}{2}$, whilst the degree of every node is $n - 1$.

In a **connected network** there is at least one path between every two nodes. If a network is not fully connected, then it can be partitioned into **connected components** or **cliques**.

The **average degree** of a network can also give insights about the density of a network, be easily calculated as:

$$c(\mathcal{G}(n,m)) = \frac{1}{n}\sum_{i=1}^{n} k_i = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij} = \frac{2m}{n} \tag{2.44}$$

Whilst the average degree may appear insightful for some networks, in large complex networks it is likely that the degree distribution has a *fat tail* and the average degree does not capture the particularities of the network well.

The **average path length** is given by the mean shortest path length:

$$l(\mathcal{G}(n,m)) = \frac{1}{n(n-1)}\sum_{i\neq j} \lambda_{ij} \tag{2.45}$$

In a **random network** (Erdős & Rényi, 1959) each node has approximately the same degree k and a mean path length $\lambda_{rand} \approx \ln n - \ln k$.

Connectance

For a simple network, connectance quantifies how dense or sparse a network $\mathcal{G}(n,m)$ is by comparing it to the fully connected network.

$$C(\mathcal{G}(n,m)) = \frac{2m}{n(n-1)} \tag{2.46}$$

A connectance of 1 means the network is fully connected. The connectance measure is very similar to the local clustering coefficient yet it is applied over the whole network.

The densest network with n nodes is the fully connected graph $\mathcal{G}_n$, where $a_{ij} = 1$ for all $i \neq j$. The number of links in this network is given by all the possible pairs of nodes $\binom{n}{2}$, whilst the degree of every node is $n - 1$.

Clustering coefficient

The averaged clustering coefficient of a network is the average clustering coefficient of all nodes (Watts & Strogatz, 1998), $\gamma(i)$, which is given by the ratio of all possible neighbour pairs of a node which are also connected to each other, forming a triangle.

$$\gamma(\mathcal{G}(n,m)) = \frac{1}{N}\sum_i \gamma(i) \tag{2.47}$$

Similar to connectance, we can compare the he amount of clustering of a given network to that of a random network (Erdős & Rényi, 1959).

Small-world index

In random networks all nodes have similar clustering coefficients $\gamma_{\text{rand}} \approx \frac{k}{n}$. By comparing the mean path length and the clustering coefficient for the two networks we get the small-world index.

$$\sigma(\mathcal{G}(n,m)) = \frac{\frac{\gamma(\mathcal{G}(n,m))}{\gamma_{\text{rand}}}}{\frac{\lambda(\mathcal{G}(n,m))}{\lambda_{\text{rand}}}} \tag{2.48}$$

The small-world index captures the so-called small-world effect characteristic of social networks. In a small-world network, most nodes can be reached from any other through a few steps, despite the network being large (Watts & Strogatz, 1998). The effect reminds of the phrase 'six degrees of separation' suggesting that any two people are connected by an average of six acquaintances. Small-world networks also have high clustering coefficients in spite of small average path lengths.

2.4.2 Degree distribution

The degree distribution is defined as the the fraction of nodes that have a degree k:

$$P(k) = \frac{\sum_{i=1}^{n}\delta(k_i,k)}{N} = \frac{\sum_{i=1}^{n}\delta(\sum_{j=1}^{n}a_{ij},k)}{N} \tag{2.49}$$

where $\delta(\cdot,\cdot)$ is the Kronecker function:

$$\delta(x,y) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

The analysis of degree distributions in different complex systems reveals the high prevalence of *power law distributions* which indicate the presence of the scale-free hierarchical structure relevant to many complex networks (Barabási & Albert, 1999) including but not limited to the cell, the internet (routing, domains and hyperlinks), proteins networks and citation networks, to only name a few examples. While many networks have been reported to be scale-free, this was also largely debated; as such, we should be cautious when fitting power law distributions to data (Clauset & Moore, 2005), and be careful that the appropriate statistical tests are being used and the correct assumptions taken into consideration.

A research field where applications of complex networks have contributed greatly is the neuroscientific study of brain function (Sarasso et al., 2021; Sporns, 2002). The idea of *effective connectivity* allows data extracted from brain imaging to be constructed into *functional networks* which show when two areas of the brain are functionally correlated i.e. show patterns of activation that are statistically similar or related.

The presence of hub nodes in the brain's functional network has been shown to be indicative of the most important brain areas related to various states or activities (Sporns et al., 2007). Analysing brain networks can also reveal relationships between structure and function (Sporns, 2002) and the difference in various characteristics of the structural brain network can reveal insights about brain-related disorders (Bassett & Bullmore, 2009; Griffa et al., 2013).

Degree centrality measures have been used to analyse the brain activations of musicians when improvising as opposed to a strict mode of performance. The EEG signals have been analysed using causality measures, then these causality relationships were used to construct a network of activation. It appears the musicians have larger out-degrees during improvisation, while the audience shows the opposite trend (Wan et al., 2014). It has been suggested that higher degrees imply the brain region is more strongly involved with the related regions.

Some of the above research methods and pipelines, even if originating in neuroscience, are employed in this thesis on the study of collective behaviour and collective motion. The properties of the networks constructed from pairwise measures of synchrony or from mutual information or TDMI, and even how they change over time, can reveal fine-grained details about the complex behaviours of agents and groups of agents, starting with one of the simplest to describe and yet richest examples of collective intelligence: movement.

Part I

Collective behaviour in physical systems

Chapter 3

Simple models of complex systems

Chapter Summary

Complexity theory is a scientific practice which operates on theoretical models of complex systems with the use of simulation and mathematical analysis. In order to focus on the interactions between components and the emergent properties at the system level, this process of modelling aims to represent a phenomenon in the simplest way that still preserves the relevant emergent property. This chapter presents background on how the study of simple models can reveal similarities between very heterogeneous systems and phenomena in nature, and then presents and defines mathematically two simple models with a plethora of multidisciplinary applications in the study of complex systems, namely random walkers and self-propelled particles, and outlines the simplest definitions of collective behaviour in these systems.

3.1 The need for simple models

Before studying complex collective motion in the natural world with measures of emergence, we should be testing our methods on the simplest examples. Complexity science provides the perfect toolbox for this purpose: the use of the mathematical representations of an emergent phenomenon in the form of a **model**, and in particular, the simplest model that can capture the emergent feature under scrutiny (Jensen, 2022). The methodology of complexity science uses such models in order to create a simulation of collective behaviour that can produce time series data to test our measures.

Consider a cell, an organ formed of many cells, an animal formed of many organs, a swarm formed of many animals: the agents in a complex system are complex systems themselves, which makes it too complicated to describe in all detail. Yet since at many levels of description the components are acting as one, we can simplify their description to a few collective degrees of freedom, and aim for a model in which the main emergent feature of interest manifests even if the agents are simplified.

Take the example of collective movement of birds: a detailed model of each bird's brain and body is not necessary to simulate flocking behaviour (Fig. 3.1). On the other hand, the amounts of detail included in the model can make a difference on the kind of behaviour we wish to describe. It is enough to simply define a rule of alignment for a group of agents to show swarming aligned motion (Vicsek et al., 1995); including aggregation and avoidance can model a realistic small flock, school or swarm (Reynolds, 1987); but more variables are needed to realistically describe a complex murmuration of several thousand starlings, such as the aerodynamics of their bodies, their nesting preferences, and their social networks (Hildenbrandt et al., 2010). Modelling helps us test theories of how agents interact by implementing and simulating those mechanisms and comparing their emergent behaviour with the real-world system.

This simplicity is not just a constraint induced by limitations in compute power or by the difficulties of modelling. It allows focusing our research on better understanding self-organisation and how similar emergent phenomena arise in different systems. Such models are *explanatory* rather than *predictive*. One of the advantages of using simplified models is their non-specificity: a physical model such as the random walks introduced in Section 3.2 can be used to describe phenomena as varied as the stock market (Fama, 1965), neural firing (Gerstein & Mandelbrot, 1964), or cells and animals moving or foraging (Berthelot et al., 2021; Codling et al., 2008). These models may not exactly describe the behaviours, but can still be used to explore some mechanisms behind them. When they do, one needs to be aware that the systemic mergent patterns are not be confused with the processes that may give rise to them (Benhamou, 2007).

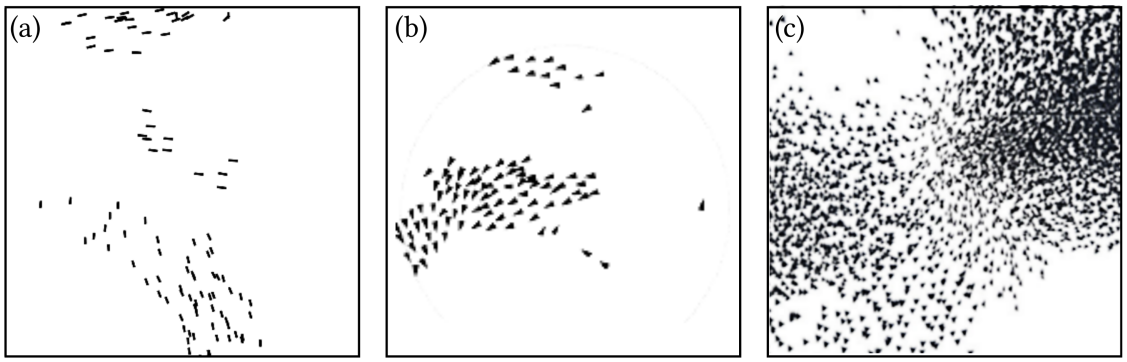


Figure 3.1: **Flocking models of increasing complexity. (a)** Author's simulation of the Vicsek model (Vicsek et al., 1995), where each particle moves randomly wth the same speed and only aligns its velocity with the mean of its neighbours on radius r. **(b)** Simulation of the Reynolds model (Reynolds, 1987), reproduced from (Bajec et al., 2007), where each bird also aligns with its neighbours, but has a different velocity, as well as a tendency to aggregate towards the flock centre of mass and avoid getting too close to neighbours. **(c)** StarDisplay model reproduced from (Hildenbrandt et al., 2010), where alignment and avoidance take into account a fixed number of neighbours. The model also considers flight aerodynamics, a bird's angle of view, and other biological constraints.

The crucial nature of interactions can be seen already from these simple models. While modelling work originally considered each agent to follow all neighbours in a given radius, i.e. *metric neighbours*, experimental work has found that birds tend to follow a fixed number of nearest neighbours, or *topological neighbours* instead (Ballerini et al., 2008). Updating models to use topological neighbours (Bode et al., 2011a; Brown et al., 2021a; Camperi et al., 2012), has created more realistic simulated displays of flocking behaviour which, in turn, have provided new insights on how to quantify the more elaborate emergent behaviours seen in real flocks.

Recent experimental work using virtual reality has been used to confirm these assumptions of how agents interact, as in the case of fish and locusts (Oscar et al., 2023), by showing the animal images of their peers pre-programmed in VR, and observing and decoding their neural activity as they compute an average direction or choose between their neighbours' directions of movement. Agents of increasing complexity may now be simulated in order to observe whether the collective behaviour still persists, but the work most often begins with a simplified model that can still capture the collective behaviour even from over-simplified parts.

Therefore, modelling can act as a useful testing ground for various theories of how the components of the system interact (Gautrais et al., 2012), but also for methods of analysis that can be used on real experimental data to capture the emergent properties resulting from these interactions. This 'bottom-up' approach became crucial to the field of artificial

life in the 1980s, and as discussed in the introduction, has started a long tradition of exchange between the experimental and computational methods of researching collective behaviour (Bajec et al., 2007).

In the rest of this chapter, some simple models where a form of organised collective behaviour emerges from the interactions of the components are introduced. We begin with a random walk model on continuous space, where the system variables are continuous yet univariate. Then, we explore simple flocking models in two-dimensional space evolving in discrete time. In this chapter, for each of these models, their local interactions or microscopic properties are stated, while the methods presented in the previous chapter are discussed in the context of their systemic features.

3.2 Random walks

A random walk is a random process describing a succession of random steps happening with a specified probability distribution as the process evolves in time. The term was introduced by statistician Karl Pearson (Pearson, 1905), and since it has seen applications in a broad range of scientific fields: the model can be used to describe Brownian motion or diffusion, walking trajectories of people ('drunkard's walk') or animals (Codling et al., 2008), or fluctuating stock prices (Fama, 1965).

Random walk models may use various probability distributions for the random step. One frequently used variant samples each step from Gaussian distributions (Fig. 3.2)

A collection of such processes can provide a simple yet insightful model for the study of complex systems, and in particular act as a *null model* to test the robustness and behaviour of measures of emergence under controlled conditions. For simplicity, we will use models in discrete time.

To test the presence of collective behaviour, simple interactions are introduced between the processes, which provide a driving force which can aggregate the random walk processes together. To study the emergence of collective group properties with reduced degrees of freedom, we define a chain of non-independent random walkers, where each walker i is coupled with its neighbours $i-1$ and $i+1$. Here, the conflicting tendencies between order and disorder are given by the interactions between particles on one hand, and the stochasticity within each component on the other.

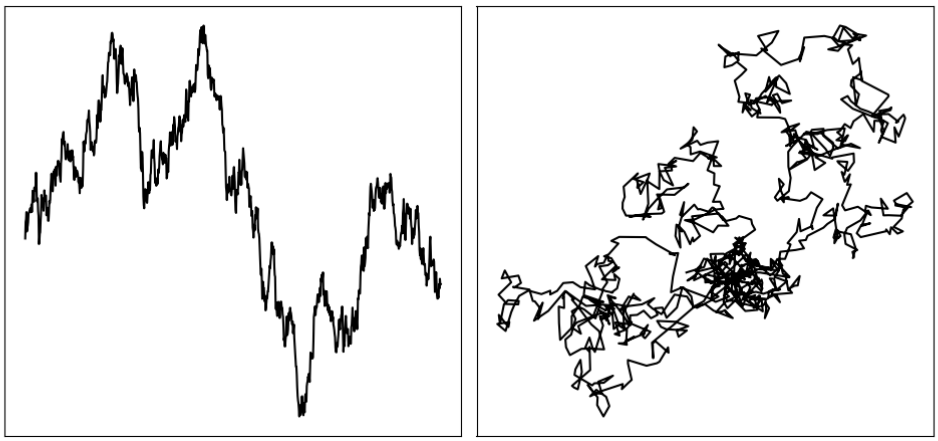


Figure 3.2: **Gaussian random walks in one and two dimensions** simulated for 1000 timesteps. **(left)** Temporal evolution of unidimensional random walk process evolving with Gaussian step $x_t \sim \mathcal{N}(0,1)$. The horizontal axis represents time. **(right)** Trajectories of a random walk process in two dimensions, evolving with step size $\mathbf{x}_t$ follwing a bivariate standard Gaussian. In spite of its simplicity, this process is prevalent in many natural and social phenomena. Random walks will be used as a 'null case' for testing measures of emergence.

3.2.1 Gaussian random walks

Consider a system of random walks where the next step η_t^i is described by Gaussian distribution of mean $\mu = 0$ and variance σ^2, evolving in *discrete* time steps $\delta t = 1$. All η_t^i are identically distributed, but a new value is sampled at each time step for each walker. This system can be described as a set of random variables X_t^i that evolve in *discrete time* via iterative difference equations, such that:

$$x_{t+1}^i = x_t^i + \eta_t^i = x_0^i + \sum_{\tau=1}^{t} \eta_\tau^i \tag{3.1}$$

With $x_0^i = 0$, each x_t^i is a sum of t i.i.d. Gaussian noise variables $\eta_t^i \sim \mathcal{N}(0, \sigma^2)$:

$$x_t^i = \sum_{\tau=1}^{t} \eta_\tau^i \sim \mathcal{N}(0, t\sigma^2) \tag{3.2}$$

To add local interactions between the particles, we introduce coupling with the nearest neighbours, an equilibrium lattice spacing constant a, and spring constant γ to drive attraction and repulsion between a particle and its neighbours. The idea is that the coupling force will drive the particles towards an ordered state where they are all equidistant by a spacing of a. Increasing the amount of coupling between by increasing γ produces more interactive systems and the emergence of collective order as can be seen in Fig. 3.3.

If we take intial conditions as $x_0^i = 0$, then a transient period is required until the walkers reach the spacing imposed by the spacing constant. Alternatively, we can take $x_0^i = i \cdot a$, which gives $x_t^i \sim \mathcal{N}(i \cdot a, t\sigma^2)$.

Then the difference equation by which the process evolves over time becomes:

$$\begin{aligned} x_{t+1}^i &= x_t^i + \gamma\left(x_t^{i+1} - x_t^i - a\right) \\ &\quad - \gamma\left(x_t^i - x_t^{i-1} - a\right) + \eta_t^i \\ &= x_t^i + \gamma\left(x_t^{i-1} + x_t^{i+1} - 2x_t^i\right) + \eta_t^i \end{aligned} \tag{3.3}$$

We setup the system with open boundaries, so for the first (i.e. $i = 1$) and the last (i.e. $i = N$) walkers in the chain we get:

$$x_{t+1}^1 = x_t^1 \ + \gamma(x_t^2 - x_t^1 - a) + \eta_t^1 \tag{3.4}$$

$$x_{t+1}^N = x_t^N - \gamma(x_t^N - x_t^{N-1} - a) + \eta_t^N \tag{3.5}$$

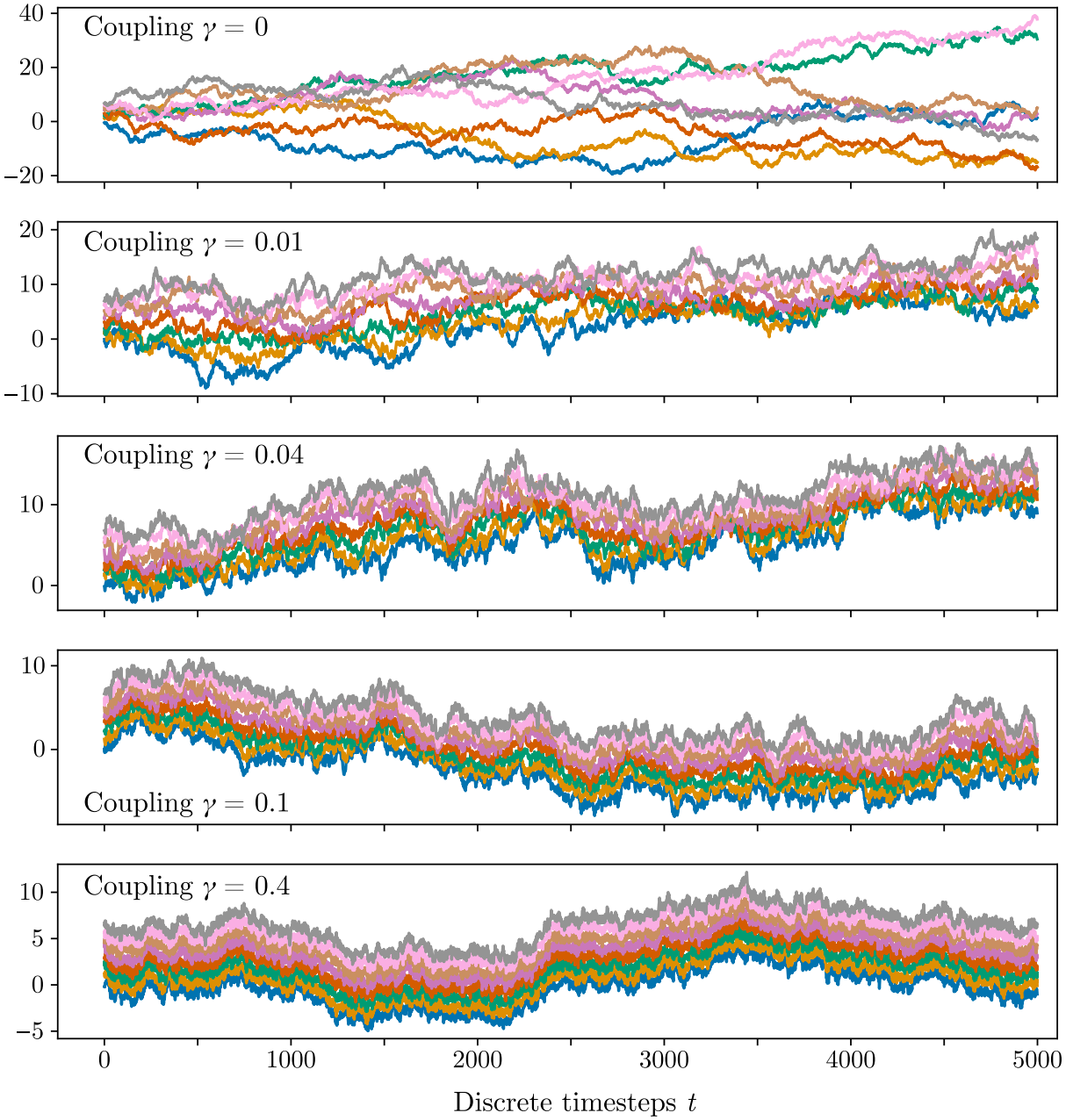


Figure 3.3: **Trajectories of non-stationary Gaussian random walks with increasing coupling** for $t = 5000$ discrete timesteps. Each of the $N = 8$ walkers starts at $x_0^i = i$, and moves with a step $x_t^i \sim \mathcal{N}(0, \sigma^2)$, with $\sigma = 0.5$. The x-axis shows the time evolution while the y-axis shows the position of each particle in the one-dimensional space. For uncoupled systems with $\gamma = 0$, the system is not showing any collective properties. When coupling is added the walkers aggregate around their centre of mass, which behaves as a random walker itself. The system is non-stationary: the particles and the centre of mass diverge from their original positions as time elapses.

To avoid difficulties introduced by the non-zero starting position in the statistical quantities, we can instead study the deviations of the particles from the initial position $x_0^i = i \cdot a$, which will maintain a mean of 0. These maintain the same recursive relation to the previous deviation as the recursive relation defining the actual position, Eq. 3.3.

$$\Delta x_{t+1}^i \equiv x_t^i - i \cdot a = (1-2\gamma)\Delta x_t^i + \gamma(\Delta x_t^{i+1} + \Delta x_t^{i-1}) + \eta_t^i \tag{3.6}$$

An important feature of this random walk process is the lack of stationarity, or the presence of time dependence, since the probability distributions for both the components and their centre of mass depend on t. In other words, the variance of the process depends on the amount of time elapsed. This can be seen in Fig. 3.3, especially for $\gamma = 0$: the position of the walkers diverges much farther than its initial condition with more timesteps. Adding coupling reduces this spread to some degree, but the group of walkers still behaves like a non-stationary random walker.

3.2.2 Ornstein-Uhlenbeck processes

Many statistical methods require an assumption of stationarity, even though, in the field, they may be appplied on data that does not meet this assumption. Quantitative analysis can be affected by making this assumption erroneously, but as long as joint probability distributions are computed correctly, information-based measures can be used to study both stationary and non-stationary processes. As such, we next test the same methods on a version of the Gaussian random walker process with stationary statistics.

To maintain stationarity, each random walker is "pulled back" to its original position by a restorative force, which we parametrise by k. This idea was introduced to model the Brownian motion of a particle in the presence of friction (Uhlenbeck & Ornstein, 1930).

Inspired by Ornstein-Uhlenbeck processes, we add a restorative force parametrised by k to the discrete-time Gaussian random walk defined in Eq. 3.1:

$$x_{t+1}^i = x_t^i - kx_t^i + \eta_t^i = (1-k)x_t^i + \eta_t^i \tag{3.7}$$

The term can also be defined non-recursively:

$$\begin{aligned} x_{t+1}^i =& (1-k)((1-k)x_{t-1}^i + \eta_{t-1}^i) + \eta_t^i \\ =& (1-k)^2((1-k)x_{t-2}^i + \eta_{t-2}^i) + (1-k)\eta_{t-1}^i + \eta_t^i \\ =& (1-k)^3 x_{t-2}^i + (1-k)^2\eta_{t-2}^i + (1-k)\eta_{t-1}^i + \eta_t^i \end{aligned} \tag{3.8}$$

Which would give the random walker's value x^i_{t+1} at time $t+1$ with respect to its intial position x^i_0:

$$x^i_{t+1} = (1-k)^{t+1} x^i_0 + \sum_{\tau=0}^{t} (1-k)^\tau \eta^i_{t-\tau} \tag{3.9}$$

Coupling is added, as before, with the two nearest neighbours using the spring constant γ, and initial positions are taken as $x^i_0 = i \cdot a$ for some spacing constant a. The central walkers would then follow:

$$\begin{aligned} x^i_{t+1} &= x^i_t - k x^i_t + \gamma(x^{i+1}_t + x^{i-1}_t - 2x^i_t) + \eta^i_t \\ &= (1-k-2\gamma)x^i_t - \gamma(x^{i+1}_t + x^{i-1}_t) + \eta^i_t \end{aligned} \tag{3.10}$$

while the equations of motion for the processes at the boundaries are:

$$x^1_{t+1} = (1-k-\gamma)x^1_t \ - \gamma x^2_t + \eta^1_t \tag{3.11}$$

$$x^N_{t+1} = (1-k-\gamma)x^N_t - \gamma x^{N-1}_t + \eta^{N-1}_t \tag{3.12}$$

As before, we can study the deviations of the particles from the initial position $x^i_0 = i \cdot a$, which maintain a mean of 0.

$$\Delta x^i_{t+1} \equiv x^i_t - ia = (1-k-2\gamma)\Delta x^i_t + \gamma(\Delta x^{i+1}_t + \Delta x^{i-1}_t) + \eta^i_t \tag{3.13}$$

This model is an example of 'diffusion with return to average', and it is also known as 'mean-preserving', since the particle tends to return to the expected value of its position (Jensen, 2022). The model uses discrete time steps and as such is a simplified version of the continuous time version. The analytical derivation of the model's equations can be seen in (Liardi et al., 2025).

Phenomenologically, we can observe the time dependence is reduced by the restorative force, which can also be seen in Fig. 3.4.

We have seen how increasing the coupling parameter creates more order in both types of random walkers, albeit the kind of order that emerges is phenomenologically different. It remains to formally define what may constitute ordered collective behaviour in the case of random walkers, but first, we introduce a simple model of collective behaviour in two dimensions.

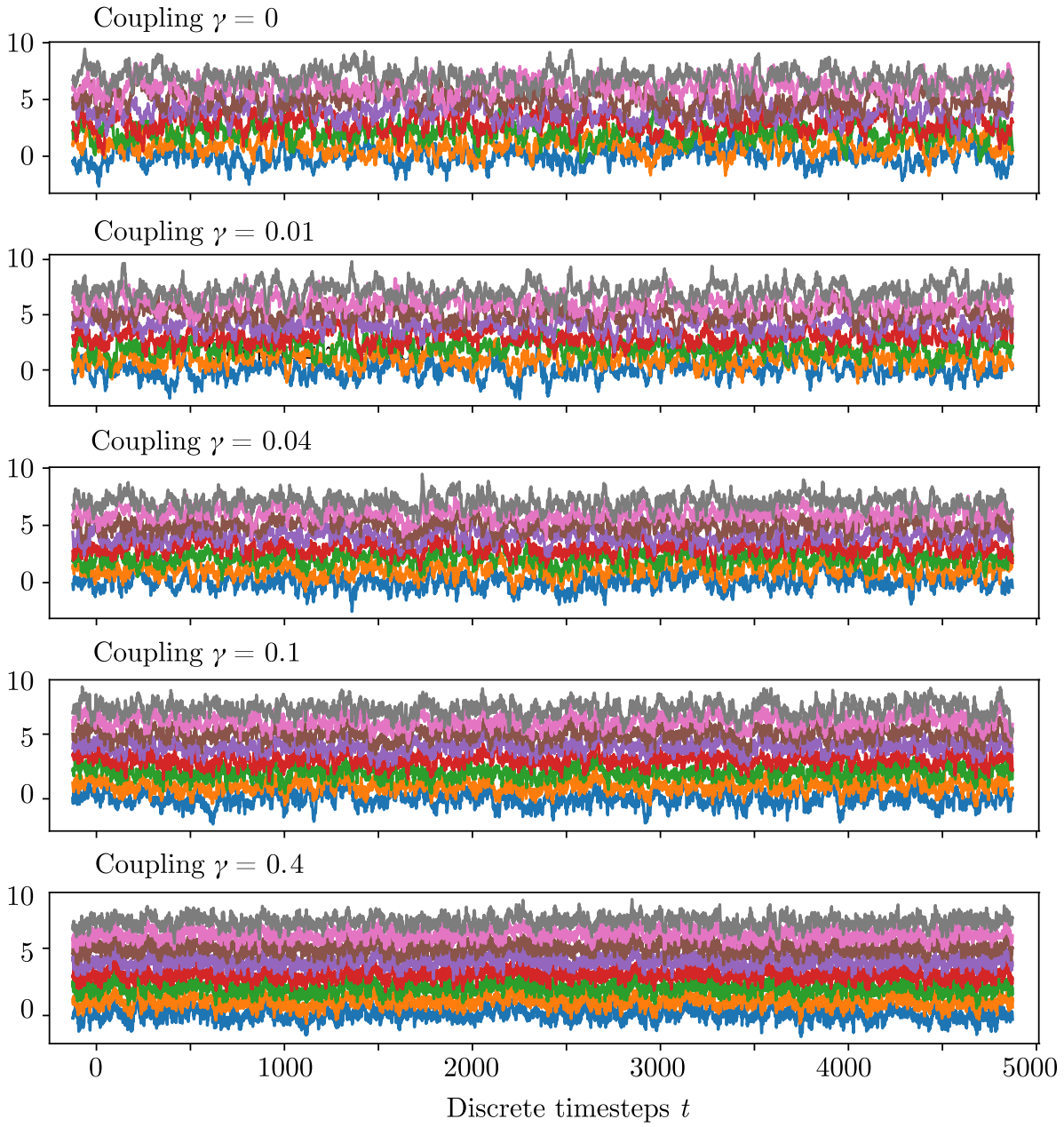


Figure 3.4: **Stationary Gaussian Ornstein-Uhlenbeck walkers with increasing coupling** for $t = 5000$ timesteps. Each walker starts at $x_0^i = i$ and moves with step $x_t^i \sim \mathcal{N}(0, \sigma^2)$ with $\sigma = 0.5$ and increasing coupling γ. The x-axis shows the time evolution while the y-axis shows the 1D position of each particle. The restorative force $k = 0.05$, although weak, is enough to keep the walkers varying around the mean. Unlike the non-stationary case, the positions of the walkers do not diverge over time. The effect of coupling seems less strong as it compounds with the restorative force.

3.3 Self-propelled particles

Moving on from one to two dimensions, we open up more ways in which the system can manifest collective behaviour. Unlike random wakers, which could only synchronise in terms of the sign of their displacement (moving to a higher or a lower value), a swarming system in two-dimensional space can manifest a much broader spectrum of collective motion that we can observe phenomenologically: picturing, for example, all the many interesting ways in which a crowd of human beings can move or walk around.

The simplest model of swarming in two dimensions was introduced by (Vicsek et al., 1995). The Vicsek model is a minimal and universal model that consists in dimensionless particles which are self-propelled, namely they move with a constant speed v without any considerations on the energy they spend. At each timestep, each particle aligns its velocity $\mathbf{v}_i$ with the mean velocity of its neighbours within a radius r. The addition of some degree of noise to the resulting angle of direction adds some stochasticity to the system, which drives the system towards disorder.

Interestingly, researchers observed a *phase transition* in this system: the self-propelled particles in the Vicsek model can manifest a 'gas-like' phase which is most disordered, and characterised by all particles headed in different directions and moving independently; at the other end of the spectrum, the 'solid' phase is characterised by the highest degree of order where all the particles are aligned and move together, fixed with respect to each other; but in between, a 'liquid' or 'fluid' phase shows that particles move collectively without being fixed with respect to each other, creating phenomenologically complex dynamics and metastable states.

This transition appears either when increasing the density of particles, or when decreasing the noise. It should be noted that in spite of the model's simplicity, the nature of this transition has been disputed and may appear to be dependent on implementation (Aldana et al., 2009). Even a fourth 'banding' phase has also been discovered in simulations with a very large number of components (Toner & Tu, 1998). There is much more to the Vicsek model than presented in this thesis. A thorough exploration of the statistical physics of the Vicsek model is provided in (Ginelli, 2016).

Thanks to this versatility and complexity, the Vicsek model and its variations have been central to many studies of collective motion in the natural world, and has been modified in different ways to express other forms of collective behaviour, for example by changing the nature of interactions between particles (Chaté et al., 2008; Czirók & Vicsek, 2000; Ginelli & Chaté, 2010) or even the topology of the space (Armbruster et al., 2017). From statistical physics to hydrodynamics to flocking, the Vicsek model is testament to the usefulness of simple models in the study of complex systems.

Albeit proposed as a model of a *physical system*, the model has been used widely also as an *agent-based model*. Besides its fascinating behaviour in the thermodynamic limit and at very high densities, many interesting kinds of collective behaviour appear in the Vicsek model when observed in different ways: at small densities, with a small number of particles, on singular realisations, and even focusing on a certain time window to observe dynamical behaviour, especially in the 'liquid' phase, where the system may behave qualitatively similar to collective motion in nature. This is why variants of the Vicsek model with tweaks in the interaction rules have been used to simulate small groups of animals, for example fish (Múgica et al., 2022; Niizato et al., 2024).

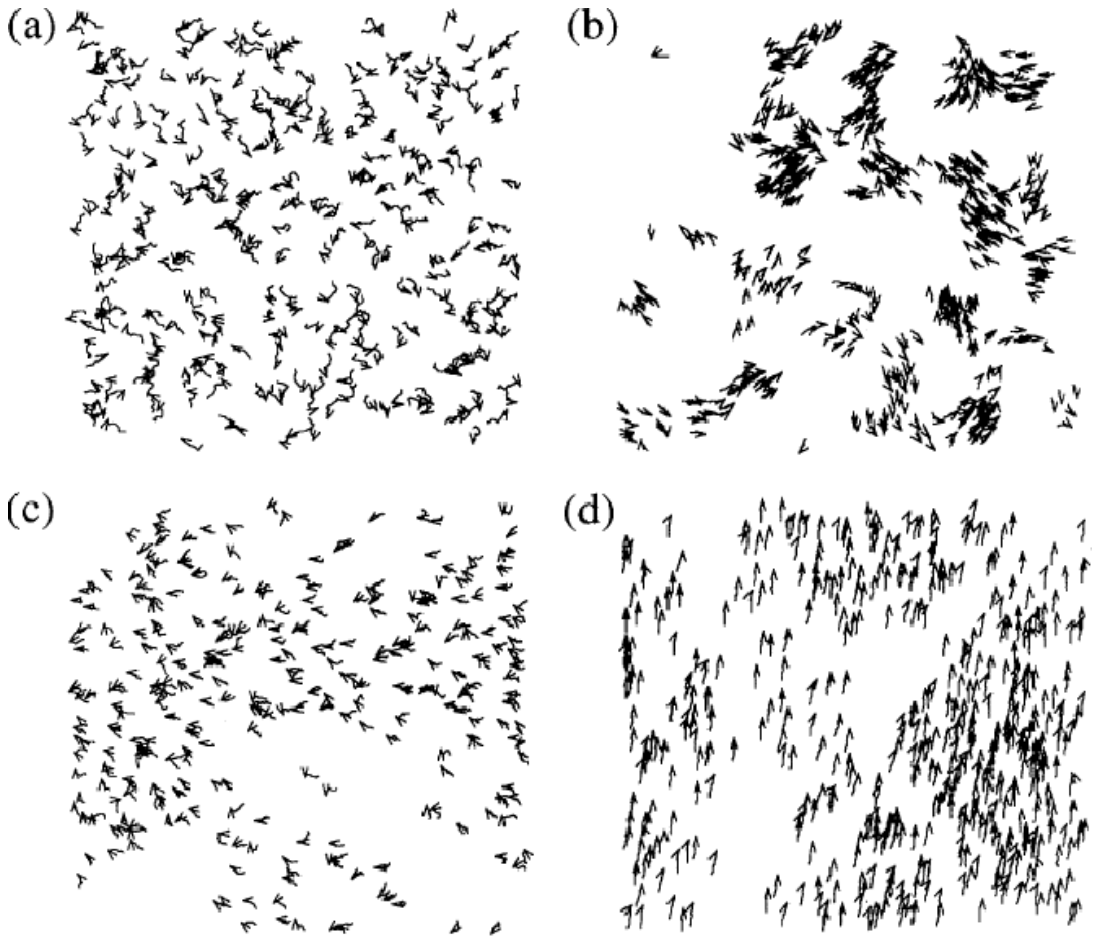


Figure 3.5: **Snapshots of the Vicsek model in different states of order or disorder**. The particles align with their surrounding neighbours until everyone moves in the same direction. Phenomenologically, trajectories produced by the model remind of animal movements: **(a)** the chaotic state is similar to the swarming of insects; **(b)** an intermediate state, where particles gather in spinning clusters, is reminiscent of birds in flight; **(c)** and **(d)** aligned states, similar to the swimming motion of bacteria. Reproduced from (Vicsek et al., 1995).

3.3.1 Standard Vicsek Model

In its original version, the system consists of N particles located at positions $\mathbf{x}_i$ with $i \in \{1, 2, ...N\}$ that move with fixed absolute velocity v in direction specified by angle θ_i in a $L \times L$ space with periodic boundaries. The time increment is set to $\Delta t = 1$. At each time step, each particle aligns its direction with its neighbours with a degree of noise.

The new positions are computed by (Vicsek et al., 1995):

$$\mathbf{x}^i_{t+1} = \mathbf{x}^i_t + \mathbf{v}^i_t \Delta t \tag{3.14}$$

where the updated velocities have direction given by:

$$\mathbf{v}^i_t = v(\cos\theta^i_t, \sin\theta^i_t) \tag{3.15}$$

$$\theta^i_{t+1} = \langle\theta_t\rangle_r + \Delta\theta^i_t \tag{3.16}$$

$$\Delta\theta^i_t \sim [-\eta/2, \eta/2] \tag{3.17}$$

where the noise term $\Delta\theta^i_t$ is sampled from a uniform distribution parametrised by noise parameter η, and $\langle\theta\rangle_r$ denotes the circular mean of the orientations of neighbouring particles within radius r. The neighbourhood is defined as:

$$\mathcal{N}^i_r(t) = \{\mathbf{x}^j_t \mid \|\mathbf{x}^i_t, \mathbf{x}^j_t\|_2 \leq r\} \tag{3.18}$$

where $\|\cdot,\cdot\|_2$ is the Euclidean distance between two points.

To make it easier to define different variants of the model later on, we rewrite Eq. 3.16 using the circular mean to compute the average angle over the neighbourhood:

$$\theta^i_{t+1} = \text{atan2}\left(\sum_{j\in\mathcal{N}^i_{r=1}(t)} \sin(\theta^j_t), \sum_{j\in\mathcal{N}^i_{r=1}(t)} \cos(\theta^j_t)\right) + \Delta\theta^i_t \tag{3.19}$$

where $\text{atan2}(y, x) = \text{Im}\log(x + iy)$ is a variant of arctan in the interval $[-\pi; \pi]$. It should be noted that for high enough density or large enough radius, the central limit theorem suggests that the average angle over the neighbourhood is Gaussian distributed.

Even though the model is extremely interesting when studied with statistical physics methods, this thesis aims to use it in a largely different way: by studying small flocks, that are not very dense, and observing if simple collective motion will emerge and whether it can be quantified or differentiated with analytical methods making use of the particle trajectories. Next we introduce variants of the model which have an effect on the phenomenology of the emergent collective motion and its dynamics in small groups.

Forward vs backward difference

A first variation to the minimal Vicsek model is due to the numerics of the computational implementation (Chaté et al., 2008; Huepe & Aldana, 2008). In the original algorithm, referred to as the 'backward difference' model, the new position at time $t+1$ is updated using the angle at time t (Czirók & Vicsek, 2000; Vicsek et al., 1995). Alternatively, in the 'forward difference' model, the angle at $t+1$ is used. The latter is used more frequently in literature, likely due to implementation simplicity.

Using the 'forward difference' minimal model, Eq. 3.15 becomes:

$$\mathbf{x}_{t+1}^{i} = \mathbf{x}_{t}^{i} + \mathbf{v}_{t+1}^{i}\Delta t \tag{3.20}$$

This has been observed to produce slightly less condensed clusters than the original (Huepe & Aldana, 2008), but this happens in systems with a large number of particles and should not affect the systems studied in this thesis.

Intrinsic vs extrinsic noise

It has been shown that the Vicsek model displays different behaviour depending on what type of noise is being used. In the literature, these have been referred to as intrinsic or scalar noise, and extrinsic or vectorial noise respectively. In the original model, the intrinsic noise is added to the average angle, but this may have an unwanted effect on system behaviour when a larger amount of noise $\Delta\theta$ is added to a small average velocity (as in the case of unordered systems) (Aldana et al., 2007). In contrast, extrinsic noise is used to perturb individual particles before averaging.

It has been shown that intrinsic noise changes the nature of the phase transition (Aldana et al., 2009; Pimentel et al., 2008). Some of the particular behaviours of the extrinsic noise implementation are explored in (Huepe & Aldana, 2008), whilst the behaviour of the two types of noise in the thermodynamic limit is also thoroughly discussed in (Ginelli, 2016).

In the current work, an implementation with **intrinsic noise** and **forward difference** is chosen due to its simplicity. As such, every time the 'Vicsek model' is mentioned without any specifics, it should be assumed to mean the Vicsek model implementation with intrinsic noise and forward difference.

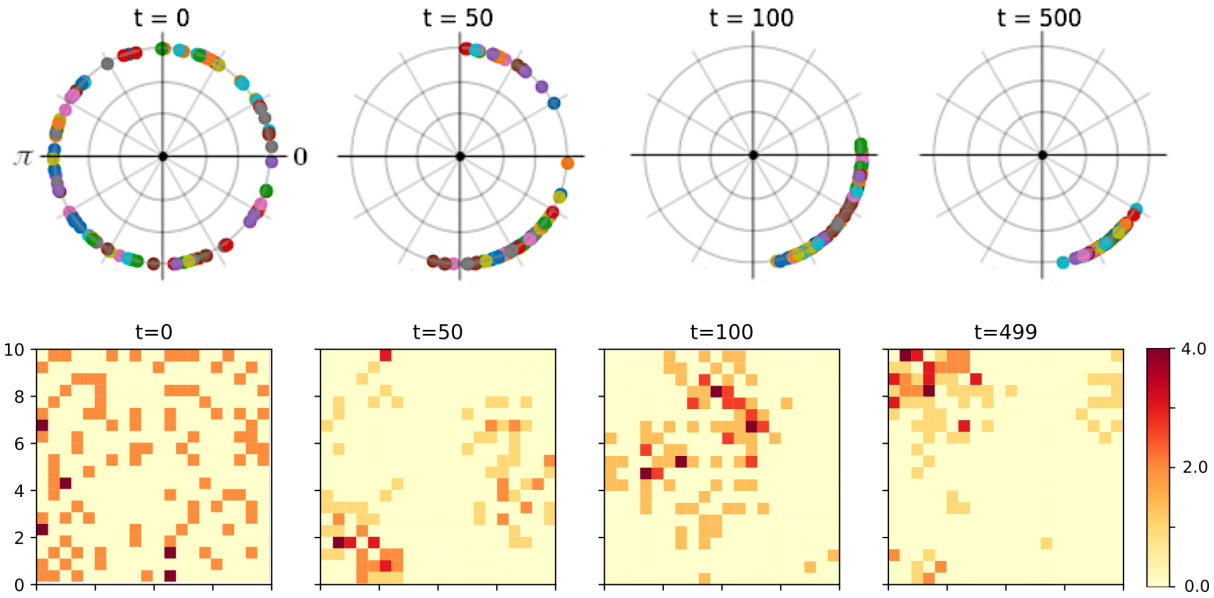


Figure 3.6: **Collective motion in the standard Vicsek model** with periodic boundaries and metric neigbourhoods, with $N = 100$ particles, density $\rho = 1$, velocity $v = 0.1$, metric radius $r = 1$ and noise $\eta = 0.4$. Histograms show particles' angles of direction **(top)** and position **(bottom)**. As the system is not very large and not very dense, after 500 timeseps, the particles have aggregated towards a unified direction. Interestingly, while there are no driving attraction forces to create spatial cohesion, the particles do aggregate in small, higher-density groups.

3.3.2 Periodic vs reflective boundaries

The original Vicsek model is defined with periodic boundaries: when a particle touches a wall, it emerges on the other side. Therefore, particles never encounter any obstacles, while the actual spatial nature of the system can be abstracted away. Periodic boundary conditions create an effectively limitless space in the shape of a doughnut for the particles to move on, changing the way the probability distributions are to be estimated for the particles' positions; a particle in position $(0, 0)$ is very close to a particle in positions $(0, L)$, $(L, 0)$ and (L, L), which is not accounted for by the usual probability distributions. This is a case where circular statistics become relevant and need to be taken into account.

Alternatively, the space could be delimited by boundaries which turn a particle around rather than moving it to the opposite side. Exploring bounded domains allows the advantage of capturing behaviour more characteristic of real-world collective motion, which happens in a finite and sometimes bounded space – for example, fish swimming in a tank, or insects buzzing around a flower. Mixed boundaries are not addressed here but have been discussed in (Armbruster et al., 2017).

This implementation is particularly appealing as it can also be generalised to any shape of boundaries by finding an efficient way to compute the corresponding normal vectors.

To reflect particles around the boundaries, the update rule is modified following (Arm-

bruster et al., 2017). We use the velocity vectors $\mathbf{v}_t^i$ computed with the angle in Eq. 3.16, and the normal vectors to the current boundary $\mathbf{n}_t^i$:

$$\mathbf{v'}_t^i = \mathbf{v}_t^i - 2(v * \mathbf{n}_t^i)\mathbf{n}_t^i \tag{3.21}$$

We must acknowledge that different implementations of this may have different effects on the collective behaviour, and hope to mitigate this in future work. Moreover, the reflective boundaries, while simple to implement, may be too rigid to describe realistic behaviour, and may be replaced with more complex steering for obstacle avoidance as in the Reynolds flocking model (Reynolds, 1987).

It is important to note that the reflective boundaries act as a driving force of cohesion bringing the flock together spatially, but may also act as a driving force of disorder by causing some particles to break alignment with their neighbours when they reflect over walls. Placing boundaries effectively constrains the particles inside a finite space. The shape of the space also has an effect on the dynamics of the system as well, for example by sometimes causing clustering in the corners when the density is high enough, which has prompted researches to simulate the model in disc-shaped spaces with reflective boundaries (Armbruster et al., 2017).

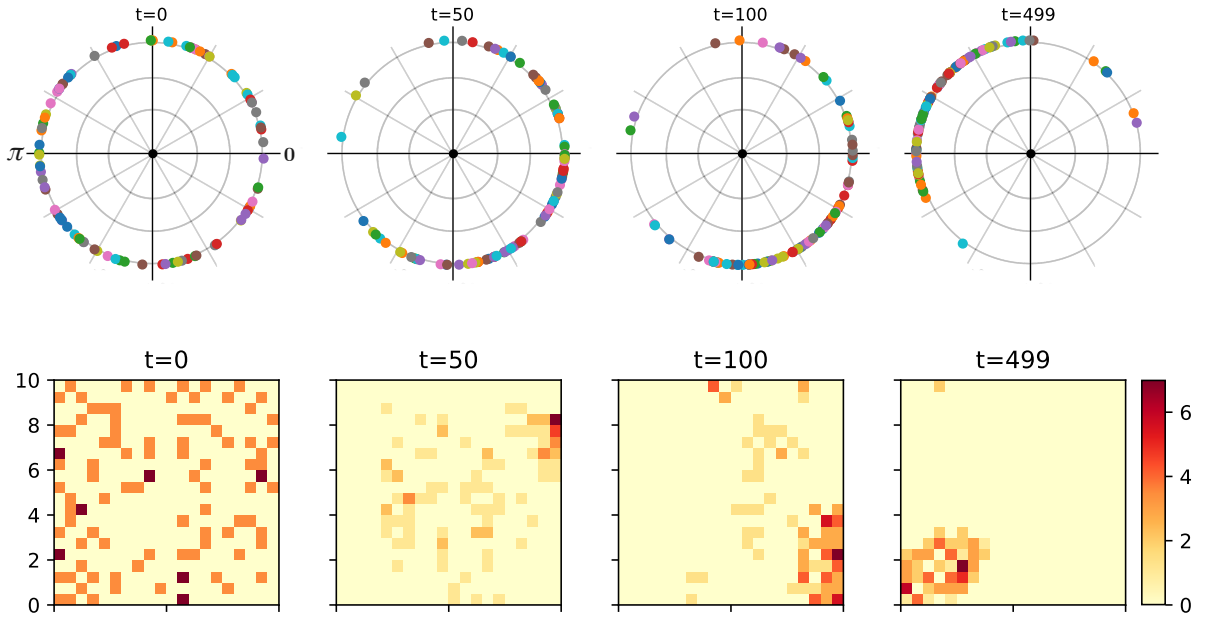


Figure 3.7: **Collective motion in the Vicsek model with reflective boundaries** and metric neigbourhoods ($N = 100$, $\rho = 1$, $v = 0.1$, $r = 1$, $\eta = 1.5$). Histograms show particles' angles of direction **(top)** and position **(bottom)**. The system evolves in a qualitatively different way from the one with periodic boundaries. The reflective boundaries introduce more disorder in the particles' tendency to align, so there is no collective alignment yet after 500 timesteps. On the other hand, the particles aggregate into more cohesive groups, especially in the corners.

3.3.3 Metric vs topological neighbourhoods

More recently when experimentally studying swarms, researchers have observed that interactions seem to occur between an individual and a fixed number of its closest neighbours, as opposed to a variable number of neighbours within a given radius (Ballerini et al., 2008). This has been further verified experimentally with VR and brain imaging studies in fish and locusts (Oscar et al., 2023).

It makes sense then to study variants of the Vicsek model with topological neighbourhoods, in which each particle aligns with the average of n closest neighbours (Ginelli & Chaté, 2010). A more complex topological model of animal behaviour can be seen in (Couzin et al., 2002) and (Bode et al., 2011a), where aggregation, avoidance, and even an angle of view are also included in the model. Combination models using topological interactions but with a metric cutoff have been successful in modelling fish in unclear waters (Grégoire et al., 2003), but such models are beyond the scope of the current work.

The important difference is that in metric interactions the number of nearest neighbours changes depending on the particles' spatial coherence. It has been argued that the change in interactions even changes the order of the phase transition (Ginelli & Chaté, 2010).

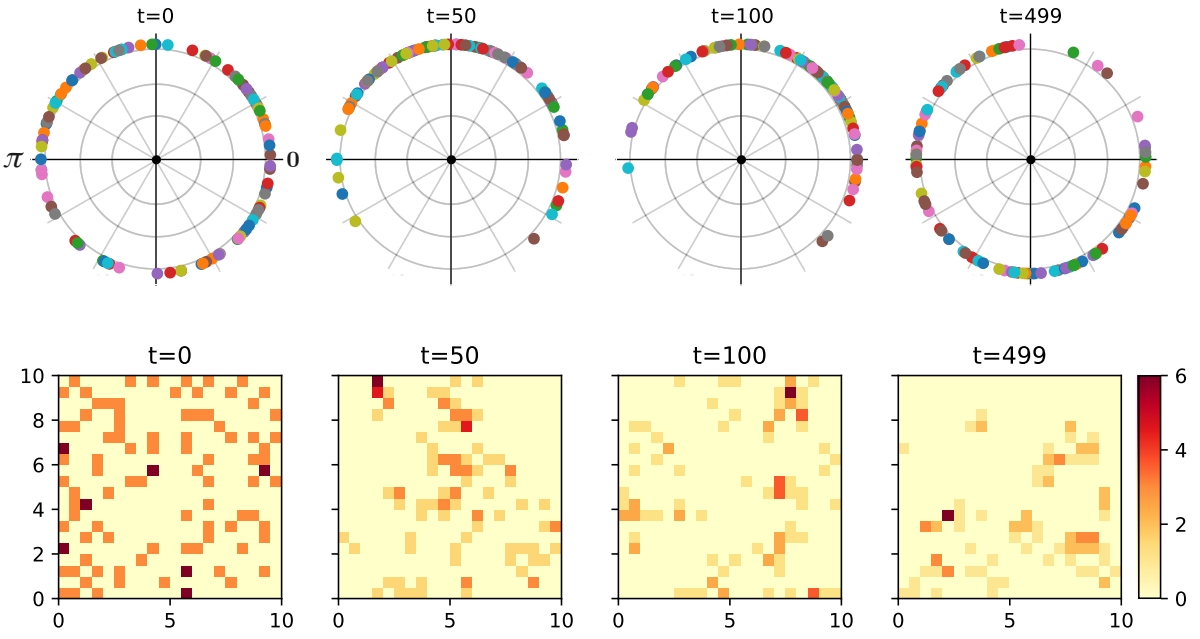


Figure 3.8: **Collective motion in the Vicsek model with topological neigbourhoods and periodic boundaries** ($N = 100$, $\rho = 1$, $v = 0.1$, $\eta = 1.5$). Each particle aligns with its nearest 3 neighbours. Histograms show particles' angles of direction **(top)** and position **(bottom)**. The system evolves in a qualitatively different way from the one with metric neighbourhoods. There is a stronger tendency to aggregate in small dense groups. The number of neighbours to align with is small so alignment does not emerge after 500 timesteps.

An analysis using information theory tools such as mutual information and transfer entropy (Brown et al., 2021a) has shown that the metric and topological versions of Vicsek also manifest diferent fine-grained information sharing patterns. To investigate these differences, we also define a new type of neighbourhood, the topological neighbourhood $\mathcal{N}_r^i$, parametrised by neighbourhood size r.

We can already see from the three case studies of three different variants of the model presented above that the system manifests qualitatively different patterns of dynamical behaviour, even in small groups of $N = 100$ particles. While the original research only quantified the collective alignment using a statistical average of the particle direction vector over all components, many types of collective behaviour, and in particular motion, can be studied in this model: the emergence of the same direction of movement, the formation of one or multiple cohesive groups, which could be aligned or not, the synchrony of sudden direction changes, and many more. In the next section, relevant statistical quantities will be introduced in an attempt to describe collective behaviour, including but not limited to alignment.

3.4 Collective behaviour in particle systems

So far in this chapter, we have defined two physical models or particle system models to study our emergence measures: the random walks and the Vicsek model. Having introduced them and observed some histograms of their evolution, it is time to more systematically define what constitutes collective behaviour in these systems.

In a one-dimensional system, the possibilities for collective behaviour are limited to the time series synchronously increasing or decreasing. But in a two-dimensional system, we may interpret some kinds of collective behaviour as collective motion, which has been quantified and studied in a variety of different ways.

3.4.1 Criticality and phase transitions

As we hinted at in the introduction, models like the ones introduced in this chapter are crucial to understanding the relationship between the mechanisms of local interactions between agents in a complex system, and the emergent behaviours that appear at the systemic level. By quantifying these emergent behaviours in the models with, say, statistical methods, we can use them as a test-bed which will help us interpret these methods in the real world.

For over a century, the field of statistical physics has been developing methods to describe the emergence of macroscopic properties in physical systems in the form of phase transitions. **Order parameters** are statistical quantities that can describe the amount of order and disorder for various conditions created by tweaking a *control parameter*, thus delimiting different *phases* characterised by different kinds of collective behaviour.

There are, of course, many kinds of emergent collective behaviour possible in physical systems, even the simplest ones we have employed in this chapter. As Vicsek *et al* found out, the **phase transition** from disordered to ordered collective behaviour in a self-propelled particle system with alignment is similar to that seen in arrays of ferromagnets (Vicsek et al., 1995).

Vicsek order parameter

Introduced in (Vicsek et al., 1995), it captures the alignment of particles by computing the size of the normalised, average direction vector of all particles. In the ordered state, the velocity of *any* single particle can also largely describe the velocity of the group. This is also referred to as *symmetry-breaking*: from a disordered phase, in which the sum of all velocities $v_a \to 0$, to an ordered phase in which all particles move in the same direction and $v_a \to 1$.

Its definition for one realisation of N particles and t timesteps is given by:

$$v_a = \frac{1}{T}\sum_{t=1}^{T}\frac{1}{Nv}\left\|\sum_{i=1}^{N}\mathbf{v}_t^i\right\|_2^2 \tag{3.22}$$

where $||\cdot||_2^2$ is the Euclidean length or L2-norm of a vector.

Taking the *ensemble average* $\langle v_a\rangle$ over a large set of realisations of the system should reveal how, as the noise is decreased or the density is increased, $v_a \to 1$ as particles align direction, transitioning from a disordered phase to an ordered one. Taking the *ensemble variance* $\langle v_a\rangle^2$ functions as a measure of *susceptibility*. It has been shown that susceptibility of the Vicsek order parameter peaks as a function of noise η at the phase transition (Baglietto & Albano, 2008). In turn, susceptibility has been related to the entropy and mutual information (Brown et al., 2018).

At this transition, we see the emergence of *critical behaviour* characterised by *long-range* or *power-law distributed correlations* (Baglietto & Albano, 2008; Baglietto et al., 2012), which are also believed to maximise information transfer (Crosato et al., 2018; Ginelli, 2016). Moreover some non-linear properties and interesting unexpected behaviours appear in this critical regime between the ordered and chaotic state such as a tendency to aggregate spatially that is not directly evident from the interaction rules of alignment (Grégoire & Chaté, 2004; Huepe & Aldana, 2008).

This critical behaviour has also been found in real world systems (Grigera, 2021), for example in starling flocks (Cavagna et al., 2010), schools of fish (Múgica et al., 2022) and audiences to sports (Farkas & Vicsek, 2006) and concerts (Silverberg et al., 2013), while the Vicsek model or other simple particle systems were used as a base for the analysis. This method allowed us to disentangle the local mechanisms producing the collective behaviour: indeed, the neighbour interactions we encode in our theoretical models seem to be similar to those producing the emergent group behaviour in the real world.

In theory, order paramers must be computed over all possible configurations on systems composed of an infinite number of particles – referred to as the *thermodynamic limit*. These methods were first developed analytically, but with computer simulations, order parameters are now also estimated from generated data. The robustness of estimation is affected by data availability: simulated systems must be large enough to capture the emergent phenomenon, and sufficient realisations of the simulation must be run to ensure many possible configurations are included. *Finite-size scaling* analysis can be performed to quantify the effect of these limitations on the study of order parameters. A huge body of work exists on the topic; a review of collective motion research using methods from statistical physics and related to the Vicsek model is in (Vicsek & Zafeiris, 2012).

Limitations of correlation lengths and order parameters

Thanks to methods from statistical physics, a rich set of underlying universal dynamics of swarm behaviour is now known. However, in spite of claims of universality, these methods do not satisfy the conditions for a substrate independent measure of emergence that is generally applicable in both simulation and experimental studies.

First of all, phase transition analysis requires working at the *thermodynamic limit* which requires a very large number of simulations and very large system sizes, making it unsuitable to studying collective behaviour in some real-world scenarios. The study of correlations, while it may be done instantaneously on a single realisation of the system (Palmieri & Jensen, 2020), it still requires the system to be very large to be robust. For example, the study of starlings showing scale-free correlations used the measured positions of more than a thousand birds (Cavagna et al., 2010). But we may want to study emergent complex behaviour which arises in much smaller systems.

We have introduced the v_a order parameter to detect alignment, but this does not describe other kinds of collective behaviour. Other order parameters exist that quantify spatial aggregation, for example (Huepe & Aldana, 2008). In general, methods from statistical physics require *prior knowledge* of the nature of the emergent behaviour in order to choose one of the many possible order parameters.

Finally, order parameter methods focus on the phase transition itself, assuming that some phases are emergent while others are not. The relevant phases are deemed to be stable, insofar that the order parameters require the system to remain either in the disordered or the ordered state. But as we frequently see with the naked eye in nature, and as we have seen in the case studies presented in the previous chapter, many interesting complex collective behaviours manifest locally and dynamically in the intermediary, possibly critical, regime between order and disorder, when susceptibility peaks, or in the 'fluid' phase or the metastable states, so we require a more localised measure.

3.4.2 Instantaneous statistical observables

Interestingly, both when applied to small datasets, or on the movement vectors of the particles over a single time step, the Vicsek order parameter can also capture some degree of instantaneous aligment. While not as robust as when averaged across many realisations and in large systems, using the statistical quantity in this way provides a first attempt at characterising datasets that can be both simulated or experimental.

While this does not address the issue of prior knowledge of the nature of the collective behaviour, instantaneous quantities based on order parameters are simple to compute in small systems as well as interpretable, and as such will be very useful to investigate known

properties and relate our novel measures to established analysis methods. Moreover, by producing time series that describe the system as a whole, we can even use these quantities to study *dynamics*.

Some relevant statistical quantities, which can be computed both instantaneously, averaged over time, or averaged over one or multiple realisations of a simulated particle system, are introduced in the remainder of this chapter, and exemplified using the case studies in Figs. 3.6 and 3.7. Same as (Huepe & Aldana, 2008), we will refer to these kinds of instantaneous statistical quantities that distinguish different types of collective behaviour as **observables**.

Alignment may be quantified using the **instantaneous Vicsek order parameter**, i.e. the magnitude of the sum vector, for a configuration at a specific time point t:

$$v_a(t) = \frac{1}{Nv} \left\| \sum_{i=1}^{N} \mathbf{v}_t^i \right\|_2^2 \tag{3.23}$$

As hinted previously, while relevant to an ensemble analysis, the Vicsek order parameter is also meaningful when used instantaneously. This is demonstrated on the Vicsek case studies shown in the previous chapter. The instantaneous observable based on the Vicsek order parameter of alignment has been computed at each timestep, showing the dynamical evolution of the system.

In the periodic boundaries case, the system evolves to the ordered state within less than 200 timesteps (Fig. 3.10a). In the reflective boundaries case the system is in an intermittent state, in which one or more aligned group forms quickly and breaks up as quickly into multiple groups (Fig. 3.10b). If the order parameter were to be averaged accross many timesteps, it would not be able to detect the collective behaviour in the second case. Reasonably, this is a different kind of *metastable* collective behaviour, characterised by a balance between order and disorder, while the periodic boundaries case produces perfectly ordered alignment.

Spread of direction can be defined as the variance of the heading angles:

$$\sigma_\theta^2(t) = \frac{1}{N} \sum_{i=1}^{N} (\theta_t^i - \bar{\theta}_t)^2 \tag{3.24}$$

This quantity is inversely related to the Vicsek order parameter, insofar as $\sigma_\theta^2(t) \to 0$ in the ordered state, and maximised in the disordered state.

$\sigma_\theta^2(t) \to 0$ as the system stabilises in the ordered, aligned state in the periodic boundaries

case (Fig. 3.10c) while in the reflective boundaries case (Fig. 3.10d), where the system does not reach an aligned state, it peaks at certain timepoints. From inspecting the simulation's behaviour visually, the two peaks around 150 and 450 occur when a large group of particles approaches a wall, and their directions suddenly change as they reflect onto the obstacle, thus triggering further sudden changes in direction in their neigbours.

Dispersion from centre of mass computed as the average distance of particles from the system's centre of mass, can be used to capture the degree of spatial aggregation or cohesion in the system:

$$\delta_{\bar{\mathbf{x}}}(t) = \frac{1}{N} \sum_{i=1}^{N} \|\mathbf{x}_t^i - \bar{\mathbf{x}}_t\|_2^2 \tag{3.25}$$

where $\bar{\mathbf{x}}_t$ is the position of the centre of mass of the flock at time t, and the quantity increasing suggests the particles' aggregation decreasing.

In the ordered case when the system settled into an aligned configuration after 200 timesteps, the dispersion parameter also stabilises (Fig. 3.10e). We recall that in the ordered state, particles act as if 'fixed' with respect to each other, which is what the more stable value of the parameter suggests. In the system with reflective boundaries, this quantity does not stabilise, as expected from its dynamics: there is no consistent mean distance to the centre of mass as there is no consistent solid group, even though the clusters may be dense themselves (Fig. 3.10f).

For more robustness in the study of systems with multiple clusters of collective behaviour, this observable can be computed over neighbourhoods, as in (Armbruster et al., 2017), or over clusters, as in (Huepe & Aldana, 2008). Alternatively, the average distance to nearest neighbour can give a more robust measure of aggregation.

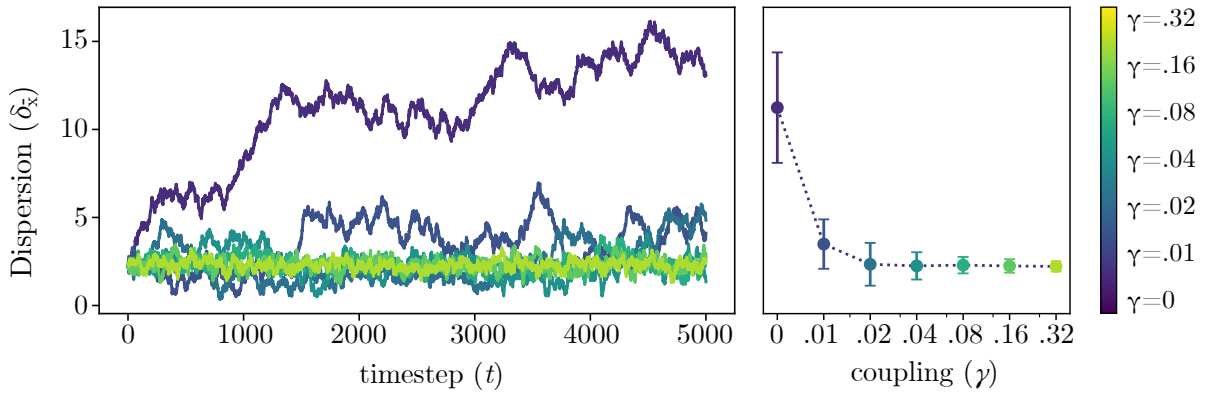


Figure 3.9: **Instantaneous and averaged dispersion from centre of mass in Gaussian random walks with increasing coupling with their neighbours**, for simulations with $N = 8$, step size $\eta_t^i \sim \mathcal{N}(0, \sigma^2)$ with $\sigma = 0.5$ and increasing coupling γ (see Eq. 3.3). As expected the dispersion decreases with increasing interactions. Averaging was done over t for all data points and error bars represent standard deviation over time.

As seen in Fig. 3.9, the dispersion from centre of mass $\delta_{\bar{x}}(t)$ is also useful in our studies of random walks in one dimension.

Mean distance to nearest neighbour can be computed directly on the data without any prior assumptions or analysis regarding how the particles are clustered or how they interact:

$$\tilde{\delta}(t) = \frac{1}{N}\sum_{i=1}^{N} \underset{\substack{j\in\{1\ldots N\}\\ j\neq i}}{\arg\min} \|\mathbf{x}_t^j - \mathbf{x}_t^i\|_2^2 \tag{3.26}$$

It has been shown that this observable originating in experimental work on fish schools (Huth & Wissel, 1994) can also be used as an order parameter (Huepe & Aldana, 2008). Huepe and Aldana also found a scaling relationship between $\tilde{\delta}$ and the average number of interaction neighbours $\tilde{\rho}$, introduced below.

This quantity, unlike the dispersion, is much more robust to quantify density even in a simulation where multiple groups have emerged. In the periodic boundaries case the particles don't really have a tendency to aggregate spatially, as such the nearest neighbour distance fluctuates around 1, which is as expected for a density of $\rho = 1$ (Fig. 3.10g). In the reflective boundaries case, which is characterised by heavy clustering, there is a consistently small mean distance to nearest neighbour (Fig. 3.10h).

Mean number of (interaction) neighbours is the average number of neighbours with which each agent interacts at a given moment in time, including itself, as well as a local measure of density for the particles. Using our notation $\mathcal{N}^i(t)$ to denote the neighbourhood of i at time t, this becomes:

$$\tilde{\rho}(t) = \frac{1}{N}\sum_{i=1}^{N} |\mathcal{N}^i(t)| \tag{3.27}$$

where $|\cdot|$ is the number of elements of a set.

This quantity is computable in systems with metric interactions and should tend to the number of interaction neighbours in a model with topological interactions.

The main downside, as the authors also emphasise in (Huepe & Aldana, 2008), is that this measure is dependent on the nature of interactions between agents, which are known in models but remain mysterious in time series extracted from complex systems in nature. Nevertheless, we may still use $\tilde{\rho}(t)$ as a general estimator of local particle density by counting neighbours on a certain radius (within a metric neighbourhood).

When used in this way, $\tilde{\rho}(t)$ can differentiate between different types of emergent behaviour in intermittent or metastable states, by capturing the local density resulting from the local clustering of individuals in multiple groups. In particular, this type of order parameter differentiates the 'forward' and 'backward' as well as the 'intrinsic' and 'extrinsic' noise implementations of the Vicsek model (Huepe & Aldana, 2008).

Angular momentum captures circular collective movement which cannot be described by either cohesion, nor alignment (Couzin et al., 2002):

$$\omega(t) = \frac{1}{Nv} \left\| \sum_{i=1}^{N} \mathbf{r}_t^i \times \mathbf{v}_t^i \right\|_2^2 \tag{3.28}$$

where $\mathbf{r}_t^i = \mathbf{x}_t^i - \bar{\mathbf{x}}_t$ is the displacement vector of particle i from the centre of mass $\bar{\mathbf{x}}_t$ at time t, and $\mathbf{a} \times \mathbf{b}$ represents vectorial cross product. In a slight abuse of notation, we may use $\mathbf{a} \times \mathbf{b}$ in a two-dimensional space which returns the scalar length of the cross product vector $\|\mathbf{a}\|_2^2 \|\mathbf{b}\|_2^2 \sin \sphericalangle(\mathbf{a}, \mathbf{b})$, since there is no third orthonormal dimension to define the cross product vector.

This observable quantifies the degree of the rotation of the group along their centre of mass, and therefore can detect the milling movement which is often characterised by very low v_a and difficult to describe with measures of aggregation. An example in the natural world is the cyclone configuration shown by herding reindeer (Espmark & Kinderås, 2002) in which all individuals gallop around the centre of mass of the group, or the milling of schools of fish (Lopez et al., 2012).

The current definition of the Vicsek model cannot produce the milling configuration at which this parameter excels. The observable was used to study a more complex flocking model which, beyond alignment, also drives the agents to avoid neighbours while staying close, and implements interaction rules with the use of steering vectors. By adding more kinds of interaction rules and more behavioural diversity, we also observe the phenomenology of milling. We will see in Chapter 5 such a multi-agent system which can produce milling behaviour (Reynolds, 1987).

Other more complex measures have been proposed, such as the integrated conditional density (Cavagna et al., 2008), which measures the average density in the metric neighbourhood of size r for various radii, and the packing fraction (Cavagna et al., 2008), often used in 3D domains, which is the ratio between the total volume of spheres of radius r occupied by the swarm and the volume of the domain. For example, the packing fraction for groups of starlings has been found experimentally to be 0.012 (Cavagna et al., 2008).

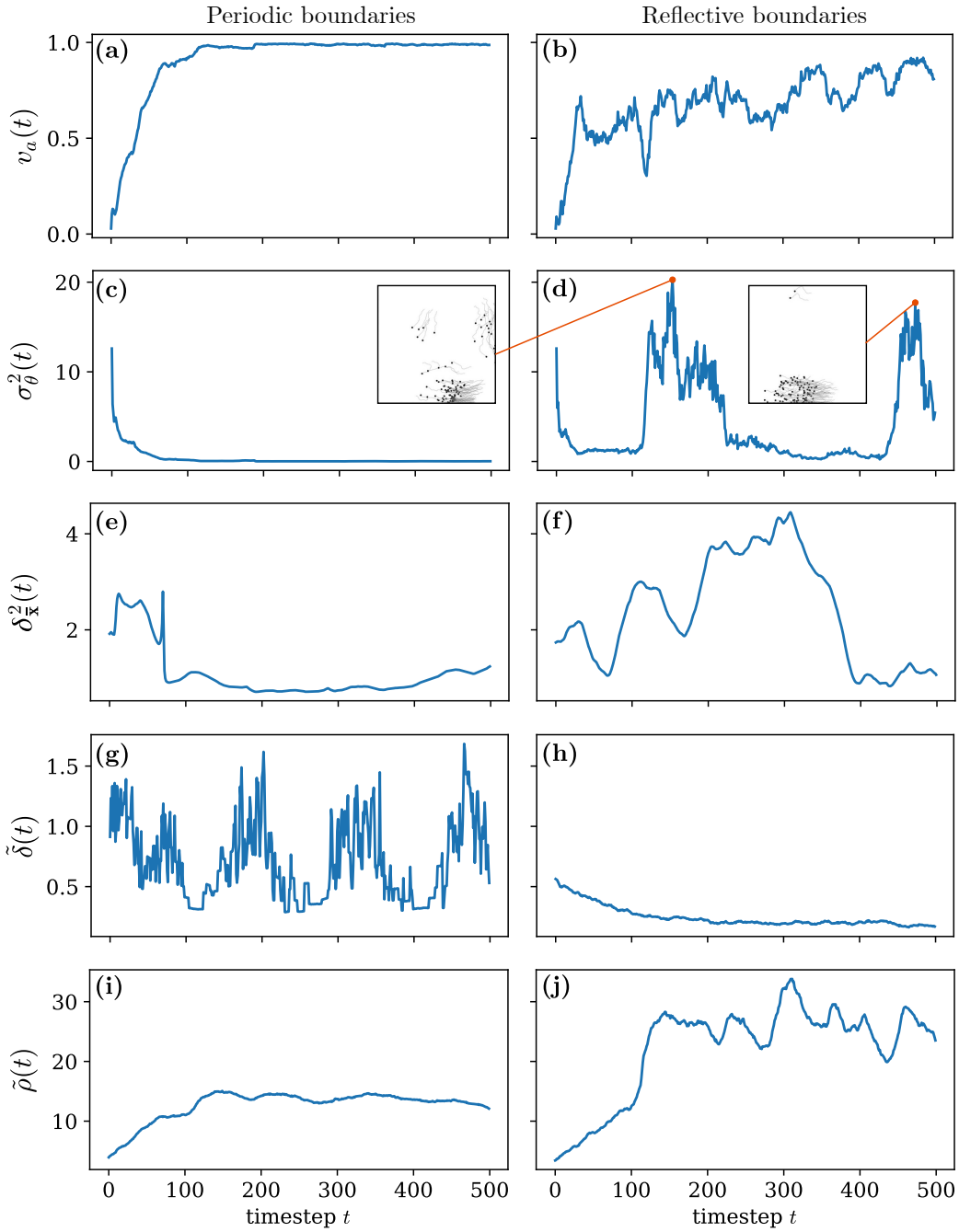


Figure 3.10: **Instantaneous observables of collective motion in periodic and reflective boundaries case studies of the Vicsek model.** ($N = 100$, $t = 500$, $\rho = 1$, $v = 0.1$, $r = 1$) **(left)** The system with periodic boundaries and less noise $\eta = 0.4$ settles into the ordered, aligned phase after less than 200 timesteps, as shown by the alignment-related observables **(a)** and **(c)**. In the ordered, aligned phase, a robust, not very dense group forms, which keeps a consistent mean distance to centre of mass **(e)** and number of neighbours on a radius r **(i)**, while the mean distance to the nearest neighbour varies somewhat **(g)**. **(right)** The system with reflective boundaries and more noise $\eta = 1.5$ is in an intermittent state, where particles aggregate in aligned groups and then break down as they hit walls, as shown by the variation in alignment-related observables **(b)** and **(d)** and the inconsistent mean distance to centre of mass **(f)**. These groups are much more dense, as shown by the decreasing mean distance to nearest neighbour **(h)** and increasing number of interaction neighbours **(j)**.

Name	Definition	Description	Ref.
$v_a(t)$	$\frac{1}{Nv}\left\| \sum_{i=1}^{N} \mathbf{v}_t^i \right\|_2^2$	Vicsek order parameter (alignment)	(Vicsek et al., 1995)
$\sigma_\theta^2(t)$	$\frac{1}{N}\sum_{i=1}^{N}(\theta_t^i - \bar{\theta}_t)^2$	spread of direction (polarisation)	(Huth & Wissel, 1994)
$\delta_{\bar{\mathbf{x}}}(t)$	$\frac{1}{N}\sum_{i=1}^{N} \|\mathbf{x}_t^i - \bar{\mathbf{x}}_t\|_2^2$	dispersion	
$\tilde{\delta}(t)$	$\frac{1}{N}\sum_{i=1}^{N} \underset{\substack{j\in\{1\ldots N\}\\ j\neq i}}{\arg\min} \|\mathbf{x}_t^i - \mathbf{x}_t^j\|_2^2$	mean distance to nearest neighbour	(Huth & Wissel, 1994)
$\tilde{\rho}(t)$	$\frac{1}{N}\sum_{i=1}^{N} \|\mathcal{N}^i(t)\|$	average number of neighbours	(Huepe & Aldana, 2008)
$\omega(t)$	$\frac{1}{N}\left\| \sum_{i=1}^{N} \mathbf{r}_t^i \times \mathbf{v}_t^i \right\|_2^2$	angular momentum	(Couzin et al., 2002)

Table 3.2: **Statistical observables used in both experimental and modelling-based swarming research.**

We have now surveyed a number of statistical scalar quantities that can describe collective behaviour in one and two dimensions. A brief outline of the measures is in Table 3.2. This is by no means an exhaustive review; many other, more complex, quantities and methods of analysis exist.

Through the case studies of the Vicsek model with qualitatively different phenomenology, we have illustrated how these different quantities describe different kinds of collective behaviour, but also their limitations in quantifying certain intermediary or metastable states between order and chaos. Nonetheless, many of these measures can be used instantaneously to describe dynamics. These statisical observables are dependent on prior knowledge of the collective behaviour to be investigated. In the next chapter, more agnostic measures will be used, aiming to detect emergent collective behaviour without prior knowledge of its phenomenology.

Chapter 4

Quantifying emergence in simple models

Chapter Summary

Measures of complexity, synergy and emergence may characterise emergent behaviour in a complex system in different ways. In this chapter, the models introduced in the previous chapter are used as a test-bed and null case to test information-theoretic emergence measures, and an unexpected behaviour of the emergence criteria is found. The aim of this chapter is to reveal and discuss concerns about the assumptions and interpretations of information-theoretic measures when analysing complex systems, using the example of mutual information-based synergy-redundancy measures.

Having just introduced some simple models that can be characterised by emergent collective behaviour, as well as some canonical methods to measure the observed collective behaviour in the models, we can now proceed to use the theoretical toolbox introduced in Chapter 2 to study the fine-grained information quantities existing in the system.

As we also hinted at in Section 2.3 and in the previous chapter, it is extremely important to study behaviour in relation to mechanisms that produce it, but without confusing the two. Testing measures of emergence on theoretical models with known behaviour and known mechanisms can help us interpret their use in the real world.

In this chapter, we present simulations of the three models presented in Chapter 3 and show how the $\Psi - \Gamma - \Delta$ emergence measures introduced in Section 2.3 change with the degree of collective behaviour in the models. In particular, we focus on collective movement on one and two dimensions, using weaker or stronger agent interactions which couple their evolution in time.

Collective movement is a remarkable testbed for many studies of complex systems, as it shows a broad spectrum of spatiotemporal patterns. We will see in the next part of the thesis how movement is particularly important as it can be taken as a proxy of hidden processes or internal states, related to agency, intentions, or interactions of agents in a complex system.

We start on the simplest kinds of systems that can manifest emergence for another very important reason: to test the robustness of the novel criteria in *null models*. For example, one needs to make sure not only that criteria find emergence in systems which do manifest it, but also, that the criteria do not produce false positives. While the authors have warned that Ψ may be negative even in emergent systems, it should be unlikely that a system without emergence should produce a positive Ψ.

We also use the numerical experiments in this chapter to address a number of practical considerations when applying information-theoretic to time series in the real world. For example, estimated information quantities are affected greatly by data availability, prior assumptions of the distribution of the data, and the stationarity of the time series, since they often require the estimation of joint probability distributions from data. As such, we can use simple models to test if and how these factors affect the estimation of information-theoretic quantities enough to change the criteria for emergence.

Relevant numerical findings in this chapter are also reported in (Liardi et al., 2025). The article also contains full analytical derivations of the models and numerical results by Prof Henrik Jensen and Alberto Liardi, which are briefly mentioned in this chapter where required.

4.1 Motivation and theoretical background

In Section 2.3 some information-theoretic methods have been introduced for the study of complex systems. These methods have gained great popularity as a very useful and model-agnostic framework for the study of complex systems. To briefly reiterate, developments in the field have allowed for better estimation of mutual information from data (Kraskov et al., 2004), whilst the Partial Information Decomposition (PID) approach (Williams & Beer, 2010) and its many developments (Kolchinsky, 2022; Mediano et al., 2022; Rosas et al., 2019, 2020b) have allowed for more fine-grained characterisations of information in multivariate systems that contributes towards the development of measures of emergence.

But the relation between information-theoretic measures and causal mechanisms can be difficult and it is important to keep in mind that notions like *information flow*, *causality* or *prediction* are related to statistical interrelations captured from the joint probability distributions and may not represent physical mechanisms. As warned before, we should be careful that emergent behaviours are not confused with the mechanisms or processes giving rise to them (Benhamou, 2007; Rosas et al., 2022).

We will now elaborate on this theme by investigating simple models of complex systems where the *mechanisms* are known: on independent and coupled random walkers, both in a stationary and non-stationary case, and in the Vicsek model. More specifically, we use the $\Psi - \Gamma - \Delta$ theory of causal emergence (Rosas et al., 2020a), which was introduced in Section 2.3.3, Eq. 2.35-2.37, to identify emergent *behaviour*, and we relate our results to the underlying mechanisms programmed in the models. For reference we reproduce the relevant quantities below for some collective random variable V_t:

$$\Psi^{(1,0)}_{t,t'}(V) := I(V_t; V_{t'}) - \sum_i I(X^t_i; V^{t'}) \tag{4.1}$$

$$\Delta^{(1,0)}_{t,t'}(V) := \max_i \left(I(V_t; X^i_{t'}) - \sum_j I(X^j_t; X^i_{t'}) \right) \tag{4.2}$$

$$\Gamma^{(1)}_{t,t'}(V) := \max_i I(V_t; X^i_{t'}) \tag{4.3}$$

The associated criteria for emergence are given by the following propositions:

(1) $\Psi^{(1,0)}_{t,t'}(V) > 0$ is sufficient for V to be causally emergent.

(2) $\Delta^{(1)}_{t,t'}(V) > 0$ is sufficient for downward causation.

(3) $\Psi^{(1,0)}_{t,t'}(V) > 0$ and $\Gamma^{(1)}_{t,t'}(V) = 0$ is sufficient for causal decoupling.

4.1.1 Limitations of mutual information as interaction measure

Given two random variables X, Y, the mutual information between them assesses the amount of information that we gain about X when Y is observed, and as such is a promising method to quantify interdependencies between components based on time series data. Often in research, a high mutual information between time series is taken to describe two interacting processes.

Yet a delicate property of mutual information is that the MI between a variable Y that assumes a value $Y = y_0$ with probability 1, and another stochastic variable X, is zero. The same is the case if Y and X are independent. This may complicate the interpretation of changes in the mutual information.

As statisticians will stress that *correlation does not imply causality*, should we stress that *mutual information does not imply interdependency or interaction*? If lack of correlation does not imply independence, is this also the case for mutual information? For instance, it is well known in statistics that a correlation value of 0 between two variables does not imply independence, a typical example is to consider a uniformly distributed variable x and x^2 in $[-1, 1]$: although correlation is zero, x and x^2 are clearly dependent.

This kind of behaviour is of course very well known by information-theorists. Its mention here is to illustrate how a decrease in the mutual information between stochastic variables may indicate two opposite interpretations: both a more random relationship, or a more predictable one. We take this as the first example of how the interpretation of changes in information measures in general is a subtle art.

This is important as, in modelling studies, the amount of the interactions is often predefined by some control parameter and the mechanisms of interactions are known; but when used on experimental data, we have no direct way to derive insight on the interactions. As such we may mistakenly interpret the mutual information to be indicative of mechanisms which are missing.

4.1.2 Limitations of synergy-minus-redundancy measures

As outlined in Section 2.3.3, the $\Psi - \Gamma - \Delta$ theory of causal emergence provides practical criteria to detect emergence in experimental or simulated data. In a broader context, Ψ and Δ are a type of whole-minus-sum measure of emergence, similar to the interaction information (Williams & Beer, 2010), the redundancy-synergy index (Timme et al., 2013) and the Ω-information (Rosas et al., 2019) which quantify the balance between synergy and redundancy.

In practice, this means that if there is redundancy in the system it will be harder to detect some kinds of emergent behaviour: a rigid system where all components behave as

one will be characterised by high redundancy and little synergy, likely causing Ψ to be negative. Alternatively, a system with very little redundancy and a very low amount of interactions between the components may show a higher value of Ψ than the rigid case.

As we have also noted in Section 2.3.3, especially when working in systems composed of many components, these measures sum up the marginal mutual informations such as $I(X_t^i; V_{t'})$ or $I(X_t^i; X_{t'}^j)$ which all, effectively, contain the redundant information common to all the components. When summing $I(X_t^i; V_{t'})$ for every i, we also count the information common to all the components $(N-1)$ times. In this chapter we will dwell on these redundancies and how this 'double-counting' can be mitigated using the PID proposed in (Sas et al., 2024b).

4.1.3 Centre of mass as emergent feature in collective movement

The $\Psi - \Gamma - \Delta$ theory of emergence requires the selection of a collective systemic property as a candidate emergent feature, and tests whether this collective property better describes the system than the individual properties of the components, using quantities which are expressed in terms of time-delayed mutual information (TDMI) between the trajectories of particles at the microscopic level, and the trajectory of this system property at the macroscopic one.

As we are interested in the emergence of collective motion, which is a spatiotemporal phenomenon, we make the observation that a group of components moving as one manifests a great reduction in its degrees of freedom. Based on this observation, and similar to previous work where emergence is defined based on the relationships between the micro and macro scales (Comolatti & Hoel, 2022; Hoel et al., 2013), we select the centre of mass of the particles as a coarse-graining function or aggregate property. This is a simple average of the entire system behaviour, but has an important intepretation: intuitively, if we expect the particles to behave collectively in some way, then their centre of mass can predict the movement of the group and the individuals better than any of the individuals themselves.

We define it as $\mathbf{v}_t = \frac{1}{N}\sum_i \mathbf{x}_t^i$. The time series $(\mathbf{v}_t)$ is a realisation of a random variable $\mathbf{V}_t$, which is the average of the random variables $\mathbf{X}^i$ describing the particles' positions. The centre of mass matches the preconditions for the theory of causal emergence and is itself used in the original case studies of the criteria, as it is an aggregate property affected by observational noise which is independent at time t from the state of all the particles in the system at a future time t'.

4.1.4 Information quantities in Gaussian random walkers

The centre of mass for the Gaussian random walkers (see Section 3.2.1) is given by:

$$V_t = \frac{1}{N}\sum_{i=1}^{N} X_t^i \tag{4.4}$$

In the **non-interactive** case, the centre of mass is a random walker itself, albeit moving with lesser variance, as well as a *non-stationary process*.

$$V_t = \frac{1}{N}\sum_{i=1}^{N}\sum_{T=1}^{t} \eta_T^i \sim \mathcal{N}\left(0, \frac{t\sigma^2}{N}\right) \tag{4.5}$$

The statistical properties of Gaussian distributions allow for a theoretical derivation of the relevant mutual information quantities in the non-interactive case, as the entropy of a Gaussian distribution can be derived analytically (Liardi et al., 2025) . These theoretical results can act as a benchmark for our numerical studies:

$$I(X_t^i; V_{t'}) = I(V_t; X_{t'}^i) = \frac{1}{2}\ln\frac{N\tau}{N\tau - 1} \tag{4.6}$$

$$I(V_t; V_{t'}) = I(X_t^i; X_{t'}^i) = \frac{1}{2}\ln\frac{\tau}{\tau - 1} \tag{4.7}$$

$\forall i \in \{1, 2, ..N\}$, with $\tau = \frac{t'}{t}$ and $t' > t$.

Since there are no interactions, there should also be no mutual information between a particle and any other:

$$I(X_i(t), X_j(t')) = 0, \forall i \neq j \tag{4.8}$$

We observe that the information from 'micro-to-macro' $I(X_t^i; V_{t'})$ is the same as the information from 'macro-to-micro' $I(V_t; X_{t'}^i)$, and that the mutual information between a walker and itself in the future is the same as that between the centre of mass and itself in the future. This follows both our intuition and statistical derivation that the centre of mass is a random walker itself. The first two quantities depend on the system size, since the more variables in the system, the less they contribute towards the centre of mass.

A no less interesting finding is the dependence of the information quantities on the multiplicative time difference $t'/t = \tau$, rather than the additive time difference $t' - t$. This result captures the *scale-free* property of random walkers. As random walks are self-similar, the scales on which patterns emerge in the trajectories can vary greatly over time, with the similar patterns more likely to appear when 'zooming in or out' rather than advancing in time by a fixed number of time steps.

In the **interactive case**, a coupling constant γ is added between neighbouring processes. The probability distributions are more difficult to derive analytically, not only due to the fact that the components are no longer statistically independent, but also due to the boundary effects created by the two particles at the edge. Moreover, positions of the particles x_t^i are initialised as $i \cdot a$ and no longer have zero mean. Instead, we use $\Delta_t^i = x_t^i - i \cdot a$ (Eq. 3.6) to represent the deviation of particle i from its initial position, to preserve comparable statistics to the non-interactive case. For convenience, we continue using the notation X^i to refer to particle i in the mutual information quantities.

By approaching the derivation as $N \to \infty$ and $\gamma \to 0$ an approximation can be derived. Analytical derivations of these information quantities and Ψ, Γ, Δ can be found in (Liardi et al., 2025). We briefly outline the results in terms of the system size N, time difference $\tau = t'/t$ and the coupling constant γ:

$$I(X(t); X(t')) = \frac{1}{2} \ln\left(\frac{\tau}{\tau - 1}\right) - \gamma t\,, \tag{4.9}$$

$$I(X(t); Xj(t')) = 0\,, \quad i \neq j \tag{4.10}$$

$$I(V(t); V(t')) = \frac{1}{2} \ln\left(\frac{\tau}{\tau - 1}\right), \tag{4.11}$$

$$I(X(t); V(t')) = \frac{1}{2} \ln\left(\frac{N\tau}{N\tau - 1}\right) + \gamma \frac{t - 1}{N\tau - 1}\,, \tag{4.12}$$

$$I(V(t); X(t')) = \frac{1}{2} \ln\left(\frac{N\tau}{N\tau - 1}\right) + \gamma \frac{t' - 1}{N\tau - 1}\,, \tag{4.13}$$

Interestingly, the self-predictability of the centre of mass $I(V_t; V_{t'})$ remains independent of the system size and depends only on the time increment, while introducing interactions creates a dependence on coupling γ in the self-predictability of each particle. The subtraction of a multiple of γ from the quantity follows our intuition that the more a particle interacts with its neighbour the less TDMI it has with itself. Furthermore, this is time-dependent.

Introducing interactions also makes the $I(X_t^i; V_{t'})$ and $I(V_t; X_{t'}^i)$ quantities no longer be equal to each other, with the former showing dependence on the past time increment t and the latter showing dependence on the future t'.

Again, we observe the *scale-free* property in random walkers, but also that the quantities describing the relationships between parts and whole are no longer the same. Moreover, there is a clear dependence on the specific time points t and t', which makes it difficult to generalise system behaviour in the interactive case. Many systems in nature may be non-stationary in a similar way, but low data availability may mean that assumptions of stationarity need to be made.

4.2 Numerical methods

Having now introduced the theoretical derivation of our quantities, we also wish to test the criteria directly in data using numerical methods. The simple models were simulated to produce time series for all the components. We investigate robustness of our methods by making different assumptions about the stationarity of the data, by varying the number of simulations, and by varying the amount of interactions between the components. Simulation and implementation details are detailed in this section.

4.2.1 Implementation details

The models have been implemented in Python using `numpy`. An abstract class is used to describe the particle system, storing random seeds, model parameters, initial conditions and trajectories, and providing an abstract `update()` rule by which each component in the system evolves over time. The abstract class is inherited into specific classes corresponding to the models. The Python library includes analysis scripts for computing order parameters and visualising the dynamical behaviour of the flocks.

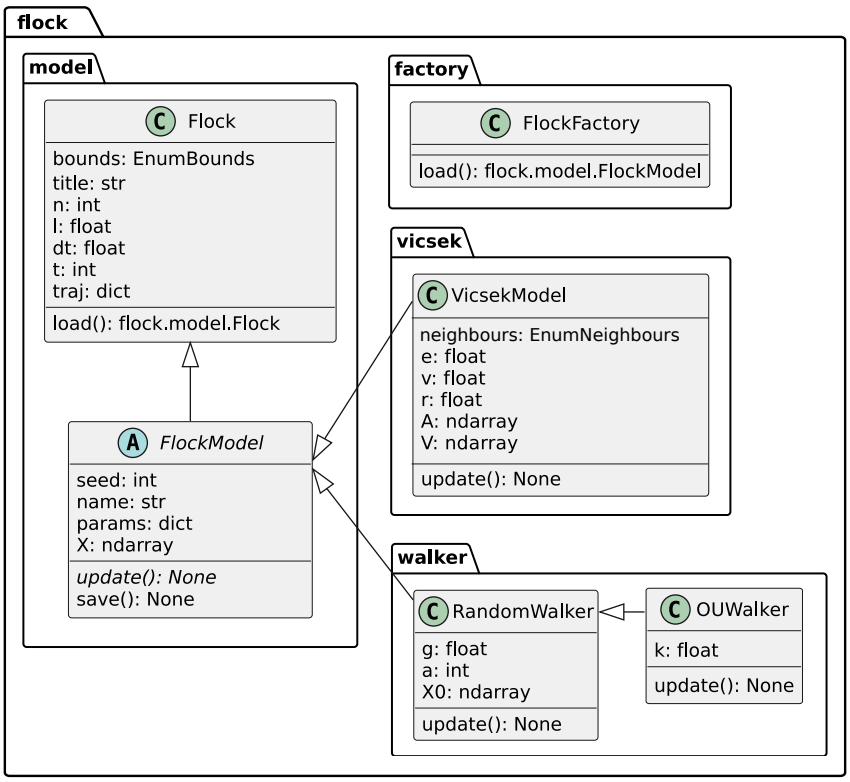


Figure 4.1: **UML class diagram for the particle systems simulations.** A `FlockFactory` class is used to load data from files in the correct structure and construct a simplified, abstract `Flock` class that can be passed on to the analysis pipeline. For the models implemented in the library, the `FlockFactory` class returns a `FlockModel`, which acts as an abstract class for the three different particle models: `RandomWalker`, `OUWalker` and `Vicsek`.

The implementation is available and documented online (Sas, 2021). The relevant classes are shown in the diagram above.

A random seed may be specified to the simulations so that the initial conditions and the random numbers sampled for the stochastic components in both models can be reproduced. At each discrete timestep, the particles are updated with new positions according to the stochastic processes that define their behaviour using the `update()` function.

The relevant equations of motion are Eq. 3.1 for the Gaussian and Eq. 3.10 for the Ornstein-Uhlenbeck random walkers, respectively. For the Vicsek model, we use the forward difference implementation, namely that we first update the angles of direction according to Eq. 3.16 and then the positions according to Eq. 3.20. Periodic or reflective boundaries, as well as metric and topological neighbourhoods, are set with class parameters `bounds` and `neighbours`.

4.2.2 Simulation: random walks

We begin by simulating the Gaussian random walkers. The number of realisations is varied to obtain different amounts of data to test the robustness of estimating information-theoretic quantities. As the systems are very simple, we can compare these numeric results with theoretic estimations when the particles do not interact with each other.

We test our measures on the *null case*, then we increase the interactions by tuning the coupling parameter γ which describes an elastic force that keeps the particles together. Since Gaussian random walkers are non-stationary unlike the way these measures are used in nature, we turn on the restorative force k to make them non-stationary, and repeat our analysis with Gaussian Ornstein-Uhlenbeck processes.

Table 4.1: Model parameters used in the random walker simulations.

Name	Symbol	Variable	Values
number of particles	N	`n`	{2, 4, 8, 16, 32, 64, 128, 256, 512}
time increment	δt	`dt`	1
duration	T	`t`	2000
noise	σ	`e`	1.0
coupling	γ	`g`	{0, .01, .02, .04, .08, .16, .32, .49}
spacing constant	a	`a`	1.0
restorative force	k	`k`	{0, .01}

The model parameters, their corresponding variables in each Python class, and the values used in the numerical studies are shown in the above table. Initial conditions are set to $x_0^i = 0$ for the non-interacting case, and $x_0^i = i$ for the interacting case. We aim for logarithmically spaced values in γ, but since the maximum value to the coupling constant is $\gamma_{\max} = 0.5$, we also study a value close to this boundary, i.e. $\gamma = 0.49$.

4.2.3 Simulation: Vicsek flocking model

We investigate the robustness of the emergence criteria against various emergent behaviours apparent in the Vicsek model. More specifically, we employ a model with periodic boundaries and metric interactions to observe the emergence of alignment, as well as a model with reflective boundaries and topological neighbourhoods to observe the emergence of cohesion. The Vicsek model allows an opportunity to iron out the idiosyncrasies of our measures, and explore how the information quantities are best applied to this positional data.

First, we consider the Standard Vicsek Model with periodic boundaries and metric interactions, as it has been the most heavily studied. We simulate small systems in three different classes of behaviour for $R = 20$ realisations each, using different sizes N with the same densities. We vary the interaction radius to produce three different phenomenological behaviours: disordered, fully aligned, and an intermediary flocking regime.

While useful for many analyses and a standard method in molecular analysis, periodic boundary conditions rarely have any physical relevance when studying real-world systems. This is very relevant when considering the estimation of joint probability distributions for computing mutual information as boundary effects may affect the estimation. As such, we employ the Vicsek model with reflective boundaries, which is more similar to how collective motion may be encountered experimentally: for example, fish in a tank.

Table 4.2: Model parameters used in the Vicsek model simulations. The system sizes, environment sizes and interaction radii are selected so all systems of different sizes have the same density and behave similarly.

Name	Symbol	Variable	Values
number of particles	N	`n`	{10,20,40,100}
size of environment	L	`l`	{5,7,10,16}
time increment	δt	`dt`	1
duration	T	`t`	5000
noise	η	`e`	0.4
speed	v	`v`	0.1
interaction radius	r	`r`	$\{0, 0.1L, 0.2L\}$

Mitigating boundary effects

Above, we have hinted at the boundary effects inherent in periodic boundary conditions. Periodic boundaries are implemented using a *unit cell* of size L by L such that when a particle passes through one side, it appears on the opposite side with the same velocity. When close to a boundary, a particle's nearest neighbour may be situated on the opposite side of the unit cell, so estimating information quantities directly on the positions will fail to catch their proximity.

A method to efficiently mitigate this difficulty was proposed in (Seth, 2010): instead of studying the positions as cartesian coordinates, they get transformed into velocities with respect to the distance from the centre of the environment $C = (L/2, L/2)$:

$$\hat{V}_t = \left(\|V_{t+1}, C\|_2^2 - \|V_t, C\|_2^2\right)/\Delta t \tag{4.14}$$

$$\hat{X}_t^i = \left(\|X_{t+1}^i, C\|_2^2 - \|X_t^i, C\|_2^2\right)/\Delta t \tag{4.15}$$

where $\|\cdot\|$ is Euclidean distance, and $\Delta t = 1$ as we use simulations with discrete timesteps.

Practically, neighbours that are close to each other at the boundaries but far away in terms of positions in the unit cell, show similar values once the distance is taken.

We also investigate how this transformation of the time series affects the results in the reflective boundaries case, which also allows computing mutual information directly on the positions and provides opportunities for comparison.

4.2.4 Information-theoretic methods

Information-theoretic analysis tools were implemented in `python` using `numpy` arrays and bindings via the `jpype1` package to the Java Information Dynamics Toolkit (JIDT) (Lizier, 2014) for estimating information-theoretic quantities from data. The implementation is available online (Sas, 2024).

In the random walkers, mutual information is computed using JIDT's mutual information calculator that assumes the underlying Gaussian distribution of the components, `ContinuousMutualInfoCalculatorGaussian`. For the Vicsek model, it is computed with the `ContinuousMutualInfoCalculatorMultivariateKraskov1`, implementing the histogram-based estimator in (Kraskov et al., 2004).

The positional time series of X^i and V, or the transformed time series $\hat{X}^i$ and $\hat{V}$, are provided as operands to the mutual information function. To compute TDMI with integer time delay dt, the time series are offset by dt before calling the function.

Data availability

To test robustness of our criteria against data availability, we simulate the models with a varying number of realisations, and compare numerical results against theoretical ones.

Computational resources

Due to requiring many parameter ranges and many realisations for the same parameters, each system is simulated or analysed in its own thread. Multiple threads are spawned in parallel to simulate or analyse multiple systems at once. Most computations were performed on machines with 32-64GB RAM. 32 cores were used to leverage parallelism, but both the simulations and the analysis (for N<1000 in 1D and N<100 in 2D) can be and have been run on a 2-core CPU laptop.

Stationarity

The estimation of mutual information from time series assumes the quantities are stationary. This, of course, is not always the case in complex systems. We have seen this in the analytical derivation of the random walkers, whose values depend on the time elapsed.

For *non-stationary* systems, the computation of TDMI is performed between states of the system at different times across different realisations. This is because estimation of probability distributions can only be done robustly at the same time instant across multiple realisations, as the probability depends on t and even more specifically, the analytical results show the mutual information depends on the exact time increments as wel as τ. The average values are obtained first by averaging pairwise results where (t, t') have the same relationship between them.

- In the case of Gaussian random walkers, as the TDMI depends strongly on τ, the averaging is done over all pairwise results where $t'/t = \tau$.
- In the case of Gaussian OU process, since we employ stationary dynamics, the time dependence is no longer multiplicative and averaging is done over all pairs where $t' - t = \Delta t$.

For *stationary* systems, the computation of TDMI can be done directly on the time series data from even a singular realisation. For robustness, multiple realisations are taken and averages are done afterwards for given values of parameters of interest. Unless otherwise specified $R = 20$ realisations are taken.

In both pipelines for stationary and non-stationary analysis, averages for information quantities are taken over the number of particles across many realisations. Standard error, unless otherwise specified, is also taken over the number of particles, after averaging the realisations.

4.3 Results: Gaussian random walks

Mutual information quantities and emergence crtieria were estimated numerically using systems of non-stationary random walks of various sizes. The restorative force was set to $k = 0$. The coupling parameter γ was set to $\{0, .01, .02, .04....32\}$. Time differences for the TDMI were taken as $\tau \in \{2, 3, ...10\}$.

4.3.1 Null case: non-interactive systems

First, the coupling was set to $\gamma = 0$ in order to investigate the *null case*. We hypothesised that in the non-interactive case where the random walks are not coupled, the centre of mass should not be an emergent feature.

Mutual information in non-interactive systems

The numerical results are mostly in accord with the theoretical estimates, with the centre of mass V and individual walks X^i showing similar mutual information quantities, as expected from their statistics.

The $I(X^i_t, V_{t'})$ and $I(V_t, X^i_{t'})$ terms are the same, and are non-zero. The quantities decay logarithmically as the time delay is increased, and we observe also the logarithmic dependence on system size predicted by the theory.

While the quantity is small and largely irrelevant when compared directly with the other mutual informations, we observe numerically a non-zero positive mutual information quantity for a walker and its neighbours $I(X^i, X^j)_{i \neq j} > 0$, even for the non-interactive case, in spite of no mechanism of coupling. This may be due to the fact that both operands are characterised by the same statistical distribution and this may create spurious correlations when doing a parametrised estimation of joint probability tables from data.

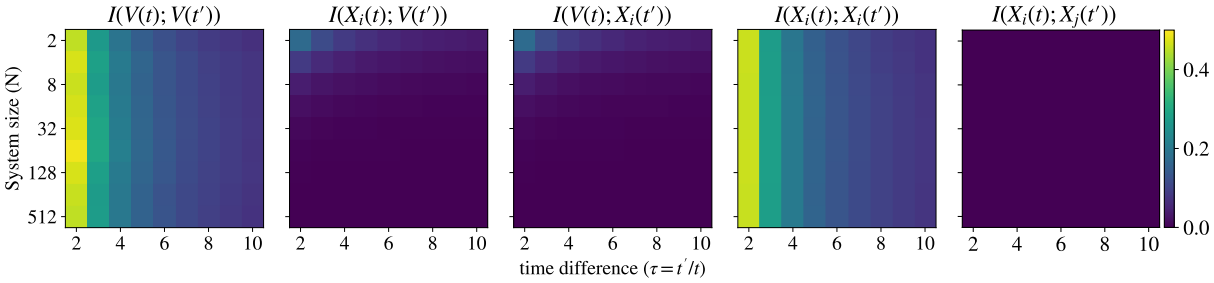


Figure 4.2: **Mutual information in non-interacting non-stationary Gaussian random walks**. The x-axis shows decay in the time difference $\tau = t'/t$ between the two measurements for TDMI, averaged over many values for t and t'. The y-axis shows sytem size. The systems were simulated for $R = 2000$ times for each parameter set, and the quantities shown are averaged over all N particles.

TDMI and data availability

As the above study generates ensembles of realisation of the systems in order to compute TDMI while taking into account the system's non-stationarity, it is important to investigate whether the amount of data available for the estimation of mutual information has an important effect on the quantities we study.

To test the amount of over-estimation, we compare with the theoretical quantities and vary the system size and number of realisations $R \in \{100, 200, 500, 1000, 2000, 5000, 10000\}$.

In the case of mutual information between two different particles, increasing the ensemble size R brings the estimation closer to 0. The quantities are small, and yet this over-estimation may end up being relevant to analysis, as these small quantities will add up when computing measures like Δ especially for systems with many components. It is clear from the two figures below how the value is affected by data availability as the estimates get more accurate with increasing number of realisations. System size does not affect the $I(X_t^i, X_{t'}^j)$ estimation in this case, as there are no interactions with neighbours.

While for $I(X_t^i; X_{t'}^j)$ the over-estimation is consistent across quantities and system size, this is not the case in the other quantities, in particular the TDMI between the centre of mass and itself. Here we see that a number of realisations under 1000 produces inconsistent quantities, sometimes over-estimating and some times not, with most over-estimation occuring in the largest system size and with the least number of realisations.

For the remaining simulations, we will settle for $R = 2000$ realisations in order to balance statistical robustness and computational demands.

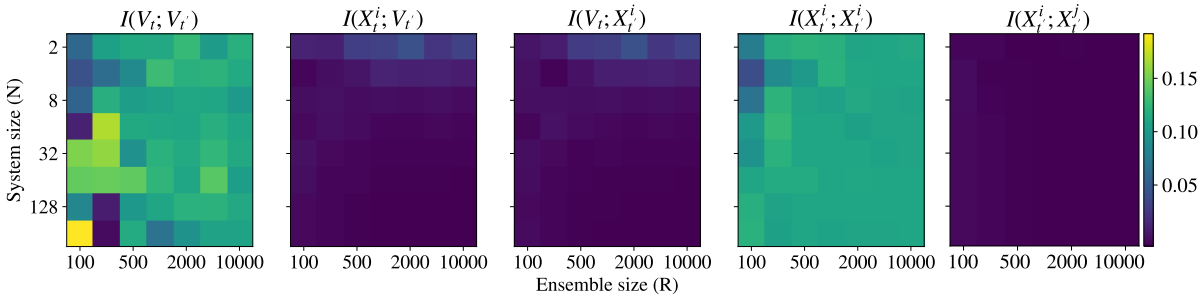


Figure 4.3: **Accuracy of mutual information estimation in non-interacting Gaussian random walks**. The x-axis shows the number of simulations R of the system that were used to estimate the mutual information. The y-axis shows sytem size. The time delay was set to $\tau = 2$. The heat maps represent the difference between the theory in Eq. 4.6 and the estimated quantities averaged over all N particles.

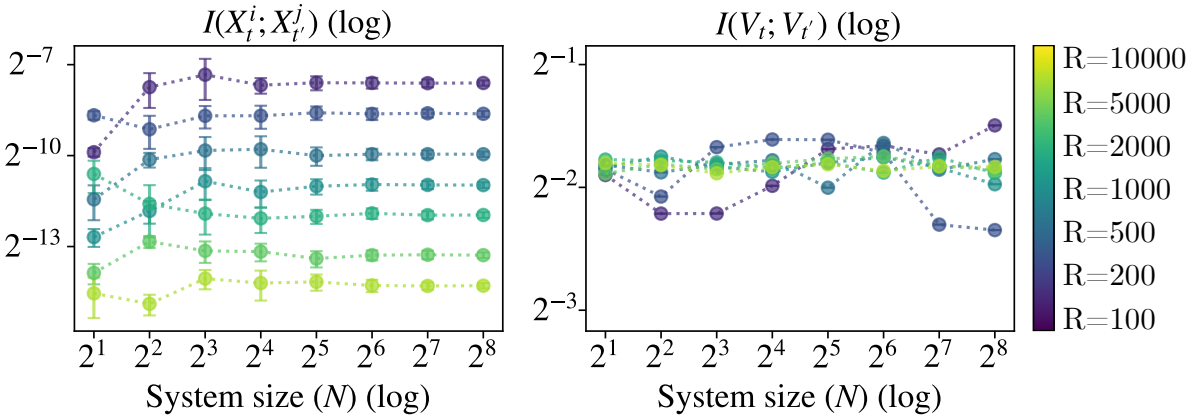


Figure 4.4: **The effect of ensemble size in mutual information estimation in non-interacting Gaussian random walks**. The time delay is set to $\tau = 2$. In the different particles $I(X_t^i; X_{t'}^j)$ case, increasing the number of realisations reduces the over-estimation. In the case of the centre of mass $I(V_t; V_{t'})$, the over-estimation is inconsistent, but becomes rather minimal above $R = 1000$ realisations. $I(X_t^i; X_{t'}^j)$ is averaged over all particles and error bars represent the standard deviation over the N particles.

Non-negative emergence measures in non-interactive systems

Continuing to numerically and analytically study the $\Psi - \Gamma - \Delta$ criteria of emergence, we start with the *null case* where the random walks are not interacting.

Having produced a theoretical derivation of the mutual information quantities in the previous theory section 4.1, we can also derive the value of the emergence criteria in terms of N and $\tau = t'/t$ with $t' > t$:

$$\Psi_{t,t'}^{(1)} = \frac{1}{2} \ln\left(\frac{\tau}{\tau - 1}\right) + \frac{N}{2} \ln\left(1 - \frac{1}{N\tau}\right) > 0, \quad \forall N \in \mathbb{N} \tag{4.16}$$

$$\Delta_{t,t'}^{(1)} = \frac{1}{2} \ln\left(\frac{N(\tau - 1)}{N\tau - 1}\right) < 0, \quad \forall N > 1 \tag{4.17}$$

$$\Gamma_{t,t'} = \frac{1}{2} \ln\left(\frac{N\tau}{N\tau - 1}\right) > 0, \quad \forall N \in \mathbb{N} \tag{4.18}$$

Theoretical results and numerics agree. Both show, unexpectedly, that for all investigated system sizes and the smaller time differences, $\Psi_{t,t'}^{(1)}$ is positive, although small, of the order of 10^{-1}, and it decays with increasing τ as expected, and for the smaller system sizes it vanishes more slowly than for larger ones. According to the sufficient condition (1) above, V is a *causally emergent* feature. This contradicts our hypothesis; the centre of mass of non-interacting constituents is not emergent in any sense that involves higher-order mechanistic interactions and ordered collective behaviour. Rather, the *emergent nature* of the centre of mass lies intrinsically in being a macroscopic variable that depends on the microscopic state, in a system in which all components are statistically identical.

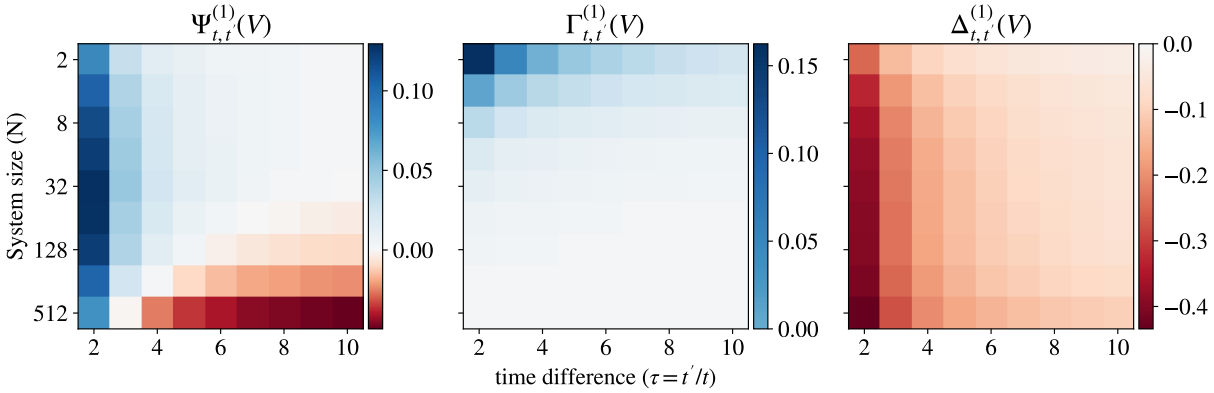


Figure 4.5: **Emergence criteria in non-interacting non-stationary Gaussian random walks**. The x-axis shows decay in the time difference $\tau = t'/t$. The y-axis shows sytem size. The systems were simulated for $R = 2000$ times for each parameter set and the quantities were averaged over the N components.

Negative Δ for $N > 1$ and positive Γ for small N suggest no downward causation or causal decoupling. However, we note that $\lim_{N\to\infty} \Gamma^{(1)}_{t,t'} = 0$, meaning that according to sufficient condition (3), *causal decoupling* occurs in a system of infinite size, where V acts as if it *behaves autonomously*.

Results may be explained by the observation that V itself is described by the same statistics as a random walk, albeit with smaller variance, and that in infinite systems the information shared by each component and the centre of mass vanishes. Nevertheless, an interpretation in terms of a concept of emergence as a 'whole greater than the sum of parts' remains difficult.

4.3.2 Interactive systems

Proceeding to study the effect of adding coupling between neighbouring random walks, we expect changes both in the pairwise measures and in the emergence criteria. Intuition as well as theoretical quantities suggest TDMI between different particles increases while TDMI of each particle with itself decreases as γ increases. As coupling adds mechanistic interactions between components we would like the criteria to find larger degrees of emergence with higher values of γ.

Mutual information

TDMI results are mostly in accordance to theory, as can be seen in Fig. 4.6 below.

The $I(X^i_t, V_{t'})$ and $I(V_t, X^i_{t'})$ terms both increase with γ, as stronger interactions make the different parts more interdependent and therefore more predictable, which is according to hypothesis. Moreover, they are no longer identical, with the latter term becoming larger than the former as γ increases.

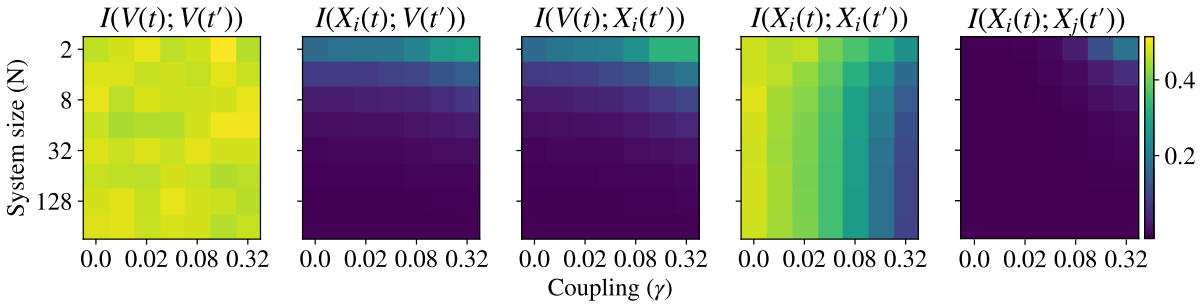


Figure 4.6: **Mutual information in interacting non-stationary Gaussian random walks**. The x-axis shows increasing coupling γ between neighbouring particles. The y-axis shows system size. Each value was computed by averaging the mutual information quantity across all components in the system, with the exception of $I(V_t; V_t')$. The time difference is $\tau = t'/t = 2$. The systems were simulated for $R = 2000$ times for each parameter set.

As predicted by derivations, $I(V_t, V_{t'})$ appears independent of the system size or coupling. The TDMI between a particle and itself $I(X_t^i; X_{t'}^i)$ decreases and decays more slowly the more coupling is added, while that between a particle and others $I(X_t^i; X_{t'}^j)$ increases. We observe the conflicting tendencies introduced by a larger system size and increasing coupling. Information between different walks vanishes in larger systems, but in the $N = 2, 4, 8$ particle systems, the quantity increases as expected.

These considerations are only possible as we know exactly there are interactions in the system as controlled by the coupling parameter γ. In a real-case scenario, not only is this knowledge not accessible, but it also might not be clear what the actual components of the system are. Thus, the interpretation of MI might not be as straightforward.

Finally, we take the simplest $N = 2$ case to observe the effect of the time delay τ in the TDMI calculations. We observe that the more time delay is introduced, the higher $I(V_t; X_{t'}^i)$ is than $I(X_t^i; V_{t'})$. Moreover, the more interactions are introduced also, the supervenient feature V maintains its self-predictability while the self-predictability of components decreases with coupling. This makes sense as by increasing interactions, each component is less self-determined, and depends more on its neighbours.

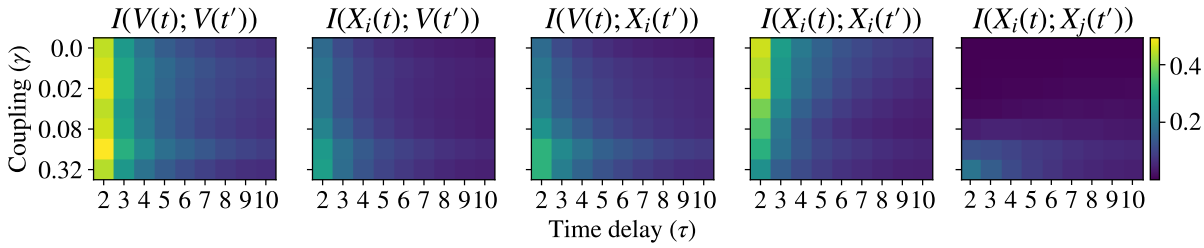


Figure 4.7: **Mutual information in $N = 2$ interacting non-stationary Gaussian random walks**. The x-axis shows increasing coupling γ between neighbouring particles. The y-axis shows sytem size. The time difference is $\Delta t = t'/t = 2$. The systems were simulated for $R = 2000$ times for each parameter set and the quantities were averaged over the 2 components.

Decreasing emergence measures in interactive systems

Moving on to interacting systems with $\gamma > 0$, one would naturally expect that even if $\Psi > 0$ in the non-interactive case, at least it should be greater in interactive systems.

Unexpectedly, this is not the case, as instead Ψ becomes smaller than the non-interactive case, making V *less emergent* the more the random walks interact. Formally, this is due to $I(V_t; V_{t'})$ not being dependent on γ, while $I(X_t^j; V_{t'})$ increases with it. However, intuitively one would expect an increase in the emergence of the system when the interactions become stronger, as the components become mechanistically interdependent.

Δ decreases and Γ increases with interactions, not affecting the conclusions drawn in non-intractive systems, that neither causal decoupling nor downwards causation criteria are met in finite systems.

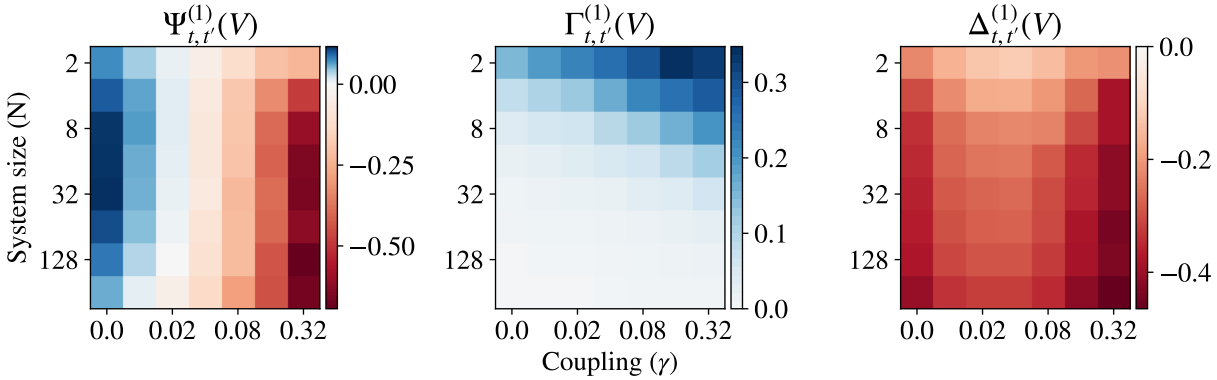


Figure 4.8: **Emergence criteria in interacting non-stationary Gaussian random walks**. The x-axis shows the coupling parameter γ. The y-axis shows sytem size. The time difference was set to $\tau = t'/t = 2$. systems were simulated for $R = 2000$ times for each parameter set and the quantities were averaged over the N components.

First-order redundancy

This result, while unintuitive, may be explained to some extent by the limitations of synergy-minus-redundancy quantifiers introduced in Section 2.3 and reiterated at the beginning of this chapter: simple systems in a highly ordered state are characterised by high redundancy and require a more accurate estimation of emergence criteria.

First we consider the redundancy across all the components, defined as the minimum mutual information: $\min_i I(X_t^i; V_{t'})$. Since all components are identical, it makes sense that they all provide some of the same reduction in uncertainty towards predicting the group, and in computing $\Psi^{(1)}_{t,t'}$ this quantity is considered N times. To compute the more accurate estimator $\Psi^{(1,1)}_{t,t'}$ we simply subtract this excess redundant information $N-1$ times, according to Eq. 2.43.

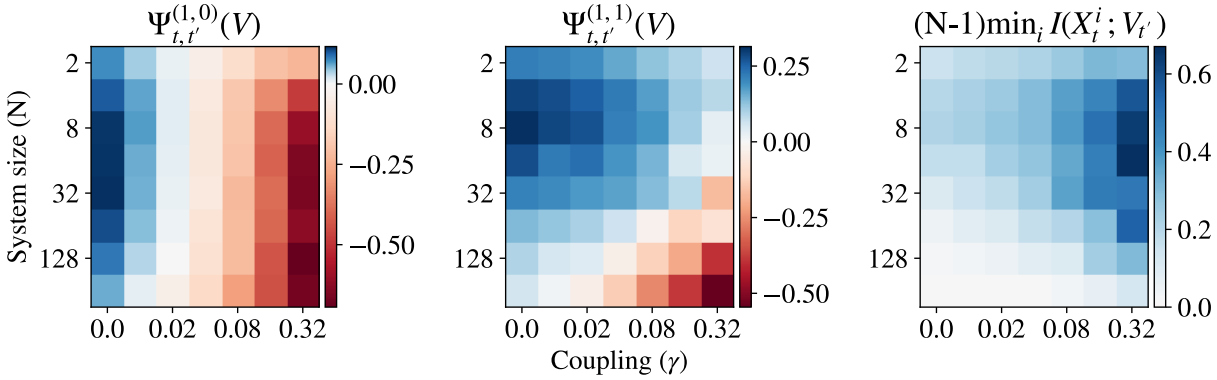


Figure 4.9: **Causal emergence and first-order redundancy in interacting non-stationary Gaussian random walks**. The x-axis shows the coupling parameter γ. The y-axis shows sytem size. The time difference was set to $\tau = t'/t = 2$. systems were simulated for $R = 2000$ times for each parameter set and the quantities were averaged over the N components. The redundancy in the third panel increases and as it is added to the $\Psi^{(1)}$ result in the first panel, we can approximate a more exact emergence criterion in $\Psi^{(1,1)}$, but this still behaves unexpectedly in the larger systems.

As the redundancy is always positive, the correction can only make the non-interactive system 'more emergent' than before. Nonetheless, a more accurate Ψ should be higher in interactive systems than non-interactive ones, since we hypothesise the systems with higher coupling would also manifest higher redundancy.

Results show redundancy increases for the larger interactions as expected. Adjusting the threshold for emergence by this redundancy produces a better approximation of Ψ, namely $\Psi^{(1,1)}$, which slows down the tendency of Ψ to decrease as the system size N increases, making the criterion more sensitive to emergence in the smaller systems now. Unfortunately, this does not reverse the general trend of Ψ to decrease as interactions are increased. This suggests finer-grained estimation is still necessary.

4.3.3 Limitations and future work

We have presented the results of an analytical and numerical study of Gaussian random walks, and observed some difficult to interpret behaviour of our emergence criteria. Further research may be required to better understand these findings, and some of the limitations and possible improvements are outlined below.

Non-stationarity

The first limitation comes from the non-stationarity of the Gaussian random walks. By taking the assumption of non-stationarity and using multiplicative time delays when estimating TDMI, we captured the scale-free property of the system, but the analysis pipeline used is not really applicable as-is to real-world collective behaviour.

By introducing a stationary version inspired by the Ornstein-Uhlenbeck processes, we will next investigate systems which are easier to quantify. Unfortunately, this only avoids the issue of practically studying non-stationary data with information theory.

One method to mitigate this issue is frequently used in neuroscience by the method of *epoching*: by splitting the time series into non-overlapping time windows of specific sizes, we may assume that within that window, the behaviour is stationary. Following the same kind of assumption, as future work, we should study the Gaussian random walks using shorter time-windows, and compare the results with the ones presented in this chapter.

Accounting for redundancy

Due to computational and time limitations, we were unable to produce a more efficient implementation of the lattice expansion technique, therefore larger system sizes or more fine-grained estimators for Ψ and Δ were not yet studied in Gaussian random walks. While we were able to see a positive trend after computing the more accurate $\Psi^{(1,1)}_{t,t'}$ with $q = 1$, we have yet to investigate criteria that are accurate enough for larger systems.

We aim to test in the future whether fine-grained estimators (i.e. with $q > 1$) might produce higher criteria in the interactive systems than the non-interactive ones. Unfortunately, the state explosion problem is emphasised when computing more accurate criteria, with the number of combinations of atoms of multiple sizes growing factorially. Nonetheless, it would be interesting to analyse trade-offs between accuracy and computational costs, but also to identify more fine-grained properties of the lattice expansion process which may inform a more efficient implementation.

Finally, it would be valuable to also develop analytical derivations of finer-grained redundancy in the random walks.

Choosing the macroscopic feature

We note that the macroscopic feature we selected as a coarse-graining average of the system $V_t = \mathcal{F}(\mathbf{X}_t) = \frac{1}{N}\sum_{i=1}^{N} X_t^i$ also contains each individual component by summing. This is one possible explanation for the non-zero mutual information between X^i and V in non-interactive systems.

A possible way to continue this research is to test the effect of excluding term i from the average when computing each term $\sum_{i=1}^{N} I(X_t^i; V_{t'})$, and compute $\sum_{i=1}^{n} I(X_t^i; V_{t'}^{\{-i\}})$, where $V_t^{\{-i\}} = V_t - \frac{X_t^i}{N}$.

4.4 Results: Ornstein-Uhlenbeck processes

The study in the previous section found some unexpected behaviours of the emergence criteria. Nonetheless, while we chose to study the Gaussian walks because of their simplicity and the ease of developing analytical approximations of our measures, the system is a quintessential example of non-stationarity and requires some assumptions that are rarely made when statistically analysing data, even though many complex phenomena are actually non-stationary. For example, the study in the previous section benefited from somewhat large ensemble sizes to robustly approximate mutual information from data, but such data would likely not be available in experiments.

Next, we look at the Ornstein-Uhlenbeck (OU) processes introduced in Section 3.2.2, which differ from Gaussian random walks in one fundamental way: a friction-like restorative force k is added to each particle, so it is 'pulled back' towards its initial position. The walks can no longer diverge and their statistics become stationary, allowing the estimation of TDMI from single realisations and with additive time delays $\Delta t = t' - t$, which is more similar to how these measures would be applied in the real world.

From numerical simulations, we have found that a small restorative force $k = .01$ is sufficient to maintain the system's stationarity on the time scales being studied ($t = 2000$). We use the same system sizes N and couplings γ as before.

4.4.1 Null case: non-interactive systems

First we revisit the *null case* analysis done for the Gaussian random walks for the OU processes, namely observing the emergence criteria in non-interactive systems. In general the results are similar but the quantities themselves have much larger absolute values.

Mutual information

In some ways, the mutual information quantities behave similarly to the Gaussian random walks studied previously: the self-predictability of the centre of mass $I(V_t; V_{t'})$ and that of each particle $I(X^i_t; X^i_{t'})$ are independent of system size, all quantities decay over time, and the $I(X^i_t; V_{t'})$ and $I(V_t; X^i_{t'})$ quantities are again the same.

But some relevant differences are seen also: the TDMI quantities for $I(V_t; V_{t'})$ and $I(X^i_t; X^j_{t'})$ are almost two orders of magnitude larger than in the equivalent system size in the non-stationary walks, while the other quantities remain as small. Since the system is stationary, a future state is easier to predict using a past state, than in a non-stationary system, which may explain the increasing quantities.

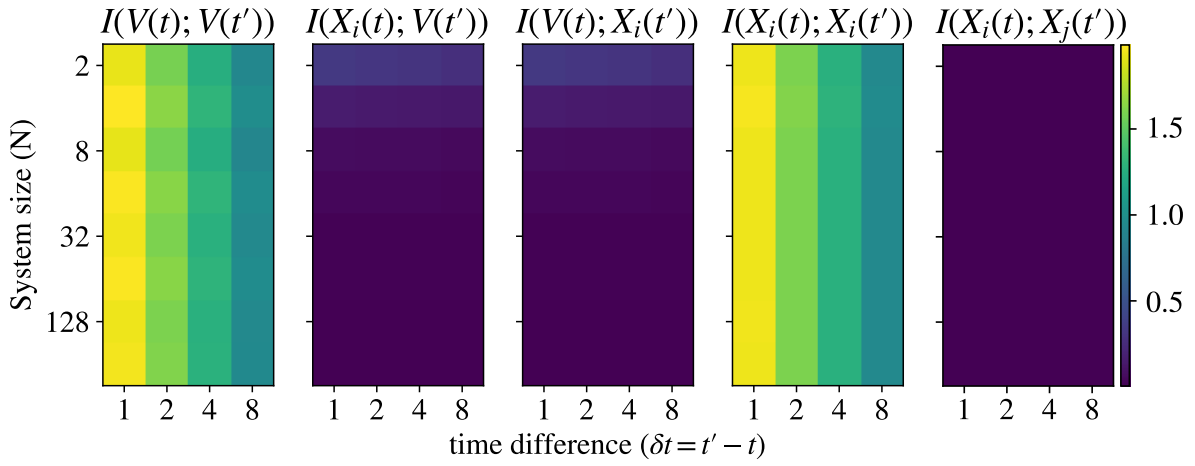


Figure 4.10: **Mutual information in non-interacting stationary Gaussian OU random walks**. The x-axis shows decay in the time difference $\delta t = t' - t$ between the two measurements for TDMI. The y-axis shows sytem size. The systems were simulated for $R = 20$ times for each parameter set, for a duration of $t = 2000$ steps, and the quantities shown are averaged over all realisations and all particles.

Unexpected emergence in non-interactive systems

We find the emergence criterion $\Psi > 0$ in this system for all the smallest time delays $\delta t = t' - t$, suggesting this system is *emergent*, even in lack of interactions. Moreover, it is much larger than in the non-stationary case. This is explained by the even larger difference between $I(V_t; V_{t'})$ and $\sum_i I(X^i_t; V_{t'})$ in this system.

Same as the non-stationary case, there is neither causal decoupling nor downwards causation, though $\Gamma \to 0$ as $\delta t \to \infty$ or $N \to \infty$, and thus the infinite system also shows causal decoupling.

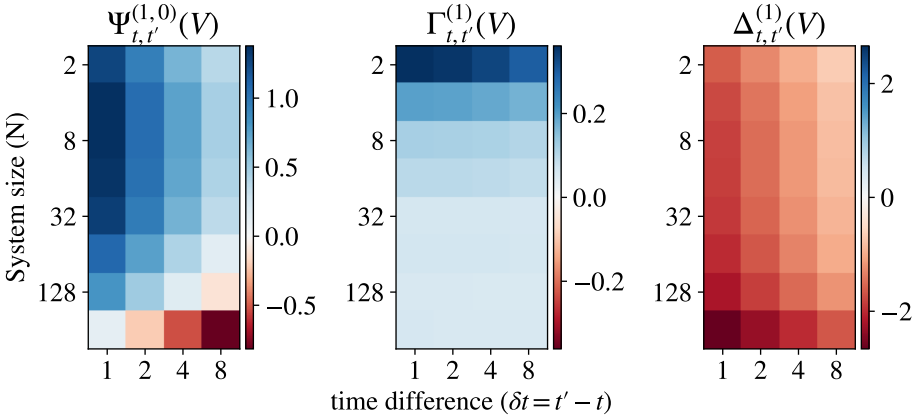


Figure 4.11: **Emergence criteria in non-interacting stationary Gaussian OU random walks**. The x-axis shows decay in the time difference $\delta t = t' - t$. The y-axis shows sytem size. The systems were simulated for $R = 20$ times for each parameter set and the quantities were averaged over the N components and the R simulations.

4.4.2 Interactive systems

As before, we study interactions by adding the elastic coupling parametrised by coupling parameter γ between neighbouring random walks.

Mutual information

Results show $I(X_t^i, V_{t'})$ and $I(V_t, X_{t'}^i)$ both increase with γ, as stronger interactions make the different parts more interdependent and therefore more predictable. The quantities are overall larger, about two orders of magnitude than the non-stationary Gaussian case. Also unlike in the Gaussian walks, the second quantity is only a little bit larger (around 10^{-4}) than the former, and the difference between them does not increase with γ.

The centre of mass term $I(V_t; V_{t'})$ remains independent of the system size or coupling, as expected, while that of each particle $I(X_t^i; X_{t'}^i)$ decreases as interactions are added. As expected, $I(X_t^i; X_{t'}^j)$ increases with coupling and decreases with system size.

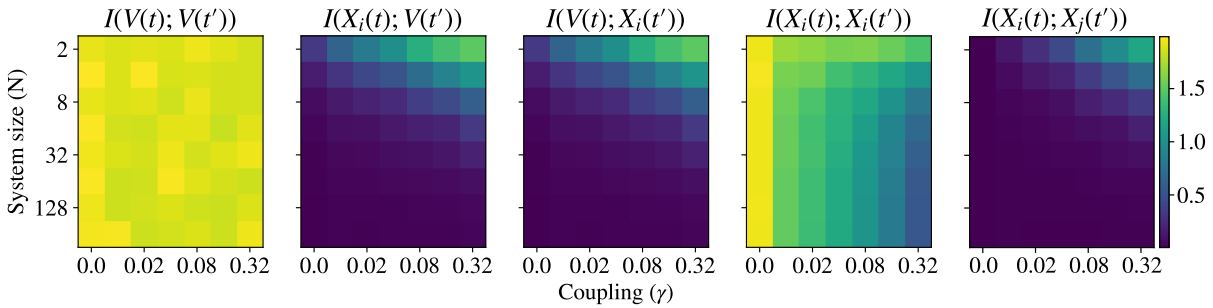


Figure 4.12: **Mutual information in interacting stationary Gaussian OU random walks**. The x-axis shows increasing coupling γ between neighbouring particles. The y-axis shows system size. Each value was computed by averaging the mutual information quantity across all components in the system, with the exception of $I(V_t; V_{t'})$, and all $R = 20$ simulations for each parameter set. The time difference is $\delta t = t' - t = 1$.

Emergence criteria

We move on to numerically study the $\Psi - \Gamma - \Delta$ criteria of emergence and how they evolve as more interactions are added between neighbouring particles.

The results are similar to the non-stationary case, with the emergence criterion Ψ also decreasing with γ, but much faster. This is due to the mutual information quantities in the sum being much larger than in the non-stationary case.

Γ behaves similarly to the non-stationary case, increasing with coupling, which is according to expectations, but also shows higher values. Meanwhile, the behaviour of Δ is again non-linear, first increasing with interactions then decreasing, while remaining negative.

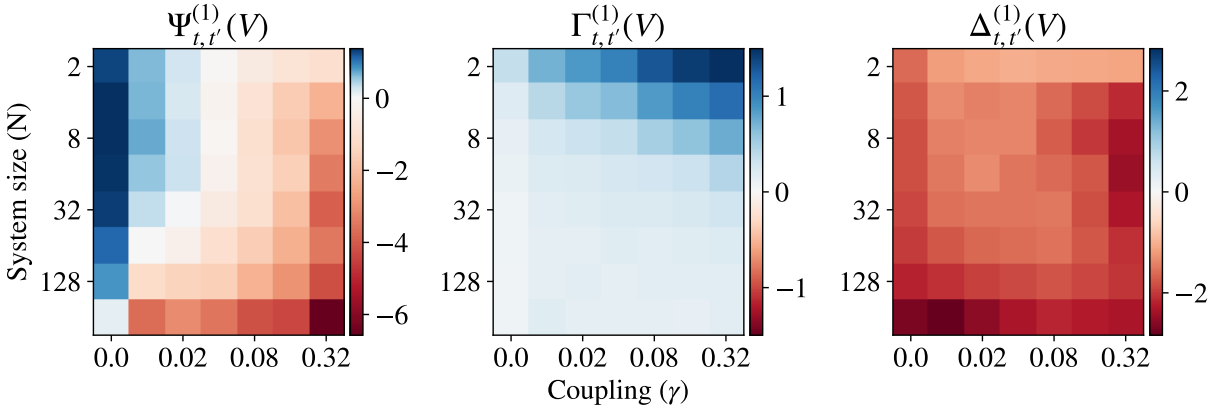


Figure 4.13: **Emergence criteria in interacting stationary Gaussian OU random walks**. The x-axis shows the coupling parameter γ. The y-axis shows sytem size. The time difference was set to $\delta t = t' - t = 1$. Systems were simulated for $R = 20$ times for each parameter set and the quantities were averaged over the N components and R simulations.

Redundancy

As expected, this system manifests more redundancy than the previous non-stationary one, with the quantities up to 4 orders of magnitude larger. Same as in the previous case, correcting the criterion with first-order redundancy only slows down the decreasing trend of the Ψ criterion.

We may now conclude that this behaviour of the Ψ emergence criterion is not caused by the non-stationarity of the data in the previous set of experiments.

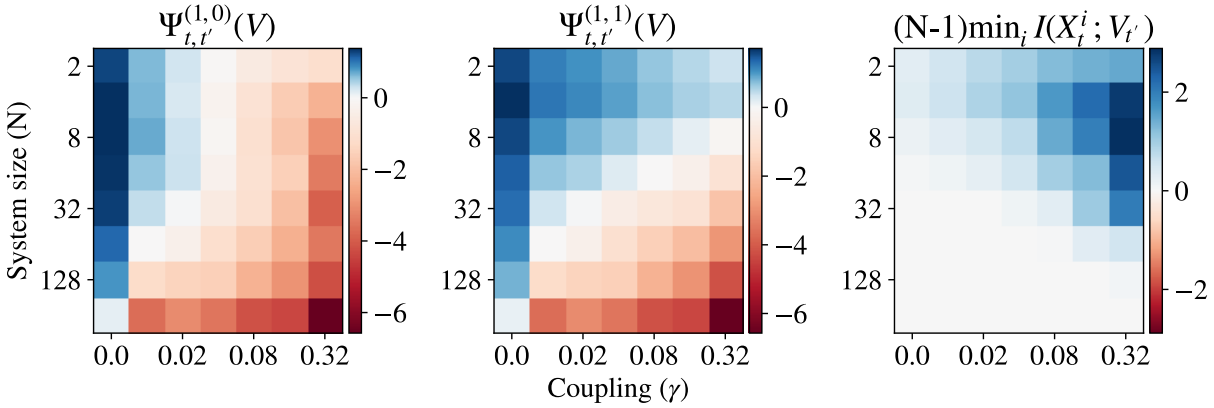


Figure 4.14: **Causal emergence and first-order redundancy in interacting stationary Gaussian OU random walks**. The x-axis shows the coupling parameter γ. The y-axis shows sytem size. The time difference was set to $\delta t = t' - t = 1$. Systems were simulated for $R = 20$ times for each parameter set and the quantities were averaged over the N components and R simulations. The redundancy in the third panel increases and as it is added to the $\Psi^{(1)}$ result in the first panel, we can approximate a more exact emergence criterion in $\Psi^{(1,1)}$, but this still behaves unexpectedly in the larger systems.

4.4.3 Limitations and future work

In this second set of experiments, the formalism of Ornstein-Uhlenbeck (OU) processes was used to construct a version of the Gaussian random walks with stationary dynamics. This was motivated by a limitation of the analysis in non-stationary systems, namely that the analysis pipeline used thousands of realisations and some assumptions which would be difficult to make in experimental data.

Nevertheless, due to time and compute limitations, we were unable to study emergence for $k > 1$ nor redundancy for $q > 1$, so we were unable to test if and for how much accuracy does the Ψ criterion become greater as interactions increase. Yet the stationary statistics make it less computationally demanding to study in the future.

Non-Gaussian statistics

The properties of Gaussian distributions make it simpler to derive analytical results as well as to estimate mutual information. Yet many complex systems are characterised by much more diverse statistics, especially in collective behaviour. Moreover, the results finding synergy in independent systems can be related to the properties of Gaussians and the concavity of the log function (Barrett, 2015), rather than to some underlying synergetic mechanism in the system.

Therefore it would be interesting to study random walks with non-Gaussian statistics, such as Levy walks, for example, as they have previously been related to animal movements (Benhamou, 2007), and to investigate whether the synergy persists in the null case for other statistical distributions.

Mechanism vs. behaviour

A most important thing to consider is again the interpretation of the measures. We had set out to use the $\Psi - \Gamma - \Delta$ criteria of emergence to detect collective behaviour where the agents behave as one with reduced degrees of freedom. Such behaviour is characterised by local coupling mechanisms that may even be considered higher-order when multiple components interact synergetically.

However, we have uncovered that in the case of the Gaussian random walks, regardless of their stationarity, the emergence criterion Ψ is always positive in systems without any mechanistic interactions. The criterion captures some collective statistical properties of the system in spite of no underlying collective behaviour. As before, we need to be careful of the distinction between behaviour and mechanism (Rosas et al., 2022), and potentially aim to disentangle it in the future through the use of measures that are more sensitive to mechanism, such as measures drawn from Amari's information geometry (Amari, 1982).

Higher-order measures

The $\Psi^{(1)}$ measure considers there to be emergence whenever there is synergy arising from two or more components. Due to computational limitations and the lack of a universal definition for multivariate mutual information, the criteria for emergence were strictly built from pairwise information atoms. This allows for an unambiguous definition of our measures and facile estimation, but unfortunately cannot identify synergetic relationships between three or more variables.

Future work should thus investigate emergence in larger groups of components rather than just using a pairwise mutual information, such as by using definitions of the emergence criteria for $k > 1$.

4.5 Results: Vicsek model

In the previous two sections, the emergence of collective behaviour in one-dimensional variables was investigated using the average or centre of mass of the variables. As variables are driven to be more similar to each other by increasing coupling, we have found the Ψ emergence criterion unintuitively decreases as more interactions are added.

However, the two random walker systems previously investigated are both characterised by an intriguing property: the fact that self-predictability of the centre of mass $I(V_t; V_{t'})$ is *not* affected by the interactions added between components, suggesting this may be an *autonomous* collective property. Yet in collective behaviour in general, we do not necessarily expect this. In the rest of this section, a more complex model of collective behaviour is investigated, namely the Vicsek model in two dimensions which can show *collective motion*, where it is more likely that the centre of mass is more affected by interactions.

While the main feature of the standard Vicsek model is the alignment of particles, we are interested in collective motion more generally, as the emergence of a flock structure where the particles move as one, and as such, can be described collectively by their centre of mass. In the case studies in Section 3.4, we have seen how various order parameters and statistical measures of alignment, aggregation and density can be used to describe the collective motion in this system, but also how each different quantity only captures a different aspect of it. We are, therefore, interested in applying the same method as in the random walks to test the system for emergent collective motion in general, in the hope that we can obtain a more agnostic and universal measure of *swarm behaviour* than using order parameters or statistical observables.

To explore the effect of various assumptions taken when estimating emergence in the system, but also to explore how robust the measures are for different kinds of behaviour, we employ realisations of the Vicsek model with periodic and reflective boundaries, which are characterised by different assumptions and types of collective motion.

An analysis of the mutual information between angle of direction and the emergence of the aligned phase in the Vicsek model is not undertaken, but an in-depth exploration can be found in the work of Barnett *et al* (Barnett et al., 2017; Brown et al., 2018, 2021a).

The work in this chapter is not meant to be an exhaustive analysis of the emergent properties of the Vicsek model, but rather another case study for information-theoretic measure of emergence. Interested readers should consult this thorough review of collective behaviour by (Vicsek & Zafeiris, 2012).

4.5.1 Case study: Vicsek model with periodic boundaries

We start with the model with periodic boundaries and metric neighbour interactions. This is the canonical version of the model, with a large body of work investigating its behaviour. To avoid boundary effects, the preprocessing step described in Section 4.2.3 is used.

For a more realistic simulation, small flocks of the same, low density are used. We selected three different kinds of phenomenological behaviour by varying the interaction radius proportional to the size of the environment:

- in the *disordered case* $r = 0$ and the system is in a chaotic state, lacking any tendency to aggregate or align; the analysis should reveal no emergence or pairwise mutual information between particles;
- in the rigid or *ordered case*, $r = 0.2L$ and the system is in an aligned state, with all particles going in the same direction; the analysis should reveal some degree of pairwise mutual information between particles and some degree of emergence
- in the *metastable case*, $r = 0.1L$ and the system is in an intermediary state, where the conflicting tendencies of order from the alignment and disorder from the noise create flock-like movement; this analysis should reveal the highest degree of emergence

We first evaluate each case with statistical observables: alignment v_a (Eq. 3.23) and dispersion $\delta_{\bar{\mathbf{x}}}$ (Eq. 3.25), shown in Fig. 4.15. The observables confirm an interesting side-effect of the intermediary regime in the Vicsek model, namely that the particles are more aggregated than expected as facilitated by the intrinsic noise on one hand, and coupling on the other (Yates et al., 2009).

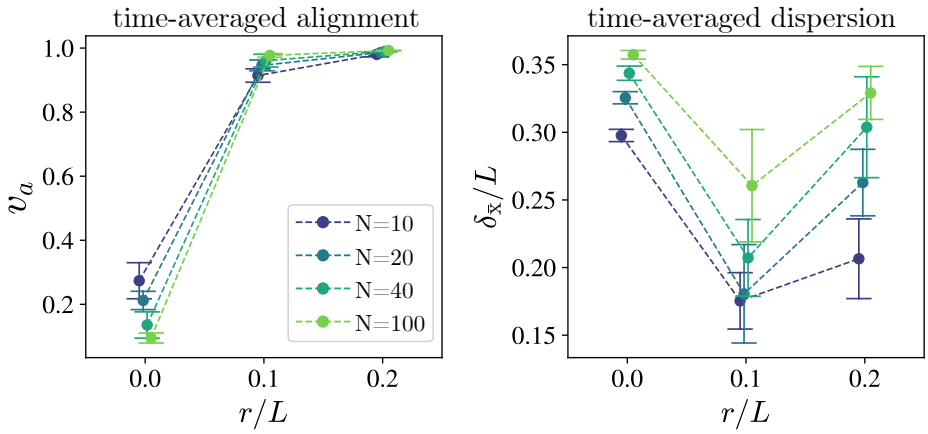


Figure 4.15: **Quantifying phenomenologically different behaviour in the Vicsek model with periodic boundaries and metric neighbours using statistcal observables**. The particles tend to align as the interaction radius is increased, yet in the regime just before alignment is met, the system manifests the most aggregation. The same behaviour occurs in all system sizes. Error bars represent standard error across simulations.

Mutual information

We first computed the time-delayed mutual information (TDMI) quantities corresponding to the components, the centre of mass, and how they predict each other's future states.

As expected, the mutual information between a component and itself $I(X_t^i; X_{t'}^i)$ reduces, while that with another $I(X_t^i; X_{t'}^j)$ increases, as the interaction radius is increased. We observe the same kind of non-linear behaviour in our statistical quantities: the intemediary regime selected as case study is closer to the ordered regime than to the disordered one.

The centre of mass term $I(V_t; V_{t'})$ is by far the highest quantity, and as hypothesised it peaks in the intermediary regime, which is characterised by more cohesion and the most complex behaviour.

We observe the same values $I(X_t^i; V_{t'})$ and $I(V_t; X_{t'}^i)$ which is unexpected. These quantities also increase with interaction radius, as hypothesised, but for the larger systems ($N > 10$) they peak before the aligment is reached. The behaviour is consistent amongst system sizes, with the larger systems showing slightly larger TDMI on average. The quantities are rather similar in spite of the different number of components. We can already intuit issues with interpreting the Ψ criterion for the larger system sizes, as the sum term $\sum_i I(X_t^i; V_{t'})$ will be disproportionately large compared to the self-predictability of the centre of mass.

Even in the non-interactive case, there is a small but non-trivial amount of mutual information both between different components, and between components and centre of mass. One reason for this may be that the mutual information captures the joint presence of the particles in the same space. In other words, the boundaries themselves reduce uncertainty to some degree. This is another example where high mutual information is not necessarily descriptive of a mechanistic relationship, but as long as we remain aware of its properties in two-dimensional spaces, its interpretation may become easier.

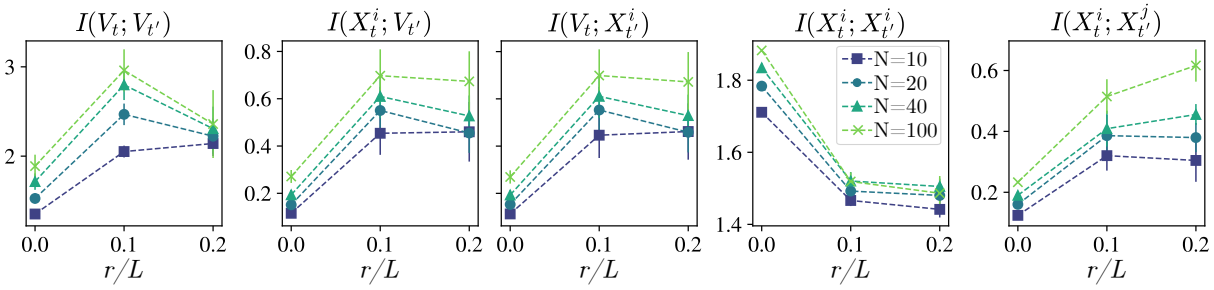


Figure 4.16: **Mutual information in the Vicsek model with periodic boundaries**. The quantities increase with system size and interaction radius, while the centre of mass term peaks in the most phenomenologically complex, intermediary regime. The positions of particles and centre of mass were preprocessed as distances from the centre of the environment. The time delay used was $\delta t = t' - t = 1$. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error over the $R = 20$ simulations.

Emergence criteria

When computing the emergence criteria, the issue of 'synergy-minus-redundancy' is apparent first. The criteria suggest there is neither any causal emergence, nor downwards causation, nor causal decoupling. The larger system sizes show negative emergence criteria almost inversely proportional to the number of components, and both Ψ and Δ continue to decrease as interactions are increased, contrary to intuition.

Similar to the random walks, we may explain the Ψ results by the fact that the sum of marginal mutual information increases much faster than the self-predictability of the centre of mass as interactions are added, and this effect is made worse as system sizes are made larger. Even more so than the random walks, this system can manifest very ordered states and is likely characterised by higher redundancy.

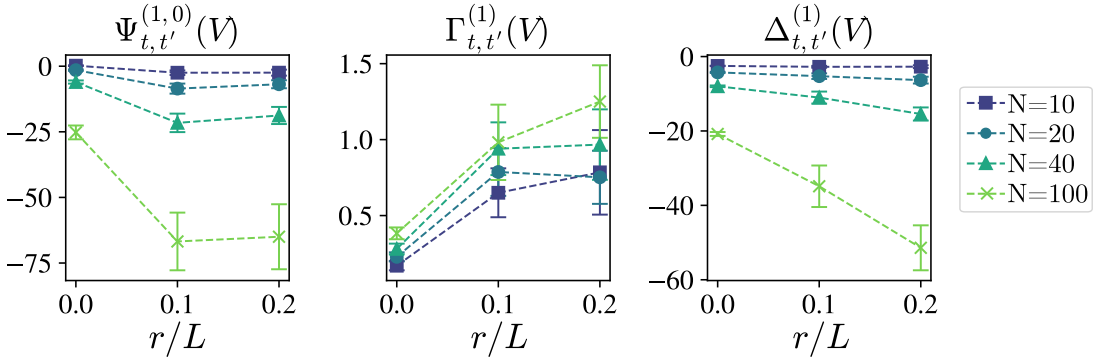


Figure 4.17: **Emergence criteria in the Vicsek model with periodic boundaries**. The time delay used was $\delta t = t' - t = 1$. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error over the $R = 20$ simulations.

Redundancy

To investigate how the results relate to redundancy in the system, the $N = 10$ case is taken, where $\Psi^{(1,q)}_{t,t'}$ is fully computationally tractable $\forall q < N$.

Applying the first correction for $q = 1$ produces a positive criterion for the non-interactive case, but not the others. As in the case of the random walks, the results are again non-intuitive: we expected Ψ to be negative in the non-interactive case; instead, it is largest for this regime.

Nonetheless, the redundancy amongst all components ($q = 1$), which is taken as the minimum mutual information multiplied by $N-1$, is proportional to the $I(X^i_t; V_{t'})$ term, and as hypothesised, is smallest for the non-interactive disordered regime and highest for the ordered regime. The non-zero redundancy in the non-interactive case reinforces the idea that indeed, there is underlying mutual information in the system which is not accounted for by any mechanistic explanation or dynamical behaviour.

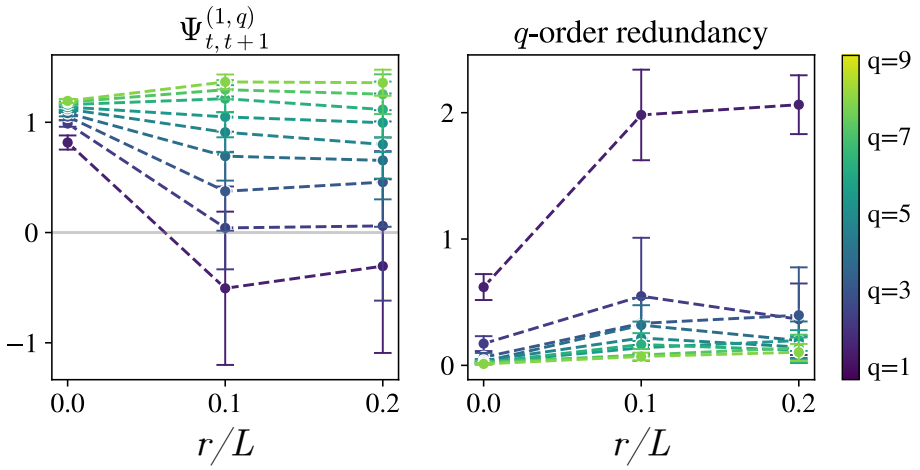


Figure 4.18: **Causal emergence and q-order redundancy in the Vicsek model with periodic boundaries**. The time delay used was $\delta t = t' - t = 1$. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error for the $R = 20$ simulations.

It is possible that generally in such systems with high redundancy, a higher degree q of accuracy is always required for the criteria to provide robust estimates. The second-order redundancy ($q = 2$), which intuitively represents the redundancy jointly provided by every group of $N - 1$ variables, peaks in the intermediary regime. Computing $\Psi^{(1,2)}_{t,t'}$ using the $q = 2$ redundancy yields a positive emergence criterion for all systems, while the most accurate Ψ criterion, $\Psi^{(1,9)}_{t,t'}$, where all the fine-grained redundancies have been accounted for, does behave according to our hypotheses.

4.5.2 Case study: Vicsek model with reflective boundaries

We continue with case studies from a phenomenologically different version of the Vicsek model. Reflective boundaries not only introduce more spatial aggregation in the system, but also allow avoiding issues related to periodic boundaries. Therefore we can study the positions directly and compare the results with those using the distance to the centre of the environment, and observe how the preprocessing affects our criterion estimations.

Apart from changing boundaries, we use the same parameters for the simulations. As before, we select three parameter ranges, yet we should note that the regimes of behaviour they create are much more complex than in the periodic bounds model:

- in the *non-interactive case* $r = 0$ and the system is in a chaotic state, lacking any tendency to align; nonetheless, the boundaries may induce a tendency to aggregate
- the *interactive case* does not necessatily mean a stable ordered phase will emerge; both $r = 0.1L$ and $r = 0.2L$ produce somewhat aligned behaviour, but there is much more variability, suggesting more heterogeneous collective behaviour.

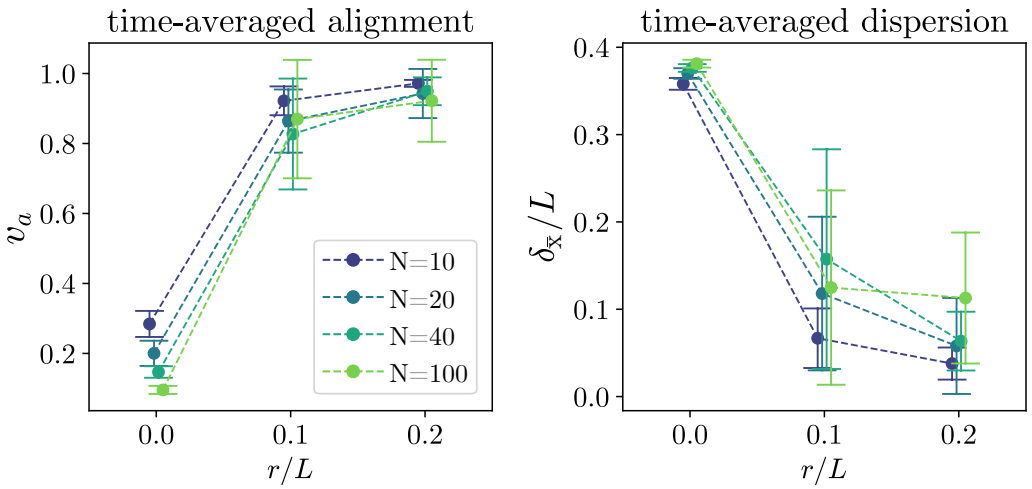


Figure 4.19: **Quantifying phenomenologically different behaviour in the Vicsek model with reflective boundaries and metric neighbours using statistcal observables**. The particles tend to align and become more aggregated as the interaction radius is increased. The same behaviour occurs in all system sizes. Error bars represent standard error over $R = 20$ simulations.

As we have seen in the case studies in Chapter 3, it is possible that one singular cohesive group never emerges in this system, due to the conflicting tendencies of order from the alignment rule and disorder from the noise, while the boundaries themselves introduce tendencies towards aggregation and against alignment As before, quantitative differences between the alignment and dispersion in the three regimes are shown in Fig. 4.19.

Mutual information

We compare the analysis using the same preprocessing pipeline as in the previous case study, with an analysis pipeline where the TDMI is estimated directly using the positions.

The first set of results can be compared directly to those obtained in the model with periodic boundaries. We find similar values for the self-predictability of the centre of mass $I(V_t; V_{t'})$ which is the highest quantity seen in the system, but now there is almost no difference between the two interactive cases. $I(X^i_t; V_{t'})$ and $I(V_t; X^i_{t'})$ are also the same in this system, and there is a lack of dependence on system size in the non-interactive case. Also, quantities are larger in this model and less proportional to system size, likely because particles are, on average, more aggregated because of the boundaries.

As expected, the mutual information between a component and itself $I(X^i_t; X^i_{t'})$ reduces, while that with another $I(X^i_t; X^j_{t'})$ increases, as the interaction radius is increased. Nonetheless the quantities behave differently than in the periodic boundaries experiment: the self-predictability of each component is smaller for the two interactive cases, and the mutual information between a particle and another is higher, again, likely because of the higher aggregation or less dispersion observed in their positions.

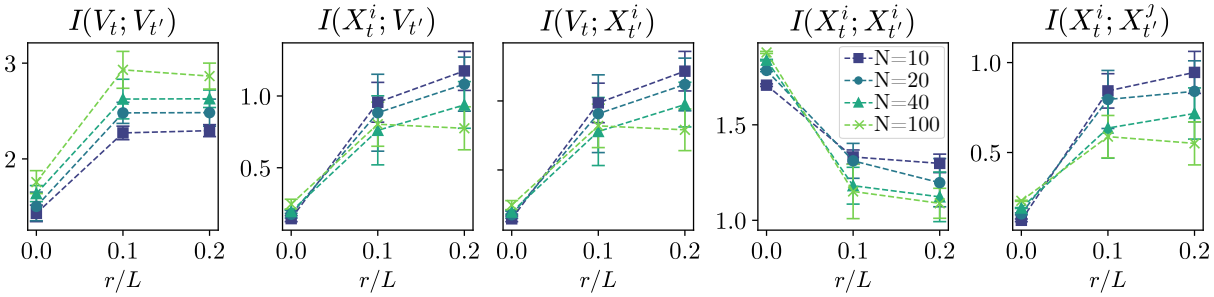


Figure 4.20: **Mutual information in the Vicsek model with reflective boundaries using preprocessed positions**. Quantities increase with system size and interaction radius, while the centre of mass term peaks in the intermediary regime. The positions of particles and centre of mass were preprocessed as distances from the centre of the environment. The time delay used was $\delta t = t' - t = 1$. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error over simulations.

When directly estimating TDMI on positions the quantities behave very differently. There is dependence on system size in all quantities, with larger TDMI in larger systems. All TDMI quantities are large, which was expected in the self-predictability terms $I(V_t; V_{t'})$ and $I(X_t^i; X_{t'}^j)$, but not in the TDMI between a particle and another $I(X_t^i; X_{t'}^j)$ in the non-interactive case.

A possible explanation is that positions carry more redundant information than distances, through their shared history and being confined in the same small, finite space. Moreover, two-dimensional data can carry more information than univariate data. This makes the quantities difficult to compare, and makes it extremely likely that the emergence criteria will be enormously negative for all systems without adjusting for redundancy.

Unexpectedly, when using positions, the TDMI of a particle with itself and with another are *not* affected by introducing interactions, apart from the latter quantity in the largest system. The centre of mass term $I(V_t; V_{t'})$ is highest on average in the intermediary case, and about the same in the more ordered and disordered cases, which is qualitatively different from how the TDMI behaved on the preprocessed positions.

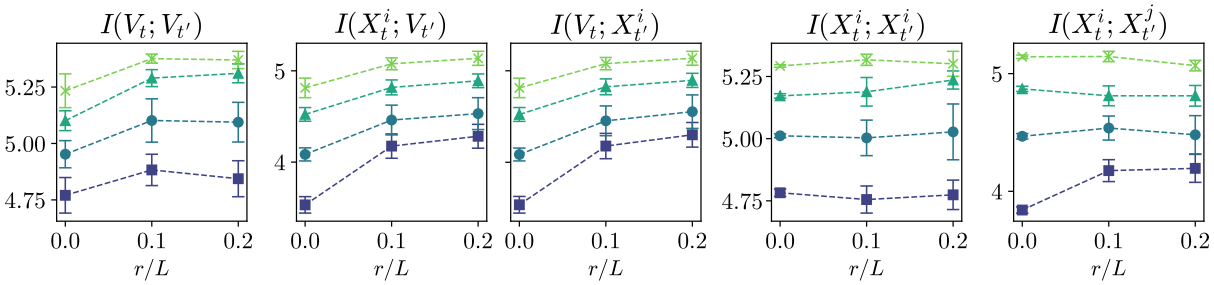


Figure 4.21: **Mutual information in the Vicsek model with reflective boundaries using raw positions**. The quantities increase with system size and interaction radius, while the centre of mass term peaks in the most phenomenologically complex, intermediary regime. The time delay used was $\delta t = t' - t = 1$. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error over the $R = 20$ simulations.

Emergence criteria

The results for emergence criteria using pre-processed positions are rather similar to those in the periodic boundaries case. Again, Ψ and Δ are smaller in the interactive cases, and we will explore the effect of more accurate estimators for Ψ momentarily.

As we intuited all Ψ and Δ are enormously negative when using positions, we will move directly into the study of redundancy for the Ψ criterion.

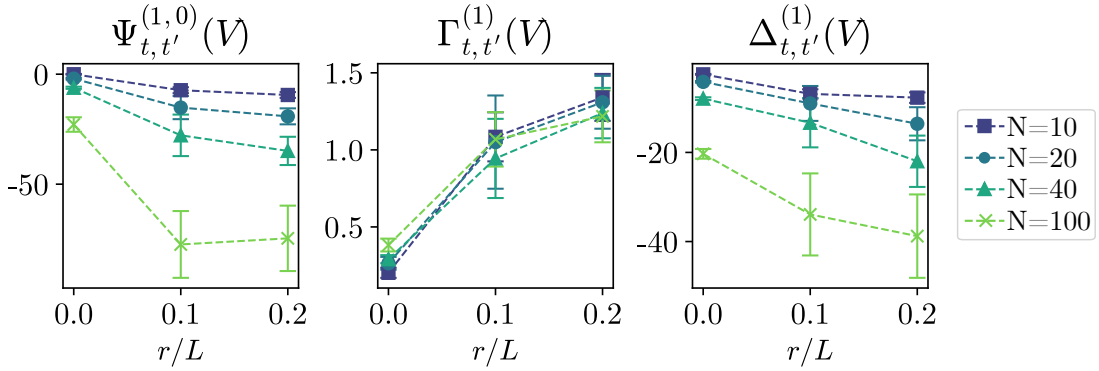


Figure 4.22: **Emergence criteria in the Vicsek model with reflective boundaries using preprocessed positions**. The time delay used was $\delta t = t' - t = 1$. Positional time series were preprocessed by taking the distance to the centre of the environment. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error over the $R = 20$ simulations.

Redundancy

We explored the redundancy in the tractable $N = 10$ case. In both cases the $q = 1$ redundancy is orders of magnitude higher than for higher q. There is much more in the interactive cases which is as expected, and three times more when using positions rather than distances.

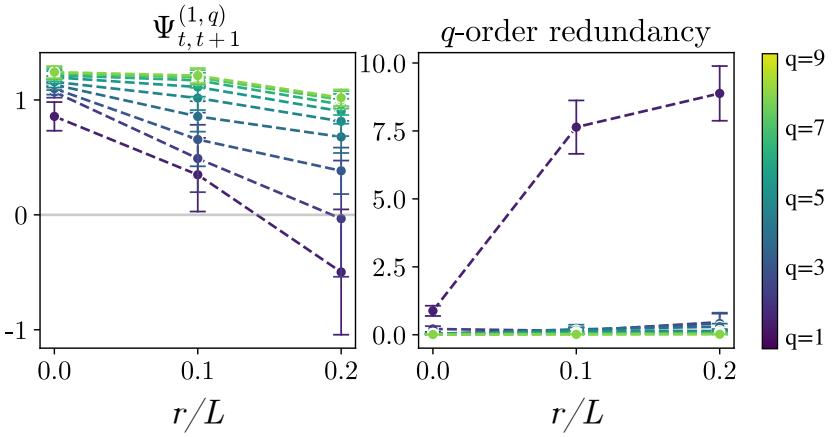


Figure 4.23: **Causal emergence and q-order redundancy in the Vicsek model with reflective boundaries using preprocessed positions**. The time delay used was $\delta t = t' - t = 1$. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error over the $R = 20$ simulations.

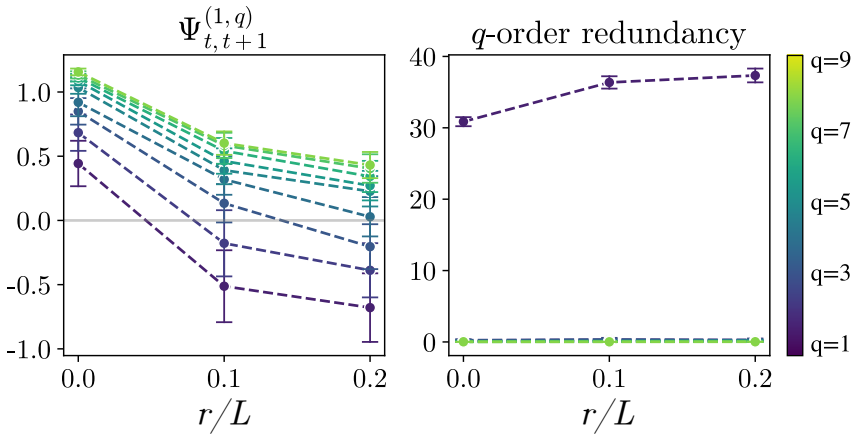


Figure 4.24: **Causal emergence and q-order redundancy in the Vicsek model with reflective boundaries using raw positions**. The time delay used was $\delta t = t' - t = 1$. Quantities shown are averaged over the N particles and $R = 20$ simulations. Error bars represent standard error over the $R = 20$ simulations.

Ajusting Ψ accordingly, the non-interactive case maintains the highest value for Ψ even after all redundancy corrections are applied. The criteria find some degree of causal emergence in all systems, though 'less' when there are more interactions. However, in this version of the model, it is easier to interpret these findings, as the spatial cohesion is more likely to be a result of the boundaries than the interactions between components.

4.5.3 Limitations and future work

We have used the Vicsek model to test the emergence criteria in a more realistic use case for collective motion and swarm intelligence. We intentionally considered small flocks at low density, and simulated them only a few times, so that we may relate our findings to collective behaviour seen in nature, as we will do in Chapter 5. Moreover, we computed the most accurate estimators of Ψ by accounting for fine-grained redundancy in the smallest systems, and found that in the Vicsek model with periodic boundaries, the most accurate criteria behave mostly as expected, with positive values for all conditions and the highest values for the interactive cases.

Nonetheless, the study is far from complete, and we outline a few more limitations and directions for future work in the Vicsek model below.

Statistical analysis

Since this chapter consists of case studies, we did not undertake a statistical analysis of the relationships between emergence criteria and quantitative observables. To better understand what kind of ordered behaviours or combinations thereof are captured by the emergence criteria, some linear mixed effect modelling with Ψ, Γ or Δ as target variables and observables as independent variables should be undertaken.

Accounting for redundancy

In both Vicsek model experiments, we studied the finest-grained estimation of $\Psi^{(1)}$, and found that the criteria behave as hypothesised but only when estimated with the highest accuracy. This analysis is difficult in larger systems, where the criterion quickly becomes computationally intractable.

Another way to address the problem of redundancy is by identifying where this redundancy comes from. As noted in Section 2.3, the TDMI cannot distinguish information that relates to actual interdependencies in the dynamics from shared information due to common history and input signals. In our case, we possibly found non-zero mutual information between components with no interdependencies because they are all confined to the same small range of values inside finite-sized, small environments.

An alternative solution may be provided by the use transfer entropy, which should be, in theory, less sensitive, and has been used in studies of the Vicsek model before (Brown et al., 2018, 2021a). As a decomposition of transfer entropy can exist using PID (Stramaglia et al., 2024), it may be possible to relate it to our emergence criteria, but this possibility, for now, remains only an idea.

Choosing different micro and macro features

A direction for future study is to use the groups' direction, or mean angular velocity, as a macroscopic feature V_t, and the orientations of the particle as the microscopic ones. This would also allow us to relate findings to aforementioned work using transfer entropy in the Vicsek model.

To do so, the estimation of joint probability distribution tables must take into account circular statistics. For example, an orientation of $0°$ and one of $359°$, which are close to each other, are numerically far away. This issue is also what makes the estimation of statistics of positions in spaces with periodic boundaries difficult. In future work, we may address it in two ways: either by using the whole velocity vectors of each component and that of centre of mass, or, similar to the preprocessing we employ for positions, to study the deviation from the zero angle, instead of the actual angle, in the time series representing the components.

Periodic boundaries

In the first experiment, the time series used were the first-order differentiated distances to the centre of the environment in order to account for periodic boundaries. This quantity captures relative movement, but valuable spatial information is lost, and it is unclear how this might affect analyses of more complex collective motion.

However, a recent improvement to the mutual information estimator proposed by (Kraskov et al., 2004) was suggested to account for estimating joint probability distributions in spaces with periodic boundaries, which could be used without requiring any data loss. We may even find this improvement to the estimator is robust when computing angles as well.

While advantageous for reducing the dimensionality of the data, using the distance to the centre of the environment to represent each component has another disadvantage: it is difficult to define practically in many cases, for example, on animal motion data where they are not confined to one space. As such, we should actually explore further possible improvements to TDMI estimation using the positions directly, as this would be the most agnostic way to apply the measures.

Data shuffling

Finally, we should mention another way to test the robustness of the emergence criteria by creating so-called *surrogate data* by delaying each time series by some random time increment. This should be done without shuffling each time series, so the temporal correlations between variables is broken, but not the auto-correlations within the same variable. Across many fields, this is a method used to test robustness of statistical inference or predictions on time series. Basically, modifying the data in this way should provide another way to remove any interdependencies and create a random null case against which we can compare results.

In the non-interactive systems, we'd expect the measures not to differ between shuffled and non-shuffled data as the signals are all random and there are no interactions and no spatiotemporal patterns to speak of. But in the interactive case, once the putative interdependencies are removed by shuffling the data, the emergent behaviour should be gone and the measure should reflect that.

This method is not necessarily required for the current modelling study, as we already have a way to establish an uncorrelated null case (e.g. by disabling interaction mechanisms). But is extremely important to experimental studies, where lack of knowledge of underlying mechanisms frequently impedes constructing a proper null case. Instead, the null or random case to compare measures against can be constructed by shifting the time series around so they no longer correspond to the same moment in time.

This method is often used in neuroscience studies, by shuffling the epochs like in (Varley et al., 2023), and was used to measure synchrony in collective movement of concert audiences: there is higher than random synchrony when they listen to music (Tschacher et al., 2023).

4.6 Conclusion

In this chapter, variations on two simple models of complex systems were used as test-beds for the $\Psi - \Gamma - \Delta$ criteria of emergence: non-stationary and stationary variants of Gaussian random walks, and the Vicsek model with periodic and reflective boundaries. While extremely promising as a substrate-indepedent theory of emergence, the criteria have shown unexpected behaviour in some simulations.

First, in both stationary and non-stationary variants of the Gaussian random walkers, the criteria found a positive $\Psi^{(1)}$ in finite-sized, non-interactive systems, suggesting the centre of mass of components is a causally emergent feature in spite of the lack of coupling between components. The result was confirmed both numerically and analytically. This is unexpected, as the center of mass of non-interacting constituents is not 'emergent' in any sense that involves interactions between components.

Instead, this is an example in which higher-order interdependencies do not correspond to higher-order mechanistic interactions: Ψ captures statistical dependencies between the components of a system, dependencies which can be present even for non-interacting constituents, or in other words without any coupling mechanism actually present (Rosas et al., 2022). Moreover, this is made more difficult by a known fact of Gaussians, namely that independent Gaussians show net synergy due to their mathematical properties rather than any mechanistic explanation (Barrett, 2015).

The second unexpected behaviour was the Ψ and Δ criteria of causal emergence and downwards causation decreasing as more interactions were added in the systems, contrary to intuition: an increase in emergence is expected when the interactions become stronger, as the components become mechanistically inter-dependent. The time-delayed mutual information (TDMI) quantities forming the criteria behaved mostly as expected, so we tried to ascribe the latter behaviour of the measures to properties of 'synergy-minus-redundancy' measures. Namely, that when the redundancy in a system greatly exceeds the synergy, the criteria do not detect the emergent behaviour.

In both random walkers and the Vicsek model, studying the minimum mutual information between all components has confirmed that there is a large amount of redundancy in this system, which can be explained by the components being very simple and identically distributed. By adjusting the threshold for emergence using the redundancy, we obtain better estimates for our criteria. Nonetheless, we need to remain aware that two variables showing mutual information with a target is not necessary redundant information, because the two variables may provide different information which MMI-PID may conflate.

One property of TDMI is that it cannot distinguish between information that relates to actual interdependencies in the dynamics, from shared information due to common history and input signals. This is important when studying collective motion, as there is a high amount of shared information in spatial data which could be a result of being confined in the same boundaries, as seen in the Vicsek model case studies. This effect becomes even more prominent when positions are used directly for the estimation of TDMI, rather than distances. Quantifying the redundancy can help mitigate this problem.

Another aspect which will become relevant in explorations of complex systems in nature is that components may have non-linear couplings and show synergy in larger groups rather than just in pairs. Using $\Psi^{(1)}$ would not capture such *higher-order* effects. For this reason, a definition of emergence as pairwise synergy may be lacking in practice, and some higher-order measures should be investigated in the future.

In the Vicsek model with periodic boundaries, the most accurate estimate for $\Psi^{(1)}$ was found to correspond to mechanistic ideas of collective behaviour of interest: the highest $\Psi^{(1,N-1)}_{t,t'}$ corresponds to the intermediary regime which shows the most complex flock-like behaviour resulting from the conflicting tendencies towards disorder induced by the individual components and those towards collective order induced by the interaction rules. However, this was only computed for the smallest case of N=10 particles, and only the most accurate Ψ behaved according to our hypotheses, but not without also showing emergence in the non-interactive case.

These unexpected results can pose serious practical issues when investigating collective behaviour. When applying the above measures to data sets for which a mathematical model is missing, we will have difficulties in distinguishing a mechanistic, causally emergent collective property with its own integrity, from a situation where a collective variable V exhibits emergent features according to the propositions (1), (2) and (3) as a mathematical consequence of V being a combination of constituent variables. This is important because some theories of causal emergence define emergent properties as a coarse-graining function over the components (Comolatti & Hoel, 2022; Yuan et al., 2024).

The numerical studies and comparisons in this chapter can constitute a set of warning signs, guidelines and considerations for the robust application of information-theoretic measures to time series data of complex system. Equipped with these insights, in the next part of the thesis, we will try these criteria on data.

Part II

Emergence of collective motion in multi-agent systems

Chapter 5

Case study: schooling and flocking

Chapter Summary

Collective motion, as a special case of collective behaviour, is a quintessential example of emergence, present at all scales in nature, from bacteria to birds, fish and herd animals, to humans. In this section, efforts to quantify emergence as well as interactions in collective movement in nature are reviewed and related to results in theoretical models, alongside with motivations for and ramifications of its study. The rest of the chapter shows results from applying information-theoretic methods tested on simple models on experimental movement trajectory data from schooling fish, as well as a more complex multi-agent model of flocking, the Reynolds model.

5.1 Collective motion in nature

Arguably one of the most important aspects of collective behaviour in the animal kingdom is *self-organisation*, where patterns emerge at the group level from the local interactions between individuals, rather than from a form of central control, authority, or *a priori* planning (Hemelrijk & Hildenbrandt, 2012; Shaw, 1978; Sumpter, 2006).

The study of complex systems so far has shown that collective behaviour can be emergent in many different ways. It can be characterised by a smaller or larger degree of self-organisation, as well as an interplay between intrinsic dynamics like the interactions between agents (for example, how a bird follows its neighbours in flight) and extrinsic drivers (a predator suddenly attacking the flock). Alternatively, this can be also seen as the interplay between following pre-established rules and improvisation in novel situations.

Collective motion is a special case of collective behaviour, where all of these interesting local and group dynamics manifest aplenty. In the case of animals, this movement is connected to everything relevant in their lives. As hinted at in the introduction, avoiding predators, foraging and migration are a few obvious examples where being together is advantageous for animals, and where collective behaviour arising by self-organisation is a necessity for survival (Sumpter, 2006). Herds of sheep, for example, show intermittent behaviour, alternating between slowly spreading in space to graze more efficiently, and aggregating back again to protect themselves from predators (Ginelli et al., 2015). Reindeer sometimes run in a cyclone configuration, milling around their young who are protected in the middle (Espmark & Kinderås, 2002). While fireflies putatively synchronise their flashes in order to make it easier for other fireflies to see each other, fly together, and find mates at night (Copeland & Moiseff, 1994; Moiseff & Copeland, 2010).

But movement can act as a proxy for so much more. Social and familial groups may be encoded in the way animals move, by choosing to stay close to kin, something sheep, some species of fish and birds, and dolphins do. In reverse, modelling animal behaviour while taking into account social networks produces more accurate simulations of their collective, emergent actions (Bode, 2011). Animals can also encode their collective memory through their movement, for example by remembering past group configurations (Couzin et al., 2002). Another example is the 'collective memory' developed by slime moulds, which forage as individuals, then exchange information via cellular signalling in order to compute shortest paths to food (Sims & Kiverstein, 2022).

One of the reasons to study collective motion as an emergent phenomenon is the simplicity of the time series involved. The trajectories produced by birds and fish are not fundamentally different from those shown by the Vicsek model. On the other hand, this behaviour is incredibly rich, and maps to important social and even psychological as-

pects of the animals that are much more difficult to study. Understanding how animals move together may also reveal how they organise their social structures, how they make decisions, how they plan collective action and how they respond to danger.

At the level of local interactions, the study of swarm intelligence has made great leaps using the conceptual framework of emergence. Following many years of mathematical modelling and comparing emergent behaviour in simulation and experimental research, scientists have come to agree that the collective behaviour of animals emerges from local interactions between neighbours. For example, the alignment rule in the Vicsek model is seen in the real world: recently, a state-of-the-art study has confirmed that following neighbours is one of the leading mechanisms of animals self-organising (Oscar et al., 2023). Using two-photon mesoscopy, the reseach team was able to monitor brain activity of zebrafish in a specially designed, virtual reality (VR) tank. By modelling VR fish with controlled movements, they were able observe both behaviour and neural responses in the real fish, and to propose a neural model of how the fish decide the direction of swimming based on the movement vectors of its two closest neighbours.

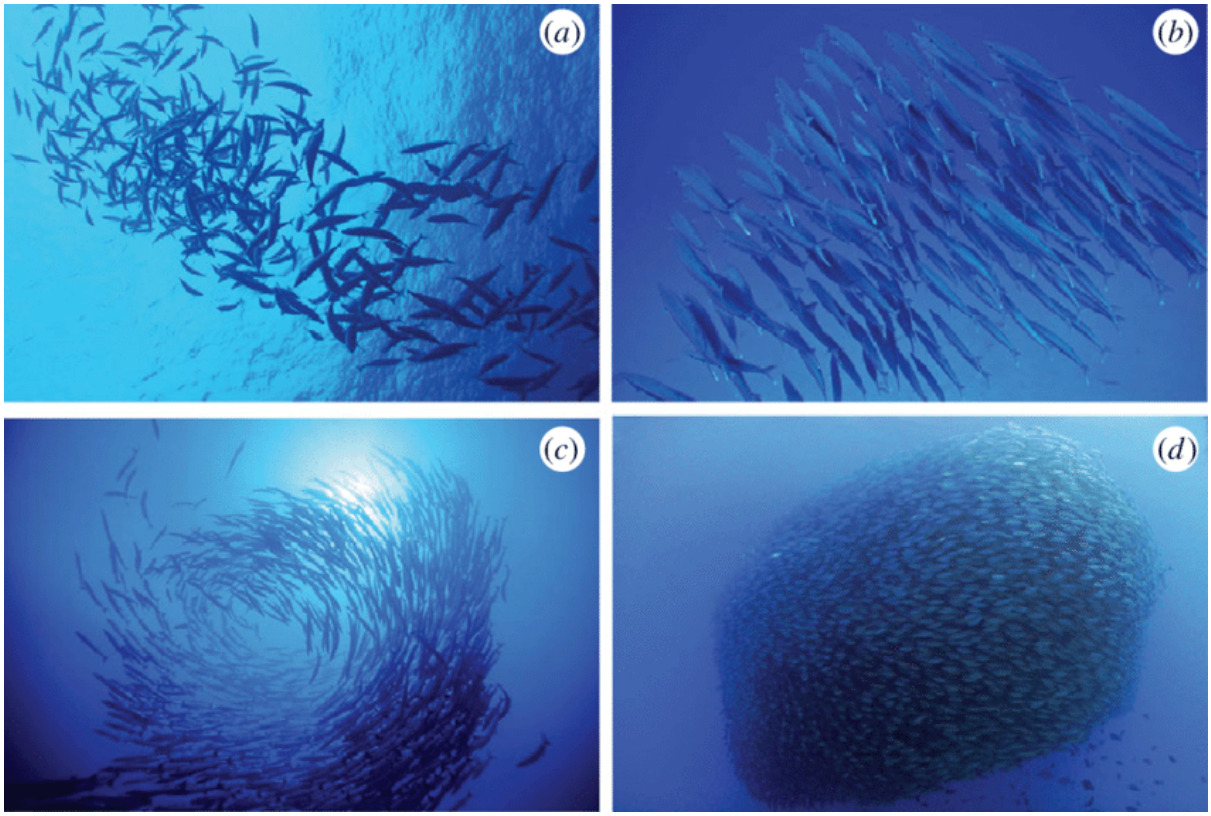


Figure 5.1: **Different types of collective movement in schooling fish** reproduced from (Lopez et al., 2012) (a) flock-like movement with high polarization but some cohesion. (b) aligned parallel movement with low polarization. (c) 'milling' movement with high angular momentum and high polarization. (d) highly aggregated group movement known as a 'bait ball', characterised by very high cohesion.

As interactions are slowly being demystified, the quantification of emergence in these systems remains a non-trivial task. Collective motion is encountered in the natural sciences by many names: swarming, schooling, shoaling, flocking, to name a few, depending on the animals and the type of movement. Many quantifiers exist for different types of collective movement, and we have seen some of the observable statistical quantities in Chapter 3. These observables have been used to define a number of spatiotemporal configurations with some rigurous definitions (Couzin et al., 2005; Lopez et al., 2012). These configurations have been observed in models as well as data (Fig. 5.1). For example, high angular momentum and high polarization may describe a cyclone configuration (Fig. 5.1a), and low angular momentum and low polarisation may describe an aligned and highly parallel motion (Fig. 5.1b) (Couzin et al., 2005), reminiscent of the aligned phase of the Vicsek model investigated in the previous chapter.

While visually and qualitatively different across species, and even amongst behaviours shown by a single species, many dynamical patterns created by animals in motion can be characterised by universal mathematical properties: we have mentioned the emergence of scale-free correlations in both birds and fish (Cavagna et al., 2010; Múgica et al., 2022), but also criticality (Calovi et al., 2015; Mora & Bialek, 2011) and symmetry-breaking (Melfo, 2017). These same properties are shared by self-propelled particle systems in the critical regime (Ginelli, 2016). Unfortunately, measures based on correlation functions or order parameters are not very robust unless the animal groups are very large, and tend to be more useful towards simulation studies, where large groups are much easier to observe.

On the other hand, studies on simulated or experimental data using Granger causality (Seth, 2010), information theory (Brown et al., 2018) and measures of emergence from the study of consciousness (Niizato et al., 2024; Rosas et al., 2020a) are gaining attention. There are many advantages to using measures of emergence for the study of collective animal behaviour: they are more robust with small amounts of data; there is no need to choose an order parameter; and it is likely that the same methods can identify many qualitatively different types of behaviour.

Therefore, the goal of this chapter is to use the $\Psi - \Gamma - \Delta$ information-theoretic criteria of emergence (Rosas et al., 2020a) to characterise complex collective motion, while keeping cautious about interpreting the results in light of the findings presented in Chapter 4. We begin by using data from a simple model of flocking behaviour introduced by (Reynolds, 1987), then proceed to test our measures on real-world movement data of fish from (Niizato et al., 2024).

5.2 Methods

In both our case studies, we consider a system composed of 10 interacting agents. The system is measured regularly over time, and the results of those measurements are denoted by $\mathbf{X}_t = (\mathbf{X}_t^1, \ldots, \mathbf{X}_t^n)$.

We select the centre of mass of the flock as a coarse-graining function or aggregate property; this gives $\mathbf{V}_t = \frac{1}{N}\sum_i \mathbf{X}_t^i$, the same aggregate property used also in Chapter 4, Eq. 4.4. This matches the preconditions for the theory of causal emergence of (Rosas et al., 2020a), which is described in Chapter 2.3: namely it is an aggregate property affected by observational noise which is independent at time t from the state of the system $\mathbf{X}_{t'}$ at a future time.

The data preprocessing and information-theoretic analysis code were implemented in `python` using `numpy` and bindings using the package `jpype1` to a Java library for the estimation of information dynamics (Lizier, 2014). Details are in the rest of this section.

5.2.1 Simulation: Reynolds flocking model

To relate the methods to previous results, we use the improved estimators to study a simplified version of the famous flocking model by (Reynolds, 1987), used in simulation studies of swarm intelligence, computer games, and animation sequences in movies like the herd in Lion King (2001). One of the first models to realistically simulate the phenomenology of collective motion in flocks, schools and herds, the Reynolds model defines a multi-agent system of "boids" ("bird-oid objects") which move and interact with their neighbours on a given radius r, following three different types of **social forces**:

- *aggregation* (a_1): a tendency to fly towards the centre of the flock
- *avoidance* (a_2): a tendency to avoid hitting the nearest neighbour
- *alignment* (a_3): a tendency to align direction with neighbours on a radius r

The model is realistic to describe collective animal behaviour, insofar as there is a degree of momentum in their motion: forces are implemented as "steerage" towards or away from the position or direction of others. This is different from the Vicsek model, where each particle simply oriented itself towards the average direction of neighbours. This model creates more realistic spatial patterns of flocking behaviour, and may also be closer to the temporal patterns emerging in the movements of real animals, depending on parameter choices.

The simulation data is the same as in the original work (Rosas et al., 2020a): $N = 10$ boids

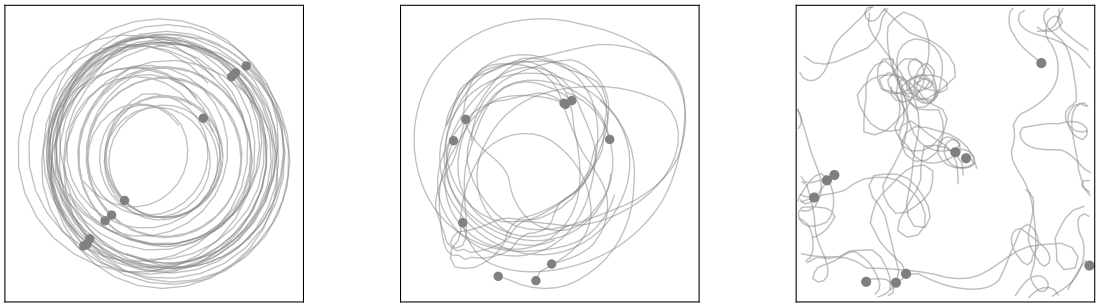


Figure 5.2: **Phenomenonologically different instances of the Reynolds flocking model under increasing avoidance.** The three simulations are computed with the same aggregation and alignment parameters, varying avoidance (a) No avoidance ($a_2 = 0$): we observe very rigid milling behaviour which should manifest very high redundancy. (b) Intermediary avoidance ($a_2 = 0.1$): reminds of a flock of birds flying around their nest, or fish in a tank. This behaviour should be characterised by a balance of shared and synergetic information. (c) Higher avoidance ($a_2 = 0.2$): almost random behaviour, which should be characterised by small redundancy and small synergy.

were simulated in *two dimensions* only, on a torus of side length $L = 200$, initialised with the same velocity, with random initial orientations and positions; the interaction radius was taken as $r = 20 = L/10$. The aggregation ($a_1 = 0.15$) and alignment ($a_3 = 0.25$) parameters were kept fixed, while the avoidance parameter was varied ($a_2 \in \{0.0, 0.1, 0.2\}$) to create more or less 'rigid' flocks. The system was simulated producing trajectories of length $T = 5000$, and for statistical robustness $R = 20$ realisations were produced for each set of parameters.

Increasing the avoidance parameter (a_2) will encourage the boids to distance away from each other, and as such, will decrease the effect of the alignment force. Manipulating this parameter produces qualitatively very different behaviours: for low avoidance the boids gather in a cyclone, known as milling behaviour; for high avoidance, the boids no longer fly together; but for an intermediary parameter one can observe a chimeric behaviour where the conflicting tendencies between order and disorder create an adaptive and complex behaviour similar phenomenologically to we see in nature. Snapshots of characteristic collective behaviour are in Fig. 5.2 below.

5.2.2 Experimental data: schooling fish

As a secondary case study, we look at small schools of $N = 10$ *ayu* (Japanese sweetfish) who are swimming together in a tank. The data was obtained experimentally by Niizato *et al* (Niizato et al., 2024). 10 fish (7-15cm long) were placed in a $3m \times 3m$ tank of 15cm deep, and filmed from above to obtain trajectories that appear *two-dimensional*.

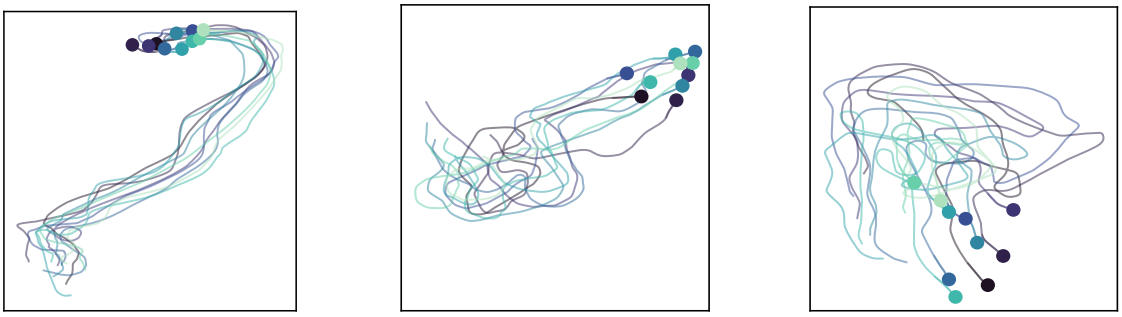


Figure 5.3: **Collective behaviour in schooling fish data with varying degrees of aggregation**. Trajectories of 200 timesteps (24 seconds) of schools of 10 fish from three different groups show increasing degrees of dispersion, or decreasing degrees of aggregation.

The fish were tracked for 8 to 12 min at 20 frames per second using computer vision, producing time series around $T = 10000$ in length. From the data made publicly available by the research team, we selected the first $T = 10000$ timesteps in six of their data sets. Please see (Niizato et al., 2024) for further experimental details.

The collective behaviour shown by the schooling fish is easily visible with the naked eye in Fig. 5.3. The behaviours persist for the entire time series, and all six data sets show the same kind of dynamical behaviour, but with different degrees of aggregation, from swimming very close to each other, resulting in a more rigid formation with tightly-knit trajectories, to swimming farther away and sometimes abruptly changing direction.

Unlike data resulting from a model simulaton, in experimental data we cannot as easily classify the collective behaviour in different regimes as we cannot rely on any knowledge of their interactions. Nevertheless, we may attempt to compute various statistics which provide a quantitative way to differentiate between the qualitatively different behaviours, for example, by estimating the density or spread between the fish, using statistical quantities introduced in Chapter 3.4:

- mean distance to nearest neighbour $\tilde{\delta}(t)$ (Eq. 3.26)
- spread from centre of mass $\delta_{\bar{\mathbf{x}}}(t)$ (Eq. 3.25)
- mean number of neighbours on a radius r $\tilde{\rho}(t)$ (Eq. 3.27)

Distances are computed for each fish, averaged over $N = 10$ fish, and normalised by the size of the fish tank. Instantaneous values are computed at each time t to produce a time series, then averaged to produce one value for each group of fish. We should note the density-related measure of neighbours on a given radius can be related to assumptions regarding interactions between the fish. We have selected the radius r for analysis to be proportional to the interaction radius set in the Reynolds model, namely, 10% of the size of the tank. All computations were performed in `numpy`.

5.2.3 Data preprocessing

We preprocess spatial coordinates by computing the distance from the centre of the environment in which the agents move, and first-order differentiating the resulting time series. Please see Section 4.2.3 for details. All computations were performed in `numpy` using `numpy.linalg.norm` to compute distances and `numpy.diff` to differentiate time-series.

The motivations for this are multiple: first of all, to reduce the dataset dimensionality; secondly, to avoid difficulties in estimating circular positional statistics in a space with periodic boundaries and provide robustness against boundary effects; and finally, to reduce some inherent mutual informaton which exists in multivariate and dependent spatial variables, since the centre of mass itself is mean of all the positions and as such already contains some information about each individual position. Data preprocessing and effects on the information-theoretic quantities have been thoroughly discussed in Chapter 4.

5.2.4 Emergence criteria calculation

We use the same information-theoretic criteria for emergence (Rosas et al., 2020a) introduced in Section 2.3 and investigated in Chapter 4 to test for spatial emergence in the trajectory data. The criteria are used to test whether the centre of mass of the group is causally emergent from the individual positions of the boids, using the information-theoretic quantities Ψ, Γ and Δ.

Mutual information was estimated using JIDT (Lizier, 2014), and more specifically the `ContinuousMutualInfoCalculatorMultivariateKraskov1` which implements the histogram-based estimator in (Kraskov et al., 2004), and the time delay for computing the time-delayed mutual information (TDMI) between two time series was set to $\Delta t = t' - t = 1$.

The rendundancy function chosen was the minimum mutual information (MMI). To compute redundancy of order q, first we compute the intersection information, defined as the MMI across information atoms corresponding to groupings of sources X^i of size $N - q + 1$. The analysis code for the redundancy decomposition was provided by the author and is publicly available at (Sas, 2024). The code was tested and verified against peer-reviewed discrete information theory package `dit` (James et al., 2018a), confirming a correct derivation and implementation of the fine-grained PID lattice required by estimating intersection information.

5.3 Results

5.3.1 Reynolds flocking model

We simulated three different sets of configurations with different phenomenological behaviours, producing 60 sets of 10 trajectories of T=5000 timesteps. Ψ, Γ and Δ were computed using the preprocessed individual's trajectories as "micro" components of the system, while the group's centre of mass was used as a coarse-grained property to act as a candidate for an emergent feature. The time difference between the two time series was set as $t' - t = 1$.

Similar to previous work (Rosas et al., 2020a; Seth, 2010), we hypothesised that the intermediary configuration manifests the highest degree of emergence. Furthermore, we hypothesise that the lowest avoidance configuration ($a_2 = 0$) is characterised by higher redundancy than the others, due to the similarity in the motion of boids.

This was suggested in previous work: the low-avoidance scenario is dominated not by a reduction in synergy, but by an increase in redundancy, which effectively increases the synergy threshold needed to detect emergence. This scenario becomes apparent having computed redundancy quantities in the system: the $q = 1$ redundancy computed by the minimum mutual information (MMI) between all the boids and their centre of mass is used effectively to adjust the synergy threshold for emergence (Fig. 5.4).

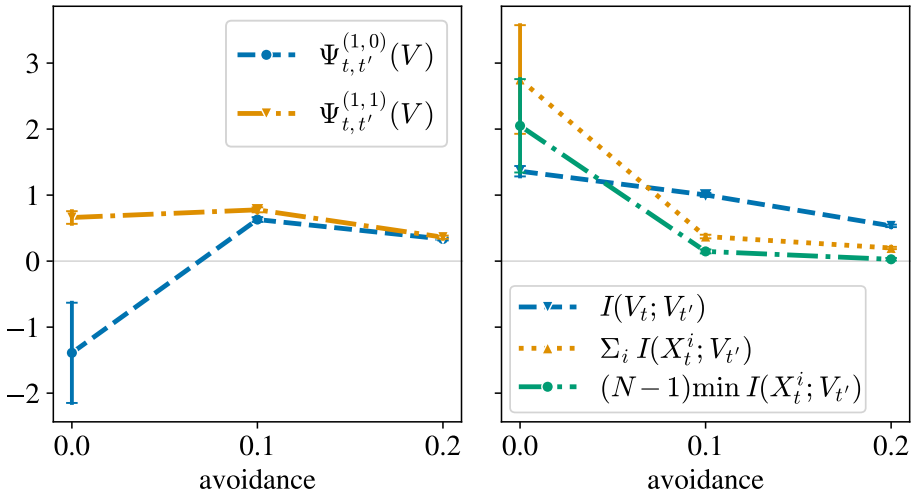


Figure 5.4: **Causal emergence and first-order redundancy in Reynolds' model.** $\Psi^{(1,0)}$ peaks in the intermediary state, and is negative in the low avoidance scenario. But when considering the first-order redundancy in the system in computing $\Psi^{(1,1)}$ the criterion also correctly finds the low-alignment case state as emergent. Error bars show standard error across $R = 20$ simulations for each parameter set.

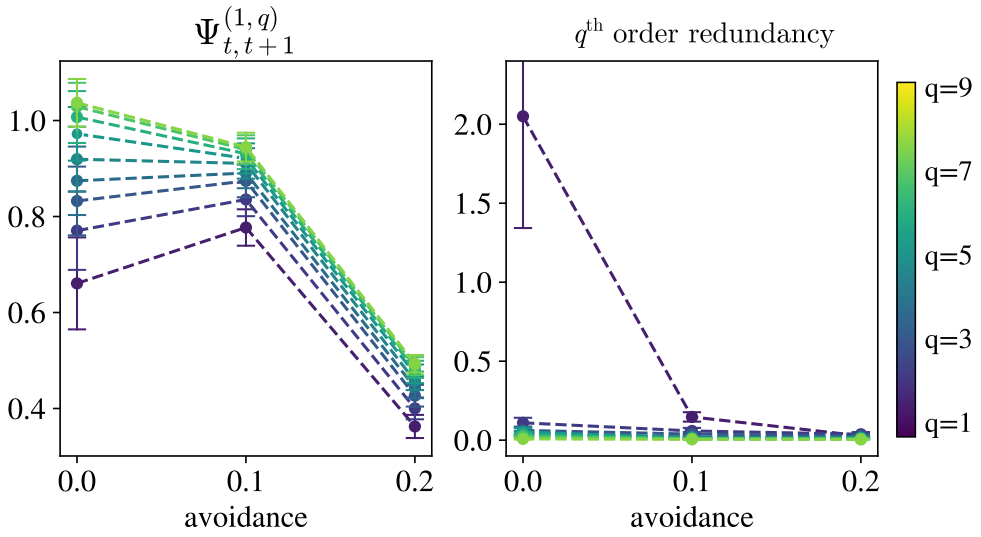


Figure 5.5: **Causal emergence and q-order redundancy in Reynolds' model.** Only the first order redudancy is relevant in this system, being orders of magnitude larger than the others, while higher orders ($q = 2$ to $q = 10$) are negligible. The system with no avidance manifests the highest amount of first order redundancy, due to the high similarity between the boids' trajectories. Interestingly, the redundancy corrections cumulate and the no avoidance case ends up showing the highest value of Ψ when all redundancy is accounted for. Error bars show standard error across $R = 20$ simulations for each parameter set.

Redundancy quantities with $q > 1$ invite interpretations regarding the fine-grained information quantities in the systems. We can test how groups of boids of various sizes jointly predict the centre of mass. Our results suggest that most redundancy is found for $q = 1$ (Fig. 5.5). This is in accordance with the nature of the model and its phenomenology: all boids are identical and follow the same distributions, and on average interact in the same way with all others. The interactions between boids are homogenous, while in real-world complex systems manifesting emergence, agents are likely to interact in more heterogeneous or higher-order ways, especially in dynamically complex collective behaviour. This motivates a comparison of the results obtained in the analysis of a flocking model with real-world data of flocking or schooling.

The downwards causation criterion Δ was also investigated. As the boids are identical and their trajectories are affected by each other, we hypothesised that the mutual information between their trajectories would be rather high. On the other hand, since there is no explicit causal influence exerted from the top-down by the centre of mass, the system should not be characterised by downwards causation. This is confirmed by our results of the downwards causation criterion, Δ, which is consistently below 0, as well as the high first-order redundancy amongst boids. Moreover, we observe the highest first-order redundancy is also in the rigid (no avoidance) case. As we can assess qualitatively, the trajectories of boids are very similar and as such the TDMI between them is high. There are only small amounts of redundancy of order $q > 1$ here as well.

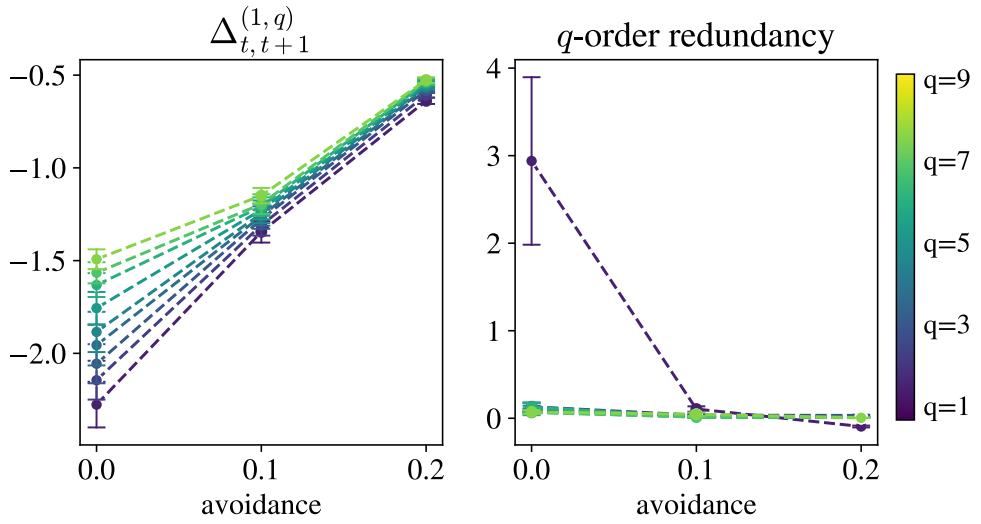


Figure 5.6: **Downwards causation and q-order redundancy in Reynolds' model.** Only the first order redudancy is relevant in this system, being orders of magnitude while higher orders ($q = 2$ to $q = 10$) are negligible. Error bars show standard error across $R = 20$ simulations for each parameter set.

5.3.2 Schooling fish

As a secondary case study, we look at six data sets of T=10000 timesteps from small schools of $N = 10$ fish swimming together in a tank. The fish clearly manifest emergent collective behaviour and as such we expect our criterion Ψ to reveal it.

We begun by estimating the Ψ measure with various degrees of accuracy q on the preprocessed spatial coordinates of the fish. First, results were averaged for all groups, expecting to observe $\Psi > 0$, even for the quantity $\Psi^{(1,0)}$ which was not adjusted for redundancy, similar to how the quantity behaves in the intermediary regime in the Reynolds' model. Instead, the causal emergence criterion was smaller ($\Psi^{(1,0)}_{t,t'} = -2.73 \pm 0.52$) and the first-order redundancy larger ($(N-1)I(X^i_t; V_{t'}) = 3.78 \pm 0.65$) than all of the Reynolds model simulations.

After adjusting the criteria using redundancy, all quantities with $q \geq 1$ are clearly positive, with $\Psi^{(1,1)}_{t,t'} = 1.04 \pm 0.31$ suggesting the causal emergence of an aggregated group around the centre of mass, and $\Delta^{(1,1)}_{t,t'} = -1.52 \pm 0.26$ suggesting there is no downwards causation. The average Ψ is closest to the value seen on average in the intermediary regime of the Reynolds model, whcih also has the most phenomenologically similar behaviour to the schooling fish. Although unlike the boids, the fish show more redundancy in their movement.

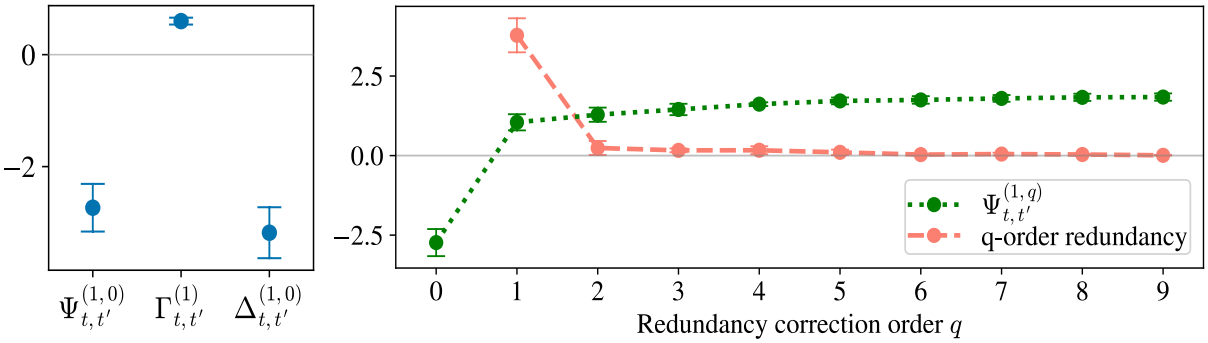


Figure 5.7: **Emergence criteria of order $q = 0$ and causal emergence and redundancy of order q in schooling fish. (left)** The emergence criteria Ψ, Γ and Δ, without accounting for redundancy, do not show this system to have an emergent centre of mass. **(right)** Ψ and redundancy have been computed for orders $q \in \{0, 1...9\}$ and averaged across the six groups. Ψ is negative unless a first-order or higher correction is applied, due to high first-order redundancy in the system.

However, we should be aware of the fact that the preprocessing step may have unexpected side-effects when applied to a dataset in which the trajectories are confined within reflective boundaries, rather than in a space with periodic boundaries.

We recall that the groups of fish showed different degrees of aggregation in their movement. We computed statistical observables related to spatial aggregation and density of neigbours in order to quantify it. As can be seen in Fig. 5.8, when averaging the instantaneous statistical observables over time, they seem to cluster similarly to the three categories we identified from the qualitative aspects of the behaviour in Fig. 5.3, which are dynamically similar to each other, but vary between looser and tigher spatial cohesion.

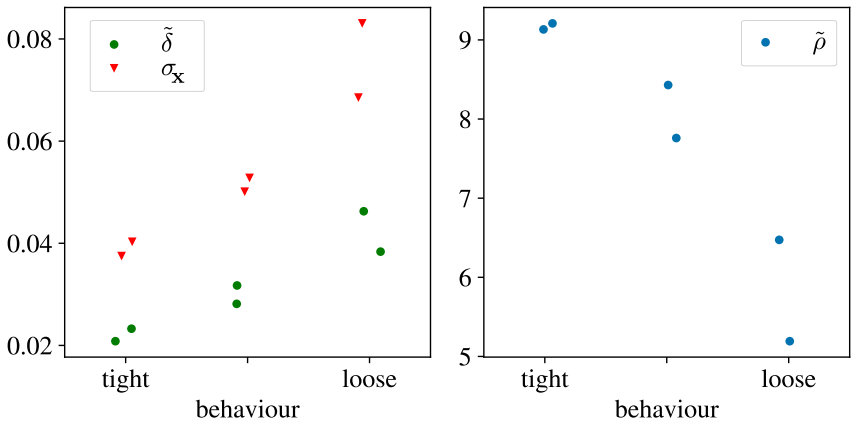


Figure 5.8: **Quantifying schooling behaviour with statistical measures. (left)** Average distances to nearest neighbour ($\bar{\delta}$) and centre of mass ($\delta_{\mathbf{x}}$) normalised by the size of the fish tank. **(right)** Average number of neighbours in a radius $r = 0.1$. The three groups show different values across the three parameters: the tightest knit groups contain almost all of their neighbours on a radius $r = 0.1$, while the loosest ones only contain half. The distance to nearest and spread also increase in the loose configurations.

With respect to information quantities, the groups do not appear to be as different from each other. Ψ is practically undifferentiated between groups, and the relationship between aggregation and redundancy is not linear, as the group of intermediate aggregation shows the highest redundancy between all components (Fig. 5.9).

This is likely because Ψ captures the behaviour better than aggregation, and the fish's behaviours are indeed dynamically similar in spite of being tigher or looser. The results do match with intuitions: the fish behaviour is not as differentiated between different degrees of spatial aggregation as it is in between the three regimes of the Reynolds model.

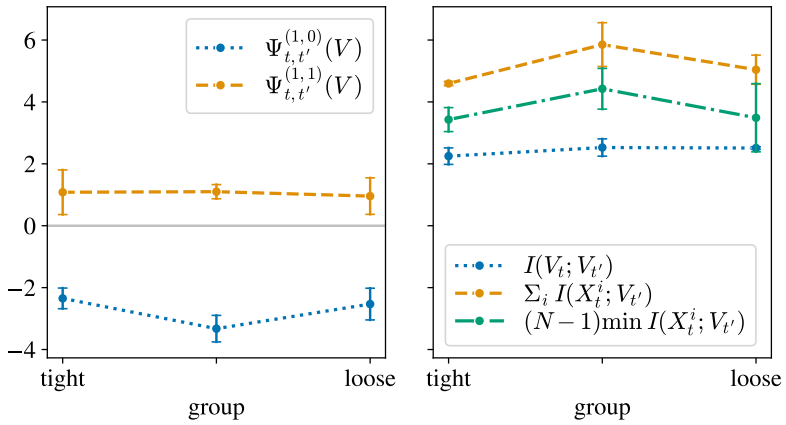


Figure 5.9: **Causal emergence and first-order redundancy in fish schools.** $\Psi^{(1,0)}$ is negative for all the schooling behaviours. Applying the $q = 1$ correction yields positive $\Psi^{(1,1)}$ for all groups, as expected. Highest redundancy is seen in the intermediary aggregation, but all are characterised by similar Ψ and higher first-order redundancy, unlike the Reynolds model.

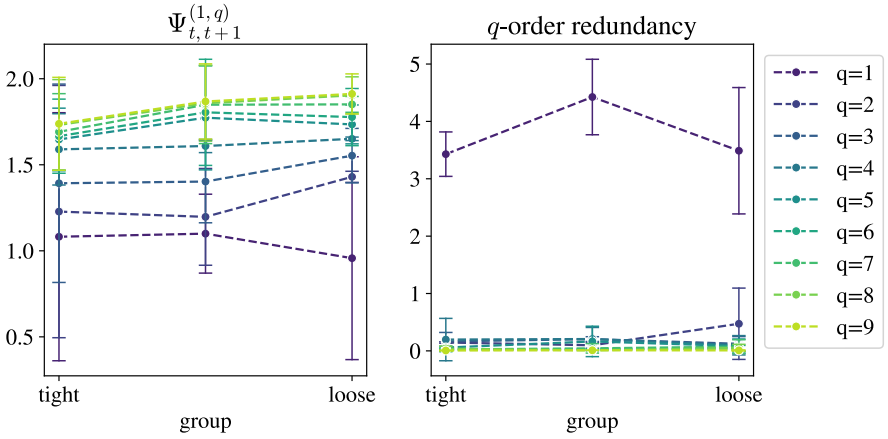


Figure 5.10: **Causal emergence and q-order redundancy in fish schools.** The most accurate Ψ is highest in the schools that are neither the most nor the least aggregated, and so is their $q = 1$ redundancy. Generally redundancy is higher than the Reynolds model especially for $q = 1$. In comparison, quantities with $q = 2$ to $q = 10$ are negligible. Error bars show standard error the two groups in each category.

5.4 Discussion

The study of complex systems with information-theoretic quantities is often made difficult by the non-linearity of measures of complexity: sometimes, a very ordered state and a very disordered state would yield similar results. 'Synergy-minus-redundancy' indices in particular, due to the subtraction of information quantities, are known to manifest such issues in practice (Rosas et al., 2020a). Systems with high synergy, but also high redundancy, and systems with little synergy and little redundancy cannot be differentiated from the index alone. This is particularly important when studying self-organising collective motion in nature where there are likely many similarities in each agent and in the spatial distribution of their positions, but also, a broad range of possible group sizes, making redundancy very likely to be high and relevant to the emergence estimation.

In this chapter, the partial information decomposition (PID) has been used to estimate redundancy in the system and to adjust the threshold for detecting causal emergence with the Ψ criterion, using the *lattice expansion* method described in Section 2.3.3. After implementing the first-order redundancy, we found causal emergence in two qualitatively distinct instances of collective motion in the Reynolds model: a rigid configuration reminiscent of milling behaviour in animals, and the intermediary configuration where the boids move together in a flock-like motion; as well as in data from schooling fish.

Without applying the redundancy correction, neither the milling configurations of the boids, nor the schooling fish, satisfy the emergence criterion $\Psi > 0$. As the systems do not manifest downwards causation, even with the redundancy corrections the Δ criterion remained below zero, but the first-order redundancy between agents was also, as expected, highest in the rigid case.

A known problem in collective behaviour research is that, while preset in the case of mathematical modelling, the mechanisms of neighbour interactions are notoriously difficult to estimate and ascertain in real data. Even in the case of a study with human subjects, who could verbally report how they were following neighbours to obtain flocking motion, scientists had difficulties in estimating which neighbours are interacting and how (Leonard et al., 2012b).

The findings provided by estimating redundancy are particularly important, as they can also be linked to the nature of interactions or hierarchical relations in the systems. High redundancy of order q may be related to interactions amongst groups of size $N - q + 1$.

In both the Reynolds model and the fish data, the $q = 1$ redundancy corresponding to the information shared by all agents is much higher than all other redundancy quantities, which are negligible in comparison. In the Reynolds model, all interactions between the simplified boids are homogenous and the agents are statistically identical, so we expect

high redundancy. The fish behaviour is characterised by even higher redundancy than the Reynolds model. This may be due to the fact that the fish themselves also have homogenous interactions, which is to be expected in their self-organising behaviour which lacks hierarchical structures or groupings between agents (Shaw, 1978).

5.4.1 Limitations & future work

One of the main limitations of the study of the Reynolds model stems from one of its strengths. We have used the same simulation data as in the original $\Psi - \Gamma - \Delta$ case study, which allowed us to reproduce the results, and to expand the findings in the original article. Unfortunately, due to this, we were restricted to an implementation with periodic boundaries, which changes the nature of the underlying statistics of the system, and makes it more difficult to directly compare with the real world data, and requires the use of preprocessing techniques. To mitigate the first limitation, the author has attempted another implementation of the Reynolds model with reflective boundaries, but at the time of writing we were unable to complete another study.

As with most case studies, the analysis on the fish data does not benefit from statistical strength. While the results are largely consistent as well as intuitive, we cannot say with certainty that they are robust and will be reproduced on other fish schools, definitely not with the same confidence as the findings in the Reynolds model. Nonetheless, this limitation is pervasive in many studies of animal and human collective behaviour, and we hope that the use of finer-grained information quantities in the system as investigated in this chapter can help improve the overall interpretability of information-theoretic analyses in case studies.

Another limitation is brought by the difficulties of estimating information quantities based on trajectories in two-dimensional space. We have found in our previous investigations in Chapter 4 that trajectories of 2D positions in a confined space are very likely to show very high amounts of mutual information. This may be an overestimation, or alternatively, an actual underlying property of the trajectories themselves when taken as two-dimensional spatial coordinates. The first order redundancy correction captures this inherent high mutual information, but then it is difficult to separate the mutual information resulting from the positions simply being close to each other and similar multivariate quantities, and that resulting from a statistical similarity in the evolution of those positions which may encode something about behaviour.

Finally, we should comment on the choice to study the emergence of collective motion in two dimensions, especially as birds and fish move in three dimensions. It is important to note that finding emergence in lower dimensions suggests it exists in higher dimensions, but not vice-versa. More over, the simplifications we introduced in the model, as well as

the two-dimensional approach to the fish experiment in (Niizato et al., 2024), also allows the findings in this chapter to be applied to collective movement of terrestrial animals or of pedestrians, as we will see in Chapter 7.

5.4.2 Conclusion

In this chapter, we have presented a case study of collective motion in animal groups using improved estimators for the causal emergence criteria Ψ and Δ, which take into account the redundancy inherent in the system. Intuitively, the redundancy correction of order q refers to the shared information (in this case, as computed by the minimum mutual information) that groups of $N - q + 1$ sources provide about the target.

To follow our goal of a substrate-independent method of emergence, we have tested this method in both a simulated multi-agent flocking model by Reynolds, and real-world experimental data of schooling fish, using time series based on the trajectories of agents to represent the components and the trajectory of the centre of mass of the group to represent the emergent systemic feature of the system.

We have shown that when applied to a dataset of simulated collective motion using the centre of mass as a candidate feature to describe emergence in the system, the most ordered configurations with low avoidance manifest the highest redundancy, and that adjusting the emergence criterion with the first-order redundancy is sufficient to find emergence in the highly ordered configuration.

We have also tested our criteria against experimental data of schooling fish. Here, all behaviour is highly emergent, and yet the first-order correction is still necessary to detect it. By studying higher-order redundancy we may find more interesting fine-grained information sharing behaviour amongst agents in the system.

Chapter 6

Case study: social structures and collective action

Chapter Summary

In the absence of pre-established hierarchical authority or coercive control, resolving collective action situations through self-organisation requires a range of alternative mechanisms, including voluntary association, mutually-agreed social contracts, or 'bottom-up' emergent social structure. In this chapter, we explore the emergence of social structure in a self-organising multi-agent system called Megabike, where cooperation or competition are expressed through movement, and we find causal emergence and downwards causation in all surviving cooperating groups. This is significant in the context of social systems in which local interactions between individuals produce beneficial leadership structures, which have, in turn, causal power over the individuals' agency, and as such expose the society to the risk of degenerative asymmetric power structures.

After thorough testing in the first part of the thesis, in the previous chapter the Ψ criterion for emergence was used to study complex motion and a comparison was made between experimental data of schooling fish and simulated data produced by the Reynolds flocking model.

The next complex system in which we use the $\Psi - \Gamma - \Delta$ emergence criteria as a case study is an autonomous self-organising system for the study of social structures and social contracts, *Megabike* (Scott et al., 2024a). In *Megabike*, agents must collectively pedal in groups on eight-rider bikes, while preserving energy, seeking resources and avoiding danger. The *Megabike* scenario features multiple inter-dependent collective action situations, including voluntary association, deliberative decision-making, social coordination, resource allocation and cooperative survival.

While fundamentally mechanistic, since the set of interactions between the components are formally defined in this model, the agents' behaviour is extremely complex and non-linear, lending itself to the study of more complex higher-order interdependencies, which we can interpret as social structures. As such, some of the findings on this model may have relevant interpretations to organisations and society: by comparing simulations in which agents self-organise and create social contracts, or elect leaders, or have a leader imposed onto them, for example.

Particularly relevant to our use of Ψ in the study of collective motion, here we have a case where movement is a direct proxy of some causal force: each agent must choose to steer, pedal or brake, and can choose to cooperate or be selfish. This manifests directly in the steering vectors of the agents, which the simulation allows us to measure. Meanwhile, the emergent collective entity which arises from the agent is obvious: the bike itself, which will move smoothly if the agents agree. This setup allows us to test the criteria of emergence in another context than by using a coarse-graining measure: for the candidate emergent system property V, we will choose the movement vector of the bike.

In the rest of this chapter we briefly describe *Megabike* and present the main motivation, results, and conclusions of a first exploration into the possibilities of studying social structure in this multi-agent system using criteria of emergence: *Megabike* was used to simulate collective action situations where knowledge alignment and consensus are reached with the help of a democratically-elected leader.

The simulation data was provided by Matt Scott and full details can be found in (Scott et al., 2024b). This chapter reproduces the main findings and discussions of the paper, which was co-written with Matt Scott and Prof Jeremy Pitt.

6.1 Emergence in social behaviour

In human social systems, once a goal has been agreed by a collective, as a product of knowledge aggregation (Ober, 2008) and/or social influence processes (Nowak et al., 2019), a plan to achieve that goal may require individuals to coordinate their behaviour, by performing specific actions at the same time, or in a particular sequence. (Ober, 2008) argues that with the appropriate epistemology, social coordination was achieved in classical Athenian democracy without formalised protocols, even in the absence of hierarchical authority or coercive control. One of the main contributing factors was *knowledge alignment*: the right people having and using the right knowledge in the right context while a lack of such common knowledge increases transaction costs and degrades organisational performance, cf. Ashby's law of requisite variety (Ashby, 1958).

Ober shows that classical Athenians made use of several mechanisms to promote accurate following, including first-choice following (alignment cascades), leader following – where people follow someone in a designated role with institutionalised power (Jones & Sergot, 1996), rule following – where coordination follows from common knowledge of simple procedural rules, and commitment following – where common knowledge of credible pre-commitments is sufficient incentive to co-operate, given the costs of non-cooperation.

A practical and simple example of these processes can be seen in an experiment where groups of pedestrians were asked to walk randomly in a large space without talking (Dyer et al., 2008), with only a few group members being informed about where and how to walk. Despite the lack of verbal communication, the group reached consensus as the informed individuals were quickly identified and followed spontaneously by the others.

This kind of social coordination is not unique to humans. For example, flocks of birds who fly in V-formation do so because careful positioning, synchronised wing-flapping and frequent positional changes all contribute to substantive – in fact optimal – aerodynamic performance and energy saving (Portugal et al., 2014). The position of the bird at the front of the 'V' has nothing to do with hierarchy or exceptional physique, or any sense of 'leadership'.

In the social sciences, there is a long history of debate on whether the top-down influence of leadership (or more generally, social structure) or the bottom-up influence of individual agency have the largest effect on group behaviour (Elder-Vass, 2010), known as the *agency-structure problem*. In this context, we pose the following questions: whether or to what extent are common knowledge, group optimisation and leadership structures *emergent properties* and how do they arise from the individuals' behaviours, and whether or to what extent do they affect, in turn, the behaviour of individuals?

The philosophy of emergence has of course also contributed to the social sciences, for

example, in efforts to reconcile the causal power of individual agency and social structures over human behaviour. An *emergentist* perspective allows social structures, in the form of institutions and normative groups (rather than a vague concept of 'society' as a whole), to be both *causally emergent* from the behaviour of individuals, in particular their interactions, but also, in turn, have an effect on individuals' agency, which is a case of *downwards causation* (Elder-Vass, 2010).

These concepts are more difficult to evaluate quantitatively, so in spite of the valuable intuitions that emergence may provide to social science, especially by studying social structures as emergent and downwards causal phenomena, most quantitative research still does not address the self-organisation processes that can produce social structure. An exception is collective movement research, such as studies of crowds and concert audiences, the social force model of pedestrian dynamics (Helbing & Molnár, 1995), or studies of human flocking (Dyer et al., 2008; Leonard et al., 2012b; Sas et al., 2024b)[1]

6.1.1 Leadership and self-organisation

An interesting contrast can be seen in the study of social systems versus natural systems. In the former, there is great emphasis on hierarchical social structures, with less focus on the processes of self-organisation producing or updating these structures; in the latter, most work assumes agents to be identical, and the contribution of hierarchical relations, social networks and leaders are less studied, even though they are of crucial importance to self-organisation (Zafeiris & Vicsek, 2017).

Some exceptions exist, suggesting the importance of social networks in the collective behaviour of animals through preference for family groups (Bode et al., 2011b). Another example are studies of effective leaders, who emerge in schools of fish to expedite group decisions when predators attack (Múgica et al., 2022). These are often the most informed individuals, who react the quickest to changes in their environment. The presence of these individuals and their recognition by the rest of the group relates to how information is shared between agents and how collective decisions and compromises are made in the presence of partial information (Leonard et al., 2012a). The same self-organising behaviour has been seen in the human groups who perceived the most informed individuals and followed them (Dyer et al., 2008).

As such, there appears to be a gap in knowledge concerning how to quantify more complex or human-centric social structures, such as an elected leader or social norms. However, rule-based, self-organising multi-agent systems (Pitt, 2021) provide an instrument where agents can self-organise in the context of conventional rules, institutionalised roles, and elaborate social structures, beyond what is typically available in either the swarming or

[1] A study of human flocking, Synch.Live, is discussed in Chapter 7

pedestrian dynamics literature; while the framework of emergence and studies in complexity science can provide a quantitative instrument for analysis.

6.1.2 Objectives and hypotheses

We define an instance of the *Megabike* scenario as a case study using multi-agent systems, where the component agents elect one of their number to a social role (the *leader*) to help constrain self-interested behaviour. Our aim is to investigate how effective collective action emerges from individuals under this leader, within an environment featuring resource scarcity, competition, social dilemmas and requirements for consensus.

Following the examples of flocks of birds and pedestrians, we take an *embodied* view of social behaviour. As such we study movement, more specifically pedalling and steering in *Megabike*, as a proxy for social actions. This enables the social behaviour of agents, which can be difficult to measure, to be related to their more easily quantifiable motion.

We need to investigate the robustness of the leadership structure, and relate its effect on decision-making and decisive action on that decision. To achieve this, we introduce two experimental conditions in our case study: *static* and *dynamic*. The dynamic case introduces extra trade-offs at both the individual and group level, between spending more energy and collecting more information, introducing more variability and a broader space to make decisions, more risk but also possibly more opportunities for successful collective action.

Consequently, we hypothesise that:

- both static and dynamic conditions will exhibit *causal emergence*, i.e. that from the combined actions of all agents, a collective behaviour will arise in the form of efficient movement through the environment;
- both static and dynamic conditions will manifest *downwards causation*, as the direction of collective movement will directly affect the possible directions the agents can physically steer in, more so than the other agents; and
- dynamic realisations, which should manifest much more diverse behaviour from the agents, should be characterised by higher measures of causal emergence, due to the presence of more *synergy* or less *redundancy*

In summary, we integrate two different methodological instruments in order to investigate emergent properties of leadership structures in social systems. The specific multi-agent systems instrument is described in the next section, while the information-theoretic instrument for the measurement of emergence is presented in Section 2.3.

6.2 The Megabike scenario

To study the above questions on causal emergence in social systems, we use *Megabike*: a self-organising multi-agent system simulation inspired by bikes that can accommodate multiple riders. In this scenario, we spawn 'bikes' which are driven by eight agents each. Driving these bikes, and communicating to other agents requires energy, of which the agents have a limited supply. These bikes thus need to collectively navigate a 2D arena in order to both obtain lootboxes, for replenishing this energy, and avoid an existential threat of a car which eliminates a bike after a collision.

Agents have the capacity to steer (at an angle from -180° to 180°) and pedal / brake (at a magnitude from 0% to 100% power), which yields a vector in 2D space. The vector that the bike travels in is the sum of the individual agent steering vectors, meaning that if agents are not in accordance, the bike is likely to move very slowly, if at all. Physical forces are also at play in this model, with the resulting movement vector of the bike sometimes of larger or smaller magnitude than the sum contributions. Consequently, the agents must collectively agree on (and each agent explicitly agrees to voluntarily comply with) the social arrangements that determine movement (through pedalling, turning and braking), and lootbox targeting.

Ultimately each agent wants to maximise its own utility, measured in terms of energy gained from lootboxes, and survivability. To complicate the scenario, each agent is ascribed a particular colour, which corresponds to a colour of lootbox. Whilst agents are able to consume lootboxes of other colours, they do not receive any energy from them.

For agents to attempt to navigate towards a lootbox, this lootbox must be within the bike's *perception radius* so the agents can become aware of it. Based on the parametrisation of this scenario, this radius can either be invariant to change or variable, where the riders of a bike are able to propose a different radius to search in.

This leads to a social dilemma, wherein agents prioritise their respective colour of lootbox, however must mutually cooperate to avoid a 'stalemate', whereby all agents pedalling in their own directions leads to zero net movement of the bike, and allows the car to gradually close in on them. Furthermore, having a large perception radius may exacerbate this issue, as agents may be 'spoilt for choice', or attempt to navigate to a lootbox (of their colour, say) that is too far to reach. Conversely, having a perception radius that is too small may lead to no lootboxes being found, giving the agents no reason to pedal.

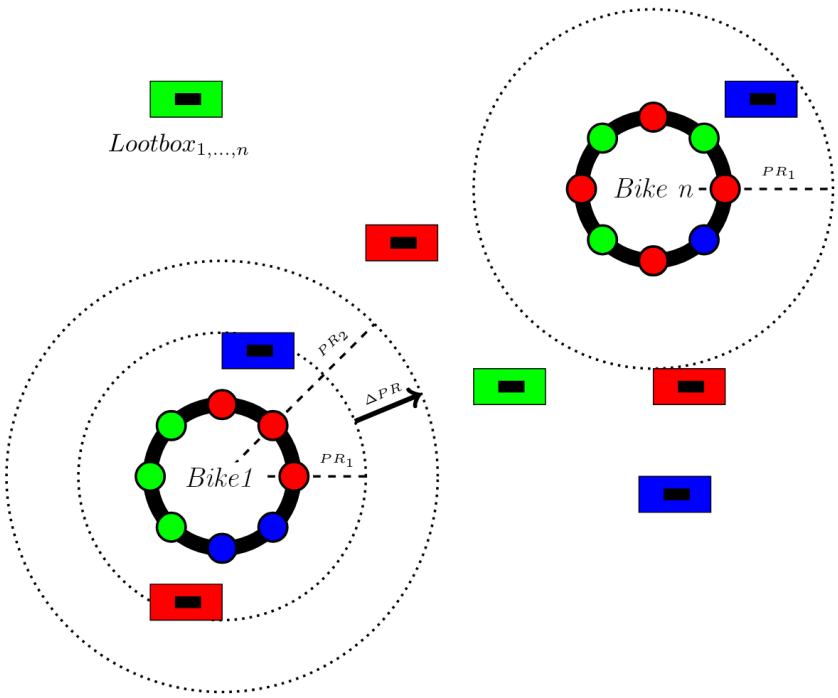


Figure 6.1: Example visualisation for *Megabike*. Bike 1 has a dynamic perception radius, expanding from PR_1 to PR_2 as the rounds progress. Bike n has a static perception radius. (Reproduced from (Scott et al., 2024b))

Although the simulator lends itself well to a diverse set of social arrangements and systems of governance, for the purposes of this paper we consider a system with a single governance strategy. In this formulation, agents elect a *leader*, who is responsible for relaying information around a bike. Due to the nature of the collective action problem posed by this scenario, the leader is needed to assist social co-ordination. To achieve this, the leader broadcasts (to their bike) a possible direction for the bike to travel. Compliant agents will agree with this request and pedal in the proposed direction, whereas non-compliant agents will ignore the request and pedal in their own direction regardless. Once these pedalling vectors have been collated, the net force exerted on the bike is a linear sum of the individuals, as above. As such, the full action space for each agent is as follows:

- *Institutional foundation* - The simulator initially spawns enough bikes for every agent to be seated. Agents are randomly distributed across bikes, so it is their task to not only negotiate whom they want to team up on a bike with, but also which social arrangements they will have. Agents may leave a bike at any time, but need to be granted access by the agents on whichever bike they attempt to join.
- *Steerage* - Once on a bike, agents submit a choice to pedal (p), brake (b) or turn (t), which make up an agent's steerage per round. These values are used to produce a vector representation, where the magnitude of steerage is $p - b$, yielding the $x - y$ components of the steerage vector as $(p - b)\cos(t)$ and $(p - b)\sin(t)$.

- *Resource allocation* - Each round, a lootbox is collected if the euclidean distance between a bike ($\vec{B}$) and lootbox ($\vec{L}$) is within the threshold ϵ units: $|\overrightarrow{BL}| <= \epsilon$. If this occurs, then agents must decide how to allocate resources amongst the bike, using their preferred social arrangements.

The act of *steerage* is directly conditioned on the information each agent has about surrounding available lootboxes. This makes the perception radius an interesting variable to manipulate, as it allows controlling the amount of information available to the group and thus the complexity of the decision-making process.

Therefore, the two experimental conditions explored in this paper are implemented through the agents' either fixed or variable radius of perception for the detection of lootboxes:

- The **dynamic** case refers to how agents may choose to increase their perception radius by spending more energy; this affects the whole megabike, as the bike's overall perception radius is an average of all agents'. This creates new oportunities for knowledge alignment and more variability in individual behaviour, which results in a perception radius that varies over time.
- The **static** case, in contrast, refers to how agents have the same perception radius through the entire simulation. Their bikes have less social dilemmas to solve but also may be characterised by less flexibility.

6.3 Methods

6.3.1 Simulation: *Megabike*

The *Megabike* simulation platform is throughly described in (Scott et al., 2024b). Below, we include the details which pertain to agent interactions.

The *agent* data structure identifies each agent, their bike if they are on one, and their energy level (0 to 100%). Agents can get access to information about the environment to some degree, such as lootbox positions, positions of other bikes and the cars. To create the social dilemma described in Section 6.2, each agent must have a varying objective function, which is operationalised through the colour of lootbox they seek. To interact with their environment, each *bike* data structure tracks the agents currently riding on it, the current elected bike leader, and the current value of the bike's pool.

In the simulation, each agent is initialised with a random colour and 100% energy. The bikes are spawned separately and agents select their bikes by *voluntary association*. Agents can communicate to establish or implement these social arrangements, using an abstract messaging structure, to self-organise for negotiating bike membership, resource allocation and steerage.

As the simulation evolves, the agents are given various opportunities for action and self-organisation. First they form into groups and negotiate their social structures and norms, after which they get the opportunity to work together on a bike until they perish, get hit by a car, or the simulation ends. The simulation loop is operationalised in Algorithm 1.

Algorithm 1: *Megabike* Scenario 'Game Loop' (provided by M. Scott)

```
1  i ← 0 ; initialise agents ;
2  // Iteration
3  repeat
4      (within agents) negotiate bike membership;
5      (within bike) negotiate social arrangements; perform role assignment;
6      j ← 0 ;
7      // Round
8      repeat
9          (within bike) decide target lootbox; each agent decides to pedal/brake/steer;
10         (environment) apply effects of actions;
11         if lootbox reached then
12             (within bike) apply resource allocation;
13         (within bike) admission/exclusion of agents;
14         j++ ;
15     until j == MaxRounds OR bike terminated;
16     i++ ;
17 until i == MaxIterations OR deadlock;
```

For this experiment, agents request to join the bike that has the greatest average risk assessment, where a risk-assessment is each agent's subjective expected probability of another agent's future performance based on experienced or reported past performance. Role assignment consists specifically of leadership election.

Social arrangements consist of proposing a new lootbox perception radius. For simplicity, the social contract that represents a static/dynamic perception radius is represented using two pieces of data: whether the contract is dynamic, as a `bool`, and the current perception radius that the megabike is allowed, as a `float`.

This setup is only one example of the many possible scenarios that can be implemented in *Megabike*. We selected leadership roles and specific social arrangements, but many other scenarios can be chosen instead. For the information-theoretic study, we shall use only steering behaviour and bike trajectory data, but many other simulation details, such as energy expenditure, lootboxes consumed etc. could be investigated.

6.3.2 Experimental design

By using the *Megabike* simulator discussed above, we perform a set of survival trials used to investigate the behaviours of agents. We subject the agents to two conditions affecting the flexibility of the perception radius agents have for discovering lootboxes. In the first trial, agents have an *static* perception radius r . This means that the euclidean distance between the agent (or bike) must be *at most* r for a lootbox to be considered accessible for voting / steering. In the second trial, we allow the perception radius to be *dynamic*. In this case, agents vote on the mutually agreed perception radius of the bike, based on their individual energy. Agents with an energy below 75% of the maximum vote to increase the radius, once per iteration, by a factor of two, starting from the initial perception radius of 50 units. Agents with a health of greater than 75% will vote to maintain the same radius, with the overall radius update factor being the mathematical mean of all proposals.

We parameterise the simulator with 80 agents and 10 bikes, with each iteration lasting for 100 rounds, and each simulation lasting for 100 iterations, for a total of 30 simulations. Across each simulation, we look at the proposed pedalling direction given by each agent, and compare this to the resultant direction that the bike travels after in.

For each simulation, we expect 80 agents to interact for 10,000 rounds and yield two vector components for each round. As such, we produce a matrix containing, for each of the 10 bikes, the steering vectors of each agent X_t^i, and a matrix containing the direction vector B_t of each bike. These time series will be used to compute information-theoretic emergence metrics.

6.3.3 Information-theoretic analysis

As in the previous chapters, we employ a non-parametric mutual information estimator by Kraskov (Kraskov et al., 2004) as implemented in the research software JIDT (Lizier, 2014), which has been previously used in flocking and swarming data (Wang et al., 2011). For robust estimation, we discard all iterations in which any agents have perished (by reaching energy level 0%), so that we have the same amount of data for all time series.

We use the steering vectors of each agent at time t, X_1^t to X_8^t, as microscopic components, and the direction vector of the bike B_t as the macroscopic, emergent collective feature of the system.

We compute the $\Psi - \Delta - \Gamma$ criteria (Rosas et al., 2020a) to investigate the relationship between the leader and the collective by principles of causal emergence, causal decoupling, and downwards causation, using a Python module (Sas, 2024) with bindings to JIDT (Lizier, 2014). Below, i ranges over the 8 agents on a megabike, and $t' = t + 1$, as we study immediate effects of agents' behaviours over the overall group behaviour, and vice-versa. As we use the spatial data with 2-dimensional coordinates directly, we reduce some of the inherent redundancy in the steering vectors with the first redundancy correction introduced in Section 2.3.

$$\Psi_{t,t'}(B) := I(B_t; B_{t'}) - \sum_i I(X_t^i; B_{t'}) + (N-1) \min_i I(X_t^i; B_{t'})$$

$$\Delta_{t,t'}(B) := \max_i \left(I(B_t; X_{t'}^i) - \sum_j I(X_t^j; X_{t'}^i) \right) + N(N-1) \min_{ij} I(X_t^i; X_{t'}^j)$$

$$\Gamma_{t,t'}(B) := \max_i I(B_t; X_{t'}^i)$$

We use Ψ to quantify how much better does the direction of the bike at a time t predicts its movements in the future at time t' than the sum of steering vectors of the agents. Therefore, our first hypothesis is equivalent to finding $\Psi > 0$ for the bike direction, while our third hypothesis is equivalent to finding consistently higher Ψ in the *dynamic* realisations, where agents can negotiate their perception radius and are flexible about which lootbox to choose, allowing more variety in behaviour and requiring more consensus reaching than the rigid cases. For our third hypothesis, we expect $\Delta > 0$ for downwards causation and $\Gamma > 0$ for no causal decoupling.

6.4 Results

This section summarises the experimental results, comparing information-theoretic emergence against the two conditions, static and dynamic, which are characterised by different degrees of flexibility in behaviour.

6.4.1 Causal emergence

We hypothesised all non-trivial systems should be characterised by causal emergence, which is confirmed by the results in Fig. 6.2, which yield $\Psi > 0$ for all simulations where all agents survived.

Moreover, consistently higher Ψ is seen in the case with a dynamic perception radius, as well a higher variance in Ψ values ($M = 1.99, s.d. = 0.93$), as opposed to simulations where the agents only had a static perception radius to base their decisions on ($M = 1.29, s.d. = 0.29$). This result is statistically significant as shown by the one-tailed independent t-test with unequal variance ($t = -3.886, p = .0002$).

It appears that Ψ is on average higher but also more varied in the simulations characterised by more complex decision-making, knowledge-alignment and consensus-reaching situations made possible by the dynamic scenarios.

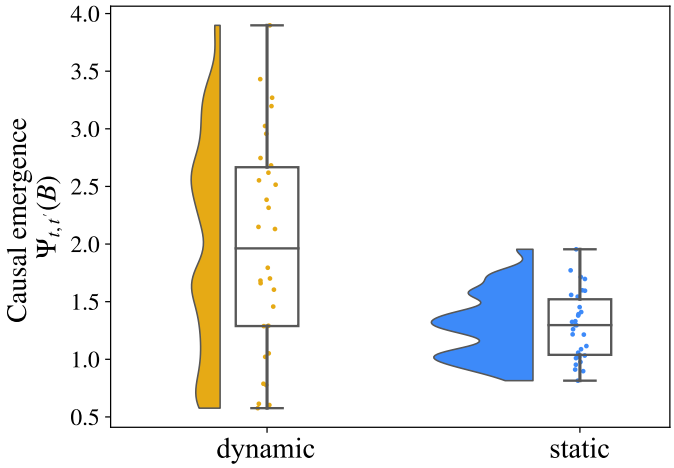


Figure 6.2: **Causal emergence in the Megabike scenario**. Histogram, box and scatter plot (aka Raincloud plots (Allen et al., 2021)) for the Ψ criterion. Since this quantity is non-zero, all systems manifest *causal emergence*. The values are significantly higher in the dynamic case ($t = -3.886, p = .0002$), and the distribution is broader, suggesting greater diversity in behaviour and information dynamics in the systems characterised by the more heterogenous behaviour in the dynamic simulations.

6.4.2 Downwards causation and causal decoupling

The $\Delta > 0$ results in Fig. 6.3a show that an individual agent's future steering direction is better predicted by the bike direction vector than any other agent's behaviour. There is a slightly higher value in those with dynamic perception radius ($\Delta = 0.025, s.d. = 0.01$) compared to those without ($\Delta = 0.02, s.d. = 0.011$). The two types of simulation don't manifest significant differences in this quantity ($t = -1.58, p = .059$), though it is worth exploring the outlier where Δ is below 0.

The $\Gamma \neq 0$ results in Fig. 6.3b show none of the simulations manifest causal decoupling. In other words, the current direction vector of the megabike can predict the future steering directions of at least one of the agents to some degree. This is according to our hypothesis, and further emphasises that there are always some interactions or so-called causal forces between individuals in this system. There is only a negligibly higher value ($\Gamma = 0.032, s.d. = 0.011$) in those with dynamic search spaces compared to those without ($\Gamma = 0.031, s.d. = 0.013$), which is statistically insignificant ($t = -0.45, p = .326$).

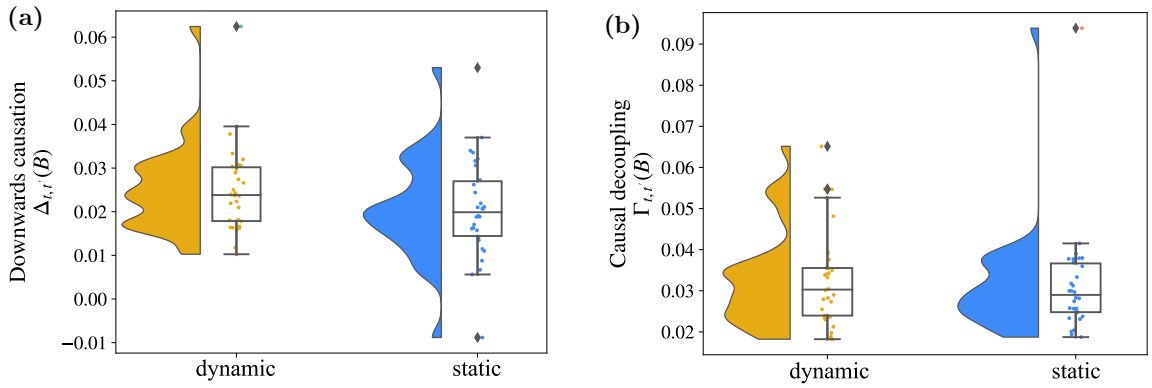


Figure 6.3: Raincloud plots for **(a)** downward causation and **(b)** causal decoupling in the two types of simulations. (a) Δ is positive, suggesting downwards causation. The mean and standard deviation are similar for the two groups of simulations. (b) Γ is non-zero, the system does not manifest causal decoupling, and the differences are non-significant between the two types of simulations.

6.5 Discussion

When looking at human societies, it is very intuitive to see that causal powers act at different levels, including within the individual (such as resulting from their genetics and state of mind), at the individual level (such as their behaviour and agency in the world), and at the group or social structure level (such as the different kinds of power individuals gain and manifest when aggregated in a family or institutions). It is also important not to neglect that between these levels of nested hierarchical structures there are complex interactions, and that the emergent properties of social systems are *multiply determined*: social structures are formed and changed by individuals, which can be seen as a result of them being *causally emergent*; but being part of a social structure may also change an individual in turn, which can be seen as an example of *downwards causation*; finally, a person may act both as an individual and as a representative of a social structure (Elder-Vass, 2010).

This view comes in stark contrast to some both individualist and voluntarist social philosophers (e.g. Weber), who believe that individual human agency explains all higher-order complexities of social behaviour (which would be a case of causal emergence only), as well as deterministic and structuralist accounts (e.g. Durkheim, Marx) who see agency as a response to social context (which would be a case of downwards causation).

The former view makes it difficult to reason about the complexity of emergent structures, with many philosophers seeing 'society' as a nebulous manifestation of individual will, and lacks the ontology to operationalise any form of social change that could result from individual behaviour. The latter view obscures the mechanisms by which these structures emerge in the first place and also the role of individual agency within these mechanisms. The issue of both approaches is that they neglect the feedback loops inherent in social systems. Meanwhile, authors like Bordieu have considered both structure and agency (Bourdieu, 1984), and recently Sawyer and Elder-Vass (Elder-Vass, 2010) have provided emergentist theories of social structures which consider both the individuals' and the structure's contributions to the dynamics of the complex system of society.

In our view, the philosophy of emergence can provide explanations to complex behaviour without explaining it *away*. When studying complex systems we are interested in observing the putative relationships between the behaviour of social entities at different levels. In this sense, we do not take a side on a strong or weak version of emergence (Bedau, 1997), but we focus on relationships and interactions in the system that produce collective effects at multiple levels: between individuals, between emergent structures such as social systems, as well as causal powers manifesting top-down and bottom-up between the individual and collective levels. In the social sciences, this approach has been named *the relational approach to the agency-structure problem* (Crossley, 2022; Elder-Vass, 2010).

In this chapter, we have presented a novel simulation environment and analysis pipeline for the modelling study of social situations from an emergentist perspective, in the form of the *MegaBike* framework and the case study analyisis using information-theoretic criteria of emergence. Assuming a robust dataset quantifying both a collective action and the actions and behaviours of each agent, the behaviour of the Ψ, Γ, Δ emergence criteria across different forms of organisation can reveal valuable insights on how social influence manifests between agents and the social structures they form.

In our specific *Megabike* case study, we chose social systems with leaders, and manipulated the perception radius of agents in order to introduce a knowledge alignment and consensus problem that the leader can mediate. We have found causal emergence and downwards causation as quantified by $\Psi > 0$ and $\Delta > 0$ in all surviving groups and higher Ψ when introducing the dynamic perception radius. Causal emergence can be related to the existence of a broader spectrum of possible decisions taken by the agents, as well as a more complex interplay between local information, the diversity of the agents' interests, and the decisions made by the leader. The higher Ψ may suggest the leader is effective in their role in solving the social dilemmas created by the dynamic scenarios, and makes good use of the opportunities for self-organisation that they offer.

On the other hand, information-theoretic downwards causation can be related to the influence the leader has on group behaviour, and completes the causal feedback loop between individual and collective agency. It should be noted that if the leader and all the agents fully agreed, the high redundancy in the system would cause Ψ to be below zero. This is relevant in a social system as adaptability of the group depends on group diversity.

6.5.1 Further work

One of the main limitations of this work also comes from one of its strengths: we studied the *Megabike* scenario from the perspective of collective movement, as that is better understood and universal in all human and animal societies; unfortunately this relies on many assumptions, such as that proximity or synchrony in behaviour with another agent is a proxy for social relations, bonds, or causal influence. While we may state that in *Megabike*, this assumption is well-founded by the nature of the model itself, its applicability may not expand further, as collective movement cannot always capture more subtle or complex social situations.

More specifically, the analysis does not keep track of any agents perishing, leaving a bike for another, or the time they wander in between bikes; nor does it consider any of the resources being gathered and how they may positively or negatively affect the agents. Furthermore, the information-theoretic analysis assumes all agents and all bikes

are statistically identical and independent, which may not be the case if a number of agents migrate from a bike to another. Finding a way to include these more complex behaviours in our information-theoretic quantification is a very exciting avenue for many more studies on various *Megabike* scenarios.

The *Megabike* scenario studied in this paper is only one insatnce of many possible social structures that can form in this multi-agent system, and, in turn, in realistic human societies. This scenario serves as a test-bed for a variety of social arrangements, some of which may not involve a leader at all. For this case study, we have considered a homogeneous set of social arrangements, wherein a single leader serves as a co-ordinator for each bike, and the agents decide to vote on how to update the perception radius for lootboxes.

Given that the *Megabike* framework provides such an expressive rule formalism (Scott et al., 2024a), it will be interesting to investigate the effect of having multiple flexible rules affording a variety of self-organisation opportunities (i.e. not just for leadership, but also for admission, exclusion, etc.), and whether or not we observe amplification or cancellation of emergent properties. It is also planned to specify a variety of governance systems in order to investigate how causality could help to distinguish between different (platonic) forms of governance, e.g. benign dictator vs. a totalitarian autocrat, or responsible aristocracy vs. oligarchy, or democracy vs. majoritarian tyranny. For example, there may be a relationship between quantifiable causal decoupling and asymmetric power structures when people are no longer represented by or have any influence on their form of governance.

6.5.2 Conclusions

In summary, this chapter has initiated a study of the complexities of social structures in the context of complex systems, using the self-organising multi-agent model and simulator *Megabike* and information-theoretic criteria for detecting causal emergence, downwards causation or causal decoupling in multivariate time series data.

The primary contributions of this paper are therefore:

- we have described and implemented a simulator for the *Megabike* scenario, a reusable, general purpose, open source multi-agent simulator for environments with (a) multiple inter-dependent collective action situations, and (b) agents capable of selecting and modifying socially-constructed roles and rules to help resolve the situations;
- we have proposed the usage of information-theoretic measures of emergence to quantify causal emergence and downwards causation in social systems as a solution to the agency-structure problem; and

- we show there is information-theoretic causal emergence and downwards causation in the behaviour of an effective leader in a set of *Megabike* simulations in a specific *Megabike* use case.

The problem of coordinating the pro-social behaviour of multiple independent actors to achieve an intended collective goal has recurred throughout place and time (Ostrom, 1990). In the scenario explored in this paper, manipulating the perception radius allows us to relate individual and structural responsibility. A higher average and variance of Ψ values characterises the *flexible* realisations, where agents may re-negotiate their perception radius used to choose lootboxes.

In human communities, hierarchical forms of coordination based on formal protocols of command and control run into the seemingly finite capacity of humans for information processing, transferring the onus of coordination onto self-organisation, the burden of which promotes expertise in bureaucracy and cornering knowledge, which in turn leads to Michels' *iron law of oligarchy* (Michels, 1962).

What can be observed in this scenario is that voluntary association with a megabike establishes a credible pre-commitment to follow rules and leadership decisions, the social contract which efficiently compute potential targets are mutually agreed procedural rules, and the emergent properties at the megabike level and its continued survival are evidence of individuals following an effective leader.

Appropriate *Megabike* scenarios can act as analogies for the technosocial systems we use to organise as societies, and can provide the test environment for the comparison of many types of social arrangements, centralised or decentralised, and power structures, symmetric or asymmetric. This can further our understanding of the complex dynamics of social structures. Using a multi-agent complex system simulation is only the beginning: information-theoretic methods are robust and often data independent, and criteria based on emergence may be applied to data from the real world, possibly even providing more accurate indexes of social or economic development.

However, the 'iron law' isn't perhaps as inevitable as its name implies: recent studies of anthropology and comparative archaeology (Graeber & Wengrow, 2021) have shown that pre-historic and indigenous communities were capable of seamlessly transitioning between centralised and decentralised social arrangements, with appropriate checks and balances to avoid getting 'stuck' in any particular form of hierarchical structure. Almost certainly such communities didn't use information theory to analyse their societies, but these results are perhaps a pointer that modern indices of democratic institutions and democratic processes could plausibly apply such tools in qualitative, quantitative and comparative assessments of a state of a democracy.

Part III

From collective motion to collective experience

Chapter 7

Case study: human groups walking

Chapter Summary

Having used simulation as a laboratory for testing emergence measures, explored their interpretations, and used them on real-world animal data, this chapter presents a new experimenal paradigm and technology for the study of collective self-organised movement in human groups, in which group members must devise strategies to achieve collective motion as quantified by the Ψ measure of emergence, and presents results of analysing the resulting trajectory data with similar methods to Chapters 4 and 5. Finally, we relate the results to collective intelligence and psychological aspects of the participants, showing that collective motion induces higher connectedness to others and is predicted by metacognitive awareness of individual strategies.

In the previous chapters, we have shown that Ψ, a synergy-redundancy index based on the mutual information, can robustly detect spatiotemporally cohesive collective motion in both particle simulations and real world data of self-organising collective motion, especially when using the redundancy in the system to adjust the threshold for emergence. Nonetheless, the trajectory data provided by the simulations or the real-world experimental observations of collective movement cannot provide enough insight into how individuals coordinate their actions and meet collective goals, or what are the mechanisms of their interactions.

One of the aims of this thesis is to explore how the principles of self-organisation in animal groups on the move can be applied to human behaviour, and whether any form of technology can foster human collective intelligence in a self-organised fashion similar to swarm intelligence in nature. Among the many types of collective behaviour in humans, the most straightforward cases of self-organisation can be observed in the case of collective motion, such as pedestrian flows, crowds at sports or artistic events, and ritual behaviours. They are also the most similar behaviours to many of those studied in the animal kingdom, and thus the obvious test-bed for our study.

Inspired by the collective intelligence shown by animals who perform transport and foraging optimisations through movement, we address the research aims by designing and executing an experiment with the goal of inducing collective walking in a human group in order to solve a spatial multi-agent optimisation problem, as quantified by the information-theoretic criterion of emergence Ψ. In other words, by posing the goal to optimise a system-level measure that is known to be high on flocking data, we can study how the participants learn and test the strategies necessary to move together – the so-called mechanisms of self-organisation.

The experiment, developed in an interdisciplinary scientific collaboration with artists, computer scientists, information theorists and cognitive psychologists, uses `Synch.Live`, a technology that induces collective behaviour in human subjects by playing a game with a group task and following a collective feedback mechanism.

This chapter will present a background to similar research work informing the experimental methodology, followed by a description of the `Synch.Live` experimental system, which was developed, assembled and implemented in-house, as well as the experimental methodology as presented in (Sas et al., 2024a). The results to the collective intelligence task are presented and discussed alongside with the cognitive and psychological aspects, and more in depth quantitative studies of the flocking movement. Finally, we present the current limitations and possible improvements to the experimental and analysis paradigm, as well as discuss possible related prosocial benefits and future directions.

7.1 Collective movement and prosocial behaviour

The behaviour of groups walking together or crowds engaging in collective activities shares many similarities with the collective motion of intelligent swarms. This has been shown by the successful use of agent-based models for simulations of pedestrians or crowds (Helbing & Molnár, 1995; Klupfel et al., 2004; Von Schantz & Ehtamo, 2019). Another way to study self-organised collective movement is through experimental studies of collective activities such as sports events, concerts and rituals. In these cases, scientists have observed and quantified interesting collective spatiotemporal patterns resulting from the very simple interactions of individuals. Fascinating examples which strongly recall swarm intelligence are waves in sports events, also known as *la ola*, which emerge as people stand up and sit down as they see nearby people do so (Farkas et al., 2002; Farkas & Vicsek, 2006), 'mosh-pits' in heavy metal concerts where people run in circles, milling in the middle of large crowds (Silverberg et al., 2013), and the flow-like movement of hundreds of thousands of pilgrims around the Hajj (Alnabulsi et al., 2018).



Figure 7.1: **Various kinds of self-organising collective movement in human groups**: **(a)** spiritual ritual practice, where pre-established rules and social norms incite expansive, but often rigid colllective activities (Boyer & Liénard, 2006); **(b)** performance arts, where synergy emerges as a combination of training and rule following with improvisation and co-creation (Noy et al., 2015; Su & Keller, 2020); **(c)** pedestrian flows, formed as people avoid neighbours and obstacles (Helbing & Molnár, 1995); and **(d)** audience waves, whose physics remind of excitable media (Farkas et al., 2002)

Previous research has also tried to recreate this collective movement experimentally by instructing people to follow simple rules and instructions, which recall the simple rules used by the simple models of flocking. For example, human groups can move like a flock if they are instructed to follow their neighbours, either in a virtual game environment (Belz et al., 2013) or physically, in the dance studio (Leonard et al., 2012b). These studies focus on how the collective motion emerges from following neighbours, rather than studying the mechanisms of interaction which, are instead, given.

The difficulty of researching interactions is present even in such a controlled study, where the rules are given to the participants. Researchers have highlighted, for example, the difficulty in estimating which other people are being followed by each participant. The dancing study (Leonard et al., 2012b) made the assumption that people would choose the two nearest neighbours within an angle of view determined by their direction of movement, and observed the temporal evolution of the interaction network by quantifying clustering coefficients and node status for each dancer, but does not explicitly quantify interactions using one of the many existing pairwise measures (Cliff et al., 2023).

Collective movement in human groups has also been related to the emergence of collective intelligence. For example, availability of information to make decisions affects the emergence of self-organising leader-follower relations when walking in a large group (Dyer et al., 2008). In this experiment, groups of people were asked to walk randomly in a large space without talking, while no interaction rules were given so people could spontaneously follow others. Only a few group members were given detailed information about where to walk. Despite the lack of verbal communication, the informed individuals were followed by others in the crowd, forming a cohesive structure, putatively suggesting the same principles of the emergence of spontaneous temporary leaders seen in bird flocks and fish schools (Couzin et al., 2005; Múgica et al., 2022).

Another experiment in the study of group behaviour and phenomenology has linked prior synchrony of movement[1] and arousal to improved cooperation in a group marching task (Jackson et al., 2018). Furthermore, these findings were related to self-organised behaviours in religious rituals, which makes it particularly relevant to our own research. This study uses collective walking both in the experimental manipulations and in the collective task of testing the cooperation of naturalistic groups of up to 50 people. First, groups were asked to walk together following an experimenter. Here they were either asked to synchronise their stride or not, while walking with slower or faster speeds for lower or higher arousal. Next, the groups received instructions to gather, disperse or cooperate (for example, to create shapes with their positions, like a circle), with groups in the synchronous and arousal condition more likely to succeed. In our experiment, we

[1]The idea that physical synchrony has benefits to collective intelligence and prosocial behaviour will be further discussed in Chapter 8.

aim to employ a similar spatial cooperative task. The researchers use a ceiling-mounted camera to perform real-time tracking, which is referred to as *in-vivo spatial tracking*. This methodology will also be employed by our experimental technology, `Synch.Live`.

Amongst the few studies directly addressing self-organised collective behaviour in groups walking together, few of them attempt to quantify the collective spatial movement of humans using measures of emergence. For our experiment, we take inspiration from the large body of work studying flocking data using quantitative measures of interaction (Brown et al., 2018, 2021a; Crosato et al., 2018; Wang et al., 2011) and measures of emergence (Mediano et al., 2022; Rosas et al., 2020a; Seth, 2010), many based on information theory. Outside fields more specifically concerned with motorisensor synchrony between pairs such as coordination dynamics (Cornejo et al., 2017), such analysis based on information theory and more specifically, measures of information synergy and causal emergence has rarely been applied to human motion in larger groups.

While many different experiments address various aspects of our research questions, a collective movement study that quantifies information patterns in collective motion and relates it to both collective intelligence and social experience remains lacking. Thus we introduce a new framework for the study of human collective behaviour, and exemplify it through a novel experimental set-up which aims to address some of these gaps in knowledge, by setting up a spatial cooperative task which can only be solved by walking together and measuring the success in the task with metrics of emergence.

Furthermore, inspired by the suggested prosocial benefits of collective movement in cultural activities and ritual behaviour from related research, we aim to investigate the relationships between the group outcome in the collective task and psychological, cognitive and phenomenological aspects of the collective activity. Our experiment should allow for a mixed data collection design where qualitative and survey data is included in the analysis and related to the quantities related to measures of emergence. We hypothesise that players who demonstrate higher empathetic perspective-taking before the game and higher metacognitive awareness during the game will contribute to a positive outcome for the group; and that succeeding in the group task will induce an overall feeling of belonging or connectedness to others.

7.2 Experimental methodology

This section describes the experimental methods, including the technology custom-built for this experiment, but also the experimental setup, participants, data collection and analysis.

7.2.1 System Design

As previously stated, the goal of this experiment was to foster collective movement in humans as inspired by the principles of self-organisation in nature. The experimental design has been developed in collaboration with the artists and psychologists in the `Synch.Live` team. Its purpose is dual: the system can function both as social sculpture artistic installation and collective intelligence experiment. Designing the system for this dual purpose allows the experience to remain as naturalistic as possible, and thus capture more realistically the complex phenomena of a collective artistic activity within an experimental paradigm.

The main elements required by the experimental technology are real time (or in-vivo) movement tracking to obtain trajectory data, real-time computation of a criterion of collective behaviour, and a means to provide incremental collective feedback. These requrements are addressed by the design and creation of a *player* headset which can be used both for real-time position tracking with computer vision, as well as a part of the feedback mechanism, and a ceiling-mounted *observer* system equipped with a camera which can perform computer vision tracking of the players wearing the headsets and compute the instantaneous value of information-theoretic emergence criterion Ψ in real-time.

Similar to the study of group cooperation where people had to arrange themselves in certain shapes (Jackson et al., 2018), our experiment also uses a centralised goal given to the whole group, namely the optimisation of Ψ. Yet in spite of a centrally given task, the lack of explicit instructions or rules about how exactly to cooperate and the lack of an explicit goal still leaves enough room for participants to attempt self-organisation. To facilitate this further, we also disallow verbal communication, also encouraging more embodiment.

The group feedback mechanism is inspired by the synchronisation of fireflies in nature. Each headset is equipped with a blinking light, and the collective degree of synchronisation of the blinking lights is to incrementally increase with the amount of collective movement. This feedback mechanism is collective and distributed insofar as one player not moving together with others would delay the synchronisation of everyone present, making it

difficult to separate individual contributions from the rest of the group. Players would likely have to distribute their attention to everyone else in order to monitor the group's progress, which creates interesting oportunities for social inclusion and participation.

The design process involved conceptualising, prototyping, testing the prototype with volunteer participants, then reiterating. Three different prototypes were created for the headset and two for the observer system.



Figure 7.2: **Prototyping technological solutions for the experimental system.** (a) Iterations for the design of the *player* headset. First a larger Raspberry Pi 3B was used and the LED lights were mounted on a headband, while the external battery had to be carried by the user. In the next iterations, the system was miniaturised with a Raspberry Pi Zero but used a soft hat. In the third iteration, a portable battery was added using the brim of a bowler hat for support. (b) Iterations for the design of the overhead *observer* system. The first iteration uses a Raspberry Pi 4 with a plastic case and alongside the Raspbery Pi High Quality camera system with a fixed 6mm lens. In the second iteration, a metal case is used, the camera system is mounted on the case with a varifocal 2.8-12mm lens, and together they can be installed on a tripod or on scaffolding using a clamp. Metal wires were added as an extra safety measure.

Technology

The `Synch.Live` experimental system is built with open technology and open source software, making use of Raspberry Pi devices and the Raspberry Pi OS Lite (v2021-01-11 *Buster*) operating system, and custom Python software which is publicly available.

The system consists of the headsets worn by the study participants (*players*) and an overhead camera and central computer (*observer*). Each of the 10 *player* systems is built

around a black hat, on which a Raspberry Pi Zero W is installed. The device is equipped with a real-time clock (RTC) module, which ensures higher accuracy timing and lower temporal drift when devices are off. Individually-addressable LED lights using the WS2801 controller are wired around the brim and on top of the hat, and a portable 1350mAh battery wires both the Pi and the lights, providing approximately 4h of gameplay. The green light on top of the hat is perpetually turned on during the gameplay to be used for motion tracking. At the beginning of each game, the clocks on the players are synchronised and the brim lights blink at the same fixed frequency with a random delay (phase) at each blink. The amount of delay is dynamically adjusted in response to the players' value of the emergence measure Ψ, such that the delay is reduced as Ψ increases, up to a full synchronisation with no delay when a high enough value of Ψ is reached.

The *observer* system uses a Raspberry Pi 4 and a Raspberry Pi High Quality Camera with C-mount lens. For the experiment, the system was mounted in a custom-built hard metal case, with a clamp to attach to scaffolding, and safety wires. A varifocal 2.8-12mm lens was used, allowing an angle of view range of 30 to 140 degrees. The *observer* system records the movement from above at 12 fps, and similar to (Leonard et al., 2012a) performs hue-based object detection in real-time using OpenCV (Bradski, 2000), and object tracking using Kalman filters (Kalman, 1960), to obtain player trajectories. The *observer* also runs a server that computes the Ψ measure and broadcasts to the players the corresponding delay parameter that governs the synchronisation of the lights through a simple HTTP endpoint.

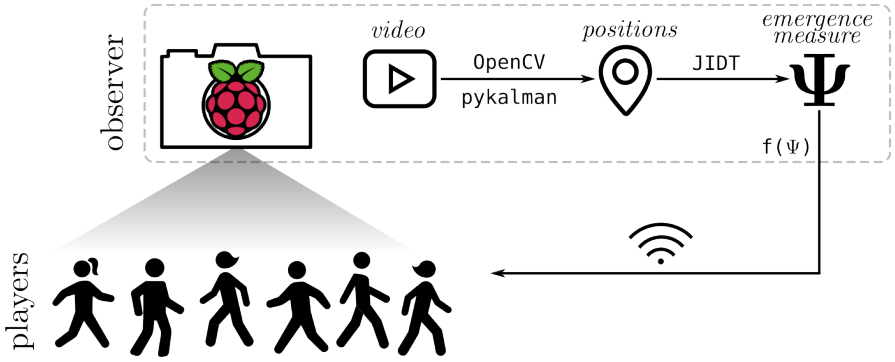


Figure 7.3: **Game loop diagram for `Synch.Live` system.** The players wear headsets with flashing lights used as tracking markers. The observer system extracts trajectories from camera footage using computer vision and Kalman filters, computes the emergence measure Ψ on the positions, and wirelessly broadcasts a synchrony parameter based on Ψ back to the player headsets.

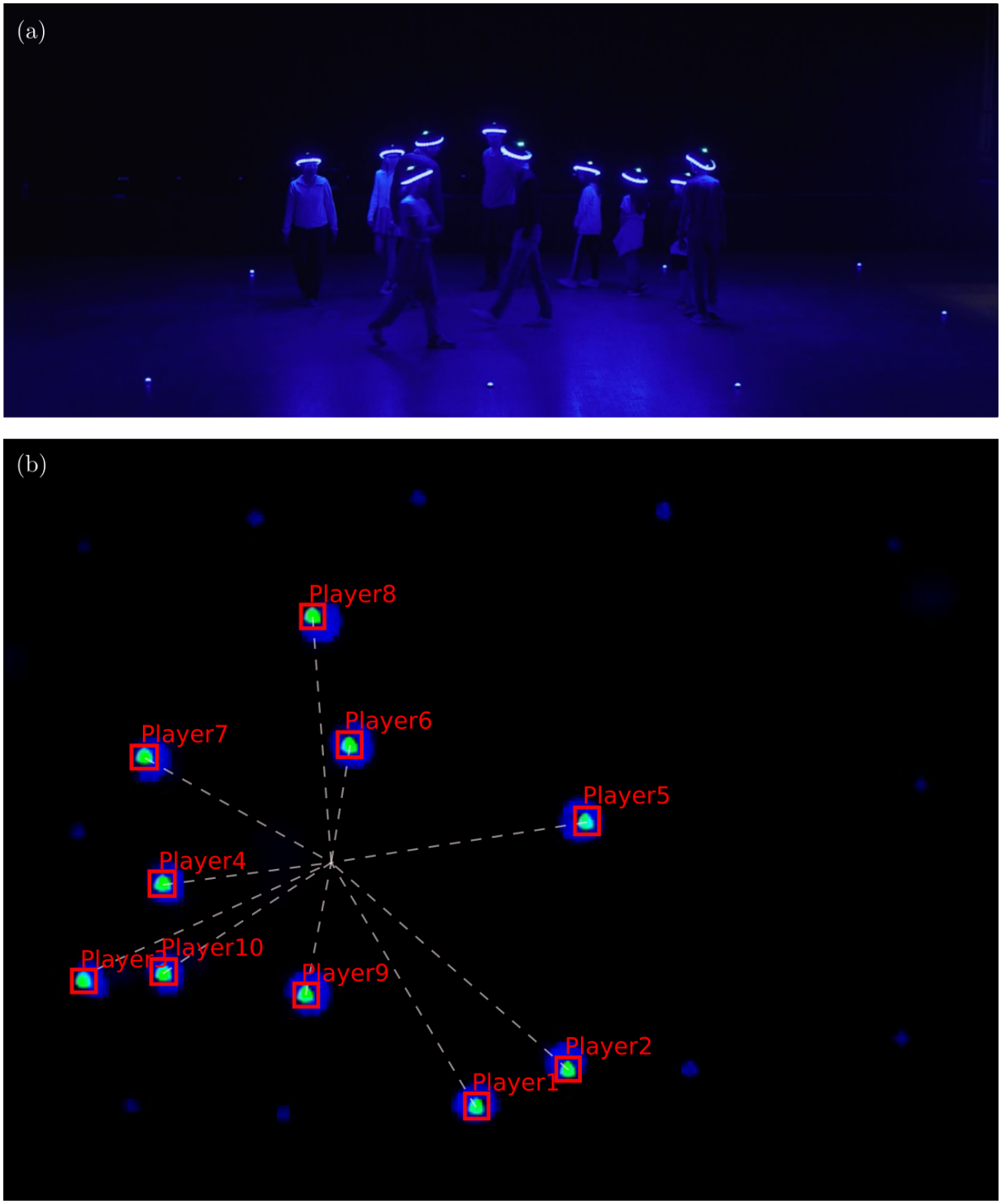


Figure 7.4: **The `Synch.Live` experimental technology in action**. (a) Photo of 10 participants wearing the headsets during an experiment. The players have just achieved a high enough value of Ψ to synchronise their blue lights, which are on at the same time in this instance. (b) Snapshot of the footage as seen by the overhead camera, taken at a very similar time in the game, overlaid with OpenCV tracking annotations. The dashed lines show distance from centre of mass, used for the computation of Ψ.

Measuring spatial emergence

To obtain a measure of collective behaviour, Ψ is calculated from the players' trajectory data as measured by the *observer* system. As seen in previous work, we take the 2D positions X_t^i of each player i at a given time t as microscopic features and the center of mass of the group V_t at a future time t' as macroscopic system feature.

Before estimating mutual information, the positions are normalised to the unit square. The future time is set as $t' = t+1$, where a discrete time increment refers to the next frame in the video, or a time window of approximately 83 miliseconds. The first 180 frames are used to estimate joint probability distributions on trajectories before computing mutual information in real time for the remaining frames.

As the redundancy inherent in a system of similar agents has been shown and discussed in Part I to grow with system size, the first-order redundancy correction was required for the robust estimation of Ψ for groups of 10:

$$\Psi = I(V_t; V_{t+1}) - \sum_i I(X_t^i; V_{t+1}) + (n-1) \min_i (X_t^i; V_{t+1})$$

As before, mutual information was estimated using JIDT (Lizier, 2014), and more specifically the `ContinuousMutualInfoCalculatorGaussian`, and the rendundancy function chosen was the minimum mutual information.

7.2.2 Experimental procedure

The experiment was performed on 18-19 June 2022, in the Great Hall of Imperial College London, UK, in the context of the Great Exhibition Road Festival (GERF).

The gameplay area was approximately 10 by 15 metres and delimited by an array of blue lights. The camera was fixed at a 8 metre height on a truss on the ceiling, and the varifocal lens was used with the widest angles of amost 140 degrees. This may have created some distortion in the image but did not interfere with the tracking. The experiment was run in the dark so the synchronous flashing of the lights is emphasised.

The participants were first instructed to answer questionnaires, then were invited into the gameplay area. They were tasked to *synchronise their lights by working together* before 10 minutes of gameplay have elapsed, following three rules:

1. No talking
2. No touching
3. Keep walking within the boundaries of the play areas

The group succeeds in the task once their motion produces a high enough value of Ψ, namely $\Psi > 3$ (with some minor variations due to technical setup e.g. 3 ± 0.1) and their headset lights are fully synchronised. After the game ends, participants are asked to fill questionnaires about their experience.

A gong sound indicates the beginning and end of the 10min period. Atmospheric music from Jon Hopkins' album *Music for psychedelic therapy* was played during the gameplay. We chose music without any clear rhythmic elements as to not affect the group coordination (Tunçgenç et al., 2021) but also inspired by successful outcomes in music-assisted psychedelic therapy (Bonny & Pahnke, 1972; Kaelen et al., 2018).

Participants

195 subjects in 20 groups signed up to participate in the experiment using the GERF website and advertising channels. Written consent was obtained from all participants. The subjects were distributed across 20 groups of $n = 9$ or $n = 10$ players, 10 on Saturday (groups A1 to A10) and 10 on Sunday (groups B1 to B10), of which 3 Saturday groups were not included (groups A2, A5, A7) due to issues with the experimental equipment. Group A10 did not complete any psychometric questionnaires. Data from a number of individual participants was also excluded due to lack of questionnaire responses, leaving $N = 109$ participants in 16 groups for analysis ($M = 6.8, SD = 1.7, n_{\text{min}} = 3, n_{\text{max}} = 9$).

Data collection

For each group, the trajectories of players and instantaneous emergence values were stored for the entire duration of the experiment.

Before the experiment, participants responded to the *perspective-taking* subscale of the Interpersonal Reactivity Index (IRI) (Davis, 1983), which measures the tendency to adopt the psychological point of view of others. After the experience, participants responded to a slightly modified version of Watts Connectedness Scale (WCS) (Watts et al., 2022), which has been used previously to quantify positive outcomes of psychedelic experience (Kettner et al., 2021), and is split in 3 subscales focusing on connectedness to self, others and the world. In particular, we specifically asked participants to rate their feelings during the experience, as opposed to the past two weeks, as in the original questionnaire. We focused only on the *connectedness to others* subscale, as it was the one most closely related to the goals in this study.

After the game, the participants' awareness of strategies used during the game was recorded through a free-form questionnaire asking the participants the following questions related to metacognition:

1. *What strategies did you use?*
2. *Were you aware of your strategy working?*
3. *What emotions did the experience induce?*
4. *Would you recommend the experience to others?*

In particular, the present analysis focused on the first two questions, relating the behaviours reported subjectively by the players to the behaviour of their group.

Ethical approval

This study was approved by the Science, Engineering and Technology Research Ethics Committee (SETREC), Imperial College London (Approval No. 22IC7800), and was conducted according to the Declaration of Helsinki.

7.2.3 Flocking study

The trajectories of players and their centre of mass can be analysed in depth with the many tools introduced in the previous chapters.

The initial analysis is performed by comparing the instantaneous Ψ with other observables of group behaviour used in swarming literature, such as the Vicsek order parameter (Vicsek et al., 1995) and density measures like the mean distance to the nearest neighbour.

We proceed by computing, beside the instantaneous synergy-redundancy index Ψ, the average values of the other emergence criteria for downwards causation and causal decoupling defined in Eq. 2.35, as well as the average pairwise information sharing, and the average amount of redundancy in the system. These quantities are compared between experimental outcomes.

The pairwise measure used to quantify the interactions is the mutual information, computed either synchronously or with a time delay, and instantaneously or averaged for the duration of the whole game.

From the pairwise measures, putative interaction networks are created using the python package `networkx`. Network backboning (Coscia & Neffke, 2017) is used to select the most statistically important edges, and effective leaders are estimated based on the players with higher node degree and status. Other network metrics as introduced in Section 2.4 are computed on the adjacency matrix or degree distribution of the interaction network.

7.2.4 Psychological data analysis

Psychometric questionnaire responses were processed to produce a value for *perspective-taking* between 0 and 5, and a value for *connectedness to others* between 0 and 100. The answers to free-form questions 2 and 4 were manually labelled as positive or negative, and used as a binary variable in analysis. Before analysis, data was standardised by subtracting the mean and dividing by the standard deviation, due to the large variety in scale between the questionnaires (on scales 0-5 and 0-100 respectively) and duration (from 50s to 375s).

The psychological data was analysed using R (v4.0.4) and the `lme4` package (v1.1-33) (Bates et al., 2015), while the significance of the statistical tests was computed using the `lmerTest` package (v3.1-3) (Kuznetsova et al., 2017).

For all studies involving game outcomes, groups with missing data or technical error were excluded, so questionnaire data from 109 participants over 16 groups was used.

Normality of the data data was tested using the Shapiro-Wilkes test (`shapiro.test` in R). To compare between groups or participants with different game outcomes in normally distributed data, we use Welch's two-sample t test using the `t.test` function in R with `paired=FALSE`. For data that is not normally distributed, we perform two-tailed Mann-Whitney U tests (also known as Wilcoxon rank-sum test) on the data from the two experimental outcomes using the `wilcox.test` R function. The Mann-Whitney U test can be used to test whether there is a difference between two groups, and the data need not be normally distributed.

Linear mixed-effects models were used with *connectedness to others* as dependent variable, game duration and *perspective-taking* as fixed effects, and group ID as random effect, using the following formula:

```
ConnectednessOthers ~ Duration * PerspectiveTaking + (1|Group)
```

To study metacognition, we counted participants based on game outcome and whether the answer to the metacognitive question (Question 2 in the free-form questionnaire) was positive or negative, resulting in four categories. The χ^2 test was used to obtain statistical significance, by using the function `chisq.test` with `correction=FALSE` in R.

7.3 Results

This section presents the successful results of the experiment as well as a trajectory analysis for the purpose of constructing interaction networks and studying leadership roles. The next section explores some cognitive and qualitative aspects of the players' experience through psychometric questionnaires and subjective reports in relation to the quantitative results.

7.3.1 Collective problem-solving through flocking motion

Out of the 16 groups, 10 of them successfully completed the task of achieving a high enough value of the emergence marker $\Psi > 3$ (Fig. 7.5a). This provides a validation of the *Synch.Live* technology, showing that collective behaviour can emerge without direct instructions and through group feedback.

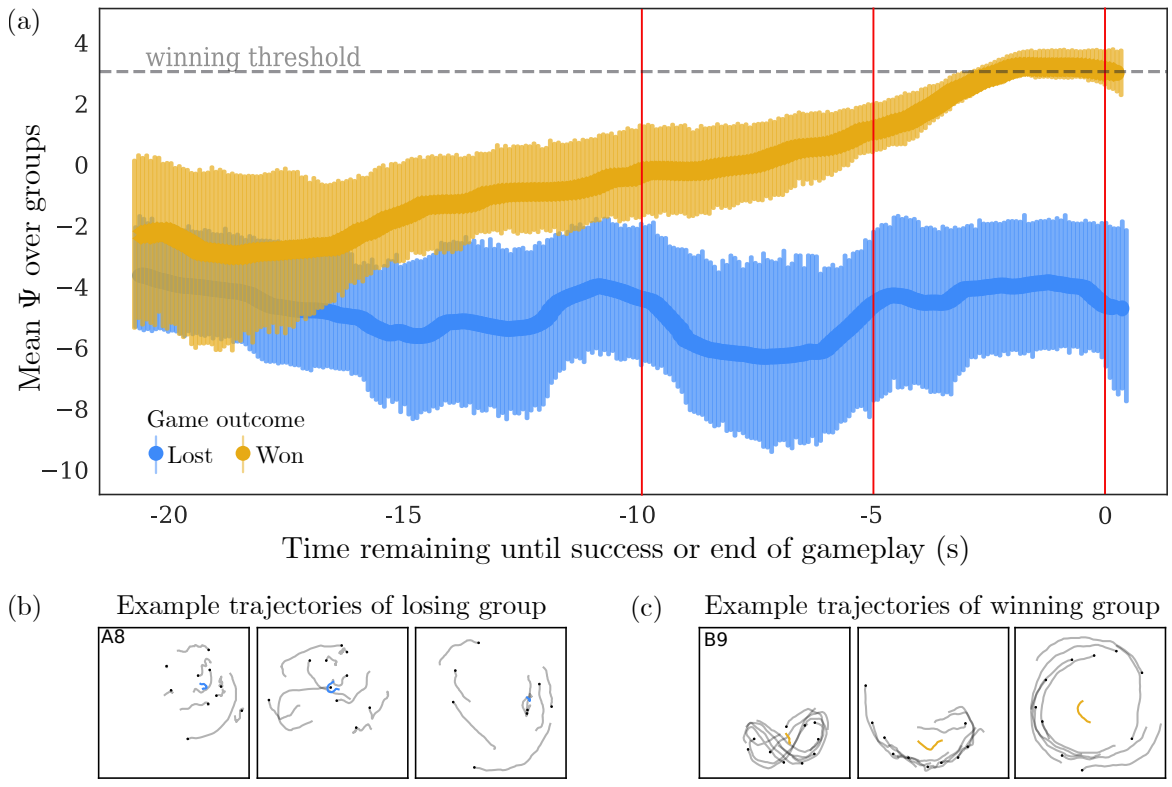


Figure 7.5: **Most subject groups succeeded in solving the task through collective motion. (a)** Average emergence measure Ψ from the last 20 s of 16 *Synch.Live* groups, separated by game outcome. Winning groups are characterised by a consistent trend of increasing Ψ. Shaded areas show standard deviation of the emergence marker Ψ across groups. **(b)** Three snapshots with 5s trajectories from an unsuccessful game, showing seemingly chaotic movement and no regular patterns in the positions. **(c)** Three snapshots with 5s trajectories from a successful game. The participants have organised without talking or touching and managed to create complex patterns such as a figure-of-eight, a school, and a cyclone.

As can be seen in Figs. 7.5b-c the unsuccessful and successful groups display qualitatively different patterns, with the latter showing not only aggregation and cohesion, but higher-order complex structures such as the figure of eight. The complexity of the movement patterns produced by the `Synch.Live` players is unlike any data produced by small simulations or even small animal groups experimentally. This unique dataset provides exciting opportunities for the quantitative study of complex collective motion.

In the analysis of this data, it is interesting to observe how optimising temporally-constrained information dynamics measures (such as the instantaneous Ψ) relates to the overall behaviour of the group for the entire duration of the game. Moreover, studying not just the synergy-related quantity, Ψ, but also the redundancy and any downwards causation in the system can reveal important insights into the way the players organise themselves, while pairwise TDMI may reveal something about pairwise relationships.

7.3.2 Flocking motion case studies

By simply exploring 30 second segments of gameplay and analysing trajectories one can see the emergence of at least three types of collective movement patterns, reminiscent of different behaviours in nature as described by (Couzin et al., 2002):

Milling or cyclone configuration, as seen in Fig. 7.6a, are characterised by high cohesion measures, high instantaneous Ψ, and a Vicsek order parameter close to 0 (low polarisation), with a high directional variance and high angular momentum. This has been seen in the behaviour of birds, fish and herd animals. Due to the entrainment of all participants in very similar movements which are very repetitive, milling appears to be characterised by high pairwise mutual information amongst most participants, high redundancy, and lack of decay in the strength of interaction even after 2 seconds of time delay. Nonetheless, as the interactions between players are strong and higher order, the Ψ is still positive in spite of high redundancy.

Swarming or cohesive configurations, as seen in Fig. 7.6b, are characterised by high cohesion measures, low polarisation, and a low angular momentum. This is more similar to the behaviour of insects. Trajectories of swarming configurations didn't necessarily result in high values of Ψ, especially as the players were confined in a small space and thus it was unclear whether the attraction between them is caused by a drive to move collectively or by the boundaries of the space. These configurations are characterised by much lower pairwise mutual information and redundancy, but also less cohesion which makes the self-predictability term in Ψ weaker.

Flow or parallel configurations, as seen in Fig. 7.6c, are characterised by high polarisation, low directional variance and low angular momentum. These movements are characterised by high redundancy due to the high degree of synchrony, and reveal in practice the dis-

advantage of using synergy-redundancy indexes to detect emergence. Nonetheless, when studying the self-predictability of the centre of mass $I(V_t; V_{t+2})$, as well as the minimum pairwise mutual information between all players, it becomes clear that this movement is highly structured and collective, with the value of Ψ being very small due to the very high amount of redundancy. These movements are similar to collective movement in bacteria, fish and birds in migration, and the flows formed by pedestrians.

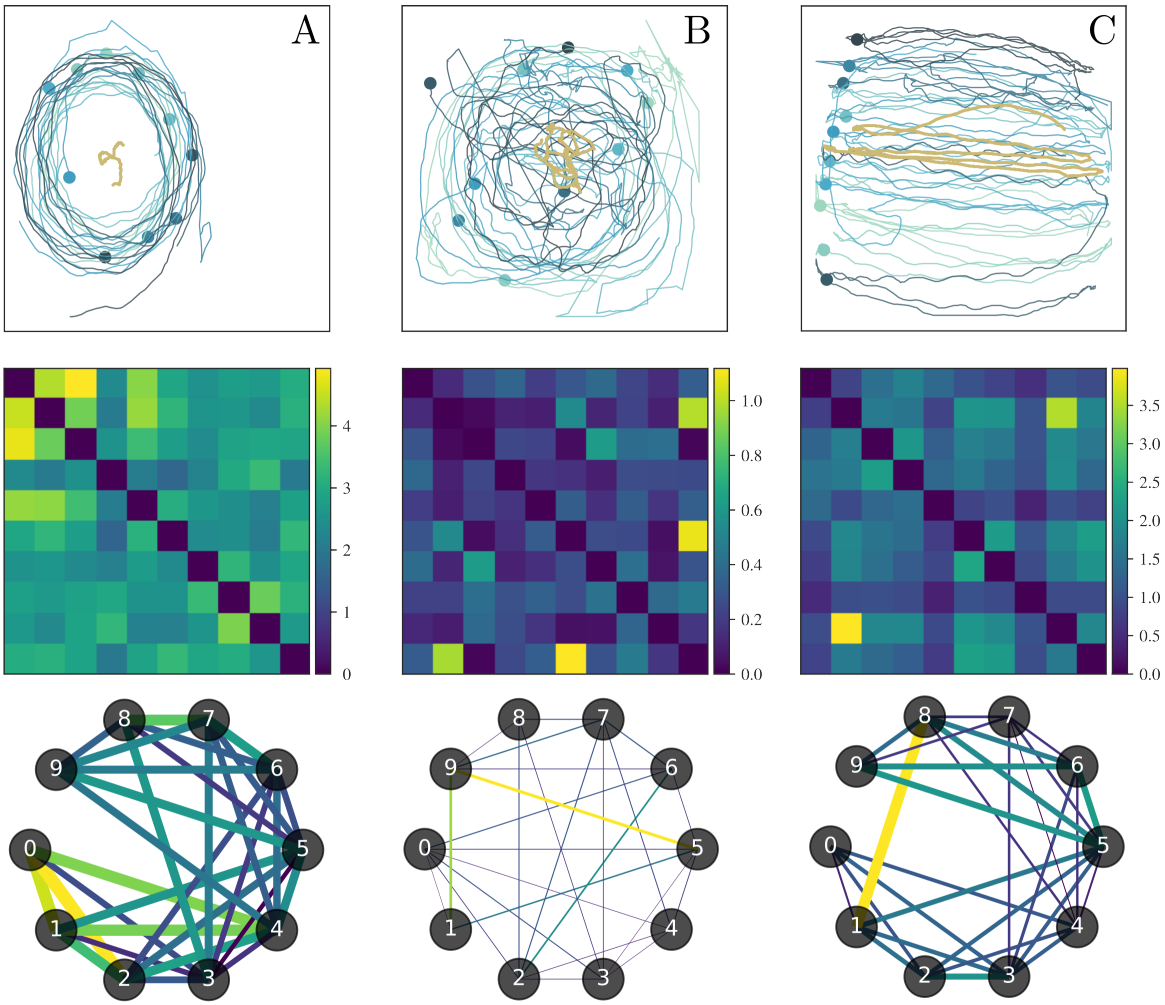


Figure 7.6: **A selection of collective movement solutions to the spatial group task. (A)** A group showing milling behaviour and associated pairwise mutual information networks. A very high amount of shared information is seen between most players. Moreover, when backboning the network, a tightly connected core remains. **(B)** A group showing swarming behaviour, characterised by much lower pairwise mutual information. The most strongly interacting players in this group had weaker interactions than the milling group. The players remain tightly connected to each other after backboning but the interactions are weaker, more uniform, and with less others on average. **(C)** A group showing parallel movement, characterised, again, by higher pairwise mutual information but a less stongly connected backboned network.

Finally, we even saw the emergence of even more complex behaviour in the form of the formation of intentional collective patterns, of which most complex was the figure of eight (Fig. 7.5c). While no metric can robustly detect such complex shapes, they are characterised by high emergence and high synergy.

When analysing the shortest winning game of group A3, which was completed by the players in less than 2 minutes by arranging into milling behaviour, manifests very strong information flow between players and even an interesting temporal prediction patterns. Compared to all other gameplays, Ψ increases after 2 seconds of gameplay instead of the power law decay seen in the other groups. Moreover, the average interaction networks between the players show extremely strong ties between many different pairs, and the higher-order redundancy is very high as well.

7.3.3 Psychology of collective behaviour

Empathy and connectedness to others

To better understand what makes certain groups of participants successful in this collective task, we assessed their tendency to adopt the psychological point of view of others. This was done through the *perspective-taking* scale of Davis' questionnaire on individual differences in empathy (Davis, 1983). We also investigated the effect of the collective experience on the participants' state of mind in relation to others through Watts' scale of *connectedness to others* (Watts et al., 2022).

A Mann-Whitney U-test shows members of successful groups had a significantly higher *connectedness to others* than non-successful groups ($W(38, 71) = 1012, p = .041$; Fig. 7.7a). The median connectedness for successful players was 68.8 ($s.d. = 18.5$), compared to 60 ($s.d. = 16.1$) for unsuccessful players. This suggests that more emergent collective movement, combined with a collective reward for achieving a joint goal, has a positive effect on the sense of feeling connected to others. On the other hand, contrary to our hypotheses, no significant difference was seen in *perspective-taking* based on game outcome ($t(82) = -1.06, p = .29$).

Additionally, we asked the question: taking into account group differences, is the *connectedness to others* of a winning participant predicted by their *perspective-taking* and the game duration? Linear mixed-effects modelling on the standardised data revealed a weak positive effect of *perspective-taking* ($\beta = 0.23, p = .052$) and a weak negative effect of duration ($\beta = -0.34, p = 0.07$) on *connectedness*. The strongest positive effect on *connectedness to others* is from the interaction between *perspective-taking* and duration ($\beta = 0.42, t(65.3) = 3.44, p = 0.001$), even though there is some variation between subjects ($s.e. = 0.12$) (Fig. 7.7b-c).

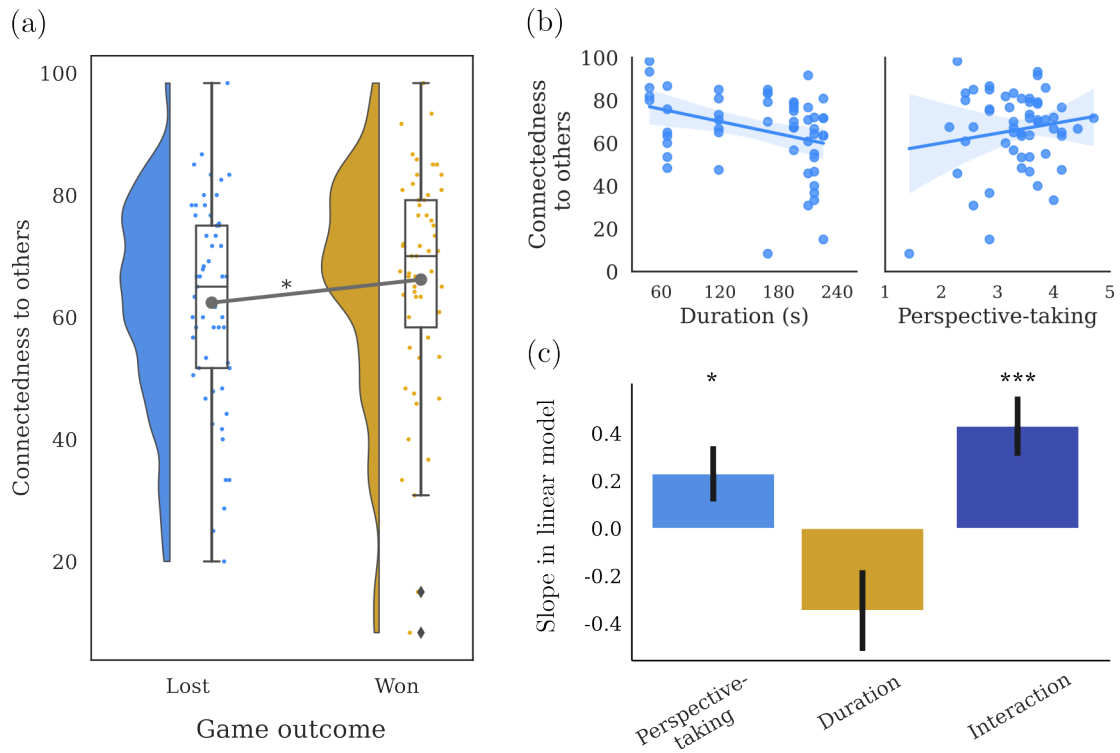


Figure 7.7: **Relating game outcome to duration, state and trait psychometric measures. (a)** Raincloud plots of audience responses to connectedness, grouped by game outcome. There is a significant difference in *connectedness to others* ($W(38, 71) = 1012, p = .041$) depending on the game outcome. **(b)** Linear regression plots showing the relationship between duration and *connectedness to others* ($F(1, 68) = 2.76, p = .19$), and *perspective-taking* and *connectedness to others* ($F(1, 68) = 1.73$), respectively, for all the players belonging to successful groups. Both are non-significant in isolation. **(c)** Bar graph showing the slopes (mean estimates) in the linear mixed-effects model (with *connectedness to others* as the target) for each variable: *perspective-taking*, duration, and their significant interaction ($\beta = 0.42, s.e. = 0.12, t(65.3) = 3.44, p = 0.001$). Error bars represent standard error for the fixed effects.

This result suggests that players with higher empathetic perspective-taking, especially when they quickly succeeded in the game, were likely to feel more positive outcomes in their emotional connection to others.

Successful players have increased metacognitive awareness of strategies

To understand individual contributions to solving the group task, we asked participants to report on strategies used and whether they were aware the strategies were successful.

Chi-squared tests of independence showed that people who were aware of using strategies were more likely to succeed in the game than those who were not aware or not sure ($\chi^2(1) = 4.91$, p = .026), as can be seen in Fig. 7.8. This indicates that participants were able to learn a solution to a challenging multi-agent coordination problem (Wong et al., 2023) based on limited information and provided through a sparse reward signal based on the emergence measure Ψ.

Moreover, by testing the dependence of the ratio of metacognitively aware players in a group against game outcome, we observed a non-significant but positive trend (p=0.11): groups with more aware players are more likely to succeed.

The study of strategies as provided by participants in the final questionnaire confirms our hypothesis that a range of explicit strategies were used to obtain complex collective movement in human groups. Throughout the gameplay, most players in winning groups paid attention to all the other players in order to observe the group synchrony, while attempting various movements and walking patterns, both in isolation or with others.

Most players reported synchronising pace or direction with neighbours, following others or imitating movements (e.g. *Following a person very closely in pace and movement*, *Synchronising movements*, *Following one small duo led to everyone joining without communicating*, *Walking along the same path*), but some also confidently lead other players (e.g. *Leading by example*). In some groups, players tried to communicate with others via gestures (e.g. *trying to listen to nonverbal guesses/ body language from other people*) and successfully organised higher order patterns such as milling configurations, circles, and even the figure of 8 seen in Fig. (e.g. *walking in a sync circle equally spaced and a similar pace*, *Walking in a constricting circle*).

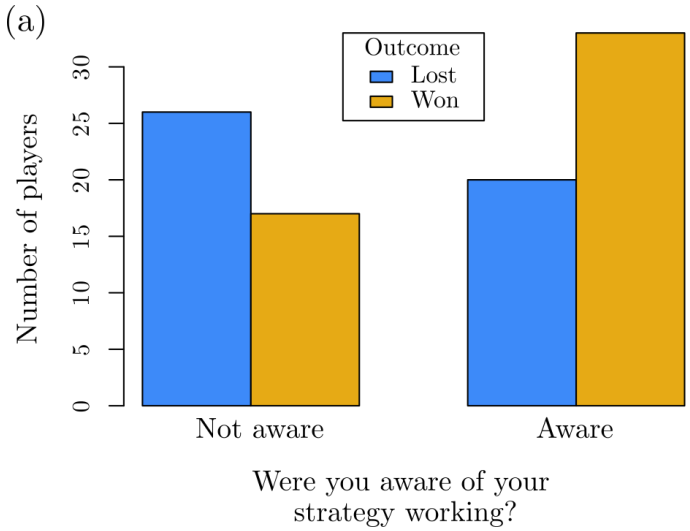


Figure 7.8: **Metacognition (strategy awareness) correlated with game outcome**. Most players who reported feeling aware that their strategies were working belonged to the successful groups, while more players who were not aware, or unsure, were part of the unsuccessful ones ($\chi^2(1) = 4.91$, p = .026).

7.4 Discussion

In the current global landscape, the study of human collective behaviour is a crucial discipline with huge consequences on social policy, government, and political issues (Bak-Coleman et al., 2021). In this work, we provided a framework for the study of collective behaviour through flocking motion in human groups, and we exemplify it with an experiment revealing its various psychological, metacognitive, and well-being aspects.

First of all, we found that humans can achieve collective movement without being told to do so explicitly. From the self-reports of participants, it appears the successful strategies are all related to paying attention to others and following neighbours, with only a few participants focusing on leadership. We are reminded of pedestrian flows and ritual behaviours, where social convention results in neighbour-following (Alnabulsi et al., 2018; Helbing & Molnár, 1995).

Pragmatically, a profound understanding of self-organised collective walking is crucial for urban planning and civil engineering, such as in the case of pedestrians walking on the Millennium bridge, who unexpectedly synchronised their stride, making the bridge shake (Strogatz et al., 2005). When maximum loads were calculated for the bridge originally, the planners did not take into account the spontaneous synchrony of steps that emerged in the pedestrians crossing it. Another example is evacuation (Von Schantz & Ehtamo, 2019), where central control is difficult and individuals often operate by instinct. A model with effective leaders has shown promising results (Ji & Gao, 2007), while canvassing large spaces in rescue operations can be successfully improved by ant colony optimisation (Morin et al., 2022).

The findings in this study can be related to many prosocial aspects of human behaviour. First of all, we may relate the solution the group task to the emergence of distibuted collective attention, where each participant had to observe everyone else in the group to assess synchrony.

Our results reveal that winning groups experienced significantly higher *connectedness to others*. This result opens up the possibility that such collective movement, incorporating group problem-solving and shared experience, could be a non-intrusive and non-pharmaceutical means of boosting well-being in a post-pandemic age of uncertainty, alienation (Dean, 1961), social isolation (Cornwell & Waite, 2009) and their negative impact on mental health (Brown et al., 2021b; Zhu et al., 2021).

We hypothesised that a higher degree of empathetic *perspective-taking* would have a significant effect on game outcome due to an improved ability to predict the others' strategies or behaviours. However, our results showed no significant difference between successful and unsuccessful groups, but only a weak trend. Instead, results showed a

significant link between *perspective-taking* and *connectedness to others* in the winning groups, with a strong interaction with game duration: players with higher empathy from groups that succeeded very quickly were more likely to feel more strongly connected to others. This could be interpreted as a form of improved social cohesion, in response to group success. Studying other psychological dimensions with well-being and social implications (such as the *Mental Well-Being Scale* (Tennant et al., 2007), *Communitas Scale* (Kettner et al., 2021), and the *Inclusion of Other in the Self Scale* (Aron et al., 1992)) is an exciting avenue for future work.

Last, but not least, our study shows that participants who were more aware of the strategies used and whether such strategies were effective were significantly more likely to succeed in the group task than those who were not aware or not sure. This result suggests the two-fold aspect of collective behaviour: namely, the interplay between individuals' agency, confidence, and meta-cognitive awareness, and their interaction with others. This connection between metacognition and success in an emergence-based social game is in line with suggestions that consciousness may have evolved to manage complex social needs (Frith, 2010, 2007, 2008; Kanaev, 2022), further supporting views of the importance of consciousness for detecting and capitalising on high-level patterns (Bor & Seth, 2012; Bor, 2012).

7.4.1 Limitations & future work

We collected no information related to age, gender, ethnicity, or social relationships with other group members. Therefore, we were unable to ascertain at the current stage the effect of underlying social networks on the outcome. Children above 12 were allowed to participate, but only adults over 18 submitted questionnaire data. As some groups had a larger number of young participants than others, the smallest number of respondents per group was N=3, while the largest was N=9. We had a total number of 135 responding subjects from the total of 195 participants. This considerably reduced the statistical power of our study and unfortunately obscured some very important winning strategy, as groups with many children are often more likely to succeed in the task.

Due to limitations in the experimental hardware and the means of data collection, we were unable to link individual questionnaire responses to individual trajectories, and had to complete our analysis at the group level. An exciting avenue for future work is to repeat the effective leadership analysis on the trajectories, and match those players with their personal responses regarding strategies and subjective ratings of their experience.

Finally, it is important to better investigate the effects of the collective activity on participants' state of mind. Currently, it is unclear whether the state of increased connectedness is a result of the collective motion and its inherent physiological synchrony, or of the social

and cognitive aspects of successful group problem-solving. It would thus be interesting to ascertain whether groups that manifest collective motion would also manifest synchronised physiological markers, such as breathing rate, heart rate variability, and arousal, and even more so to study the neural activity of the players of Synch.Live.

7.4.2 Conclusions

Our study shows how groups of people can spontaneously work together – without following a predefined leader or rules, and using only non-verbal communication – to solve a task only guided by a group feedback mechanism. The groups' solutions manifested as various forms of flocking movement displaying emergent spatiotemporal patterns. Furthermore, this collective activity has been found to induce social bonding through increased connectedness to others in successful groups.

Amongst groups, we observed a wide variety of strategies for addressing the collective challenge including imitation, improvisation, the arising of different effective leaders who proposed various strategies, and even the development of non-verbal forms of communication and planning through gestures. Moreover, success in the group task is predicted by individual awareness of strategy.

In summary, our results demonstrate that collective movement can be elicited within human groups as a solution to a collective task without explicit instructions, resulting in increased feelings of connectedness to others even in groups of strangers. Overall, this study shows the potential benefits of harnessing the study of collective movement, and not just art, sport or music, to elicit well-being and social cohesion in a divided world.

Chapter 8

Case study: Collective motion of concert audiences

Chapter Summary

Physical and physiological synchrony is pervasive in collective human activities, and manifests in many different forms. This chapter focuses on collective synchrony in concert audiences, presenting related work, and explores the collective effects of improvisatory music performance on the audience. We investigated the experience of audience members during a classical music concert by analysing the audience's subjective reports and movement patterns. Our results show that performance with improvisational elements affect movement synchronisation dynamics between audience members differently at different timescales, which are predictive of changes in the subjective perception of music.

In the social sciences as well as anthropology, it is often argued that collective behaviour in humans can have an important social function: to build and enhance social cohesion through collective experience. Extensive ethnography and anthropological research confirms how, for example, collective ritual behaviour fosters strong social ties between participants. One of the proposed mechanisms behind this phenomenon is through the interpersonal synchrony of physiology and state of mind, such as increased arousal (Jackson et al., 2018; Konvalinka et al., 2011). Meanwhile, participating in artistic activities, like watching movies (Bacha-Trams et al., 2020; Richardson, 2019) or listening to music (Tschacher et al., 2023), has also been found to produce an emergent collective state of physical or physiological synchrony.

In the previous chapter, we have seen how collective motion and solving a collective intelligence task can induce feelings of connectedness in pariticipants, and made a first step to relate our measure of emergence developed on spatial motion to something much more profound: the state of mind of the individuals. So far, in this thesis we have focused on information-theoretic measures of emergence, which have been particularly useful in the study the emergence of spatiotemporal patterns. In this final chapter, we focus more on temporal emergence, using the wavelet methods introduced in Section 2.2. In the spirit of exploring how complexity science and emergence in nature can be applied to human behaviour, we continue with a study of collective experience as related to collective motion using wavelet-based measures to study the emergence of complex, metastable synchronous behaviour at different temporal scales.

In this chapter, the wavelet coherence transform introduced in Section 2.2 is used as a measure of synchrony, to quantify the collective movement of a seated concert audience. We present a concert-experiment which not only explores synchrony in the audience as a marker of collective enjoyment, but also investigates the effect of improvisation, and more specifically, classical musical improvisation, on experience, state of mind, and motion. This is a particularly interesting approach to be taken in classical music, where audiences are seated and assumed to be passive, but also where improvisation is not as prevalent.

This chapter presents the motivations for this experiment and exciting results showing the emergence of multiscale synchronisation dynamics as quantified with the wavelet transform. The experiment was designed by Takayuki Nozawa and his team, who also provided the technology and analysis method. The full details can be read in our paper (Nozawa et al., 2023). Where text is reproduced from the paper, it contains contributions by the co-authors.

8.1 Collective movement, synchrony and experience

Collective activities involving shared experiences are ubiquitous in human culture. They are believed to play crucial roles for strengthening social bonds, a sense of group belonging, and social cohesion (Castano et al., 2003). Empirical investigations have extensively explored the impact of interpersonal synchronization of physical activity on these social dynamics. Such synchronization is strongly associated with collective subjective experiences and prosocial outcomes in many kinds of group activities (Mogan et al., 2017; Rennung & Göritz, 2016; Vicaria & Dickens, 2016). These include feelings of unity, rapport or perceived social bonding (Baranowski-Pinto et al., 2022), such as the enhanced group experience in shared social, artistic and ritual celebrations (Alnabulsi et al., 2018) which may also be characterised by shared psychological arousal (Kettner et al., 2021; Konvalinka et al., 2011).

It has been suggested that motor synchronisation between individuals emerges spontaneously from their interaction, such as synchronization of body postures during communication (Shockley et al., 2003), but also when individuals engage with a common stimulus such as music (Madsen & Parra, 2022). The relationship between synchronisation and rhythm has also been extensively explored in the tapping literature (Repp, 2005). Moreover, movement, physiological, or behavioural synchronization has been linked to collective behaviour that is very complex and manifests even in much smaller groups. For example, synchronisation appears to be important for in-person communication (Higo et al., 2014; Varni et al., 2010), rapport and education (Nozawa et al., 2019), efficient group collaboration (Gordon et al., 2020) and even developing spontaneous reciprocal feelings of attraction to another person (Zeevi et al., 2022).

Among collective activities, music making and listening occupies an important place in all known human societies (Mehr et al., 2018; Trehub et al., 2015), and often reveals, even within unique, cultural-specific approaches, universal elements of expressing and perceiving emotional cues (Clarke et al., 2015). As a group activity, ensemble music-making requires high levels of empathy (Cho, 2019; Clarke et al., 2015; Laird, 2015), coordination (Tognoli et al., 2020), and synchrony (Keller et al., 2014), which support the emergence of spontaneous leaders (Chang et al., 2017), group improvisation (Noy et al., 2015; Walton et al., 2015), and group states of flow (Csikszentmihalyi, 1990; Shehata et al., 2020). Beyond the stage, music is known to also engage audiences in a participatory, reciprocal relationship with the performers (Brand et al., 2012; Toelle & Sloboda, 2019).

Within musical praxis, group musical improvisation is a very complex, creative and highly social process, which requires years of training (Jansen, 2018) and is an exemplary case of *collective intelligence* which produces complex patterns of behaviour and rich cultural artefacts. Improvisation also has widespread appeal, as evidenced by its varied expressions

across different cultures and musical genres (Matare, 2009; Nettl, 1974) as an emergent form of collaborative social creative behaviour (Sawyer, 2000).

However, from the early 20th century until recently, the mainstream of Western classical music performance has largely adhered to notation-based performance: following the score strictly and accurately, striving for the best and most expressive performance while avoiding spontaneous, improvisatory elements (Creech et al., 2008). Even so, in the last three decades, a more improvisatory approach is regaining attention in classical music. This approach is characterised by spontaneity and risk-taking, and allows performers to deviate from the written text, according to the stylistic language in question, in an unrehearsed coordination with ensemble partners (Leech-Wilkinson, 2020). A number of studies place the omission of improvisation from classical music performance and training under question, as this practice has been shown to enhance the musical experience of both performers and audiences, as seen, for example, in the increased brain signal complexity (as quantified by entropy rate) related to improvisational states (Dolan et al., 2013, 2018). However, improvisation remains more of an exception rather than the norm in Western classical concert culture at large, unlike in several non-European music cultures such as Arabic and Indian art music.

We refer to two performance modes described above as *Strict*, and respectively, *Let-go* (Dolan et al., 2018). Comparing *Let-go* with *Strict* performances of the same repertoire piece by the same performers allows us to manipulate collective musical experiences while controlling other factors.

In the context of Western classical music, coordination of physical movements between performers has been investigated thoroughly in the joint action literature (Chang et al., 2019; Keller, 2008; Volpe et al., 2016), yet previous experiments have rarely studied whether and how physiological or movement synchrony occurs between performers and audiences, or the synchrony among listeners themselves. Recently, it has been shown that audiences synchronise on physiological signals such as heart and respiration rate in many situations of music-listening (Ardizzi et al., 2020; Bernardi et al., 2017; Czepiel et al., 2021; Madsen & Parra, 2022; Tschacher et al., 2023). But regarding their motion, audiences to classical music are still mostly assumed to be passive and static, in contrast to other musical genres (Burger et al., 2013; Ellamil et al., 2016).

In this study, we challenge this assumption and explore the effect of innovative improvisational attitude to classical music performance on the collective motion of a seated audience. For this purpose, we developed a concert-experiment where two classical repertoire pieces were played twice, each in the *Strict* and *Let-go* performance modes, in order to compare and contrast between the two modes.

Albeit many psychological studies of music and improvisation tend to focus on short segments of a few measures being performed by many musicians (Donnay et al., 2014; Vieillard et al., 2008), the current experimental design allows us to address the improvisational character of performance and study its effects on the musical experience more comprehensively in an ecological, naturalistic manner.

During the experiment, we measured the spontaneous movement of the audience. Although the audience's spontaneous physical activity should be subtle, we expect that it is linked to the music itself as well as the physical movements of performers. Thus, we hypothesise the degree of physical synchrony in the audience can differentiate the way they perceive the different performance modes.

- *Let-go* would be perceived by the audience as more innovative and improvisatory than *Strict* performances. This is in line with previous work (Dolan et al., 2013, 2018), and here we aim to confirm the results with a larger group;
- *Let-go* would induce higher movement synchrony (with performers and within the audience) than *Strict* performances;
- *Let-go* would induce larger temporal variability in the degree of movement synchrony, due to the additional moments in which the audience face unpredictability in the music as it unfolds;
- the effects on the audience's perception and physical synchrony would be positively associated

Higher movement synchrony and its temporal variability would be positively associated with the degree to which the audience perceives the music to be innovative and stimulating. We posit that such performances, by virtue of their novelty and engagement, capture the audience's attention and foster a deeper connection with the performers and, indirectly, among the audience members themselves. This higher meta-stability of the synchrony can be seen a marker of adaptability (Mayo & Gordon, 2020), and is very relevant in synergetic, collectively intelligent group behaviour.

8.2 Methods

This section briefly outlines the experimental design and analysis methods relevant to results reported in the next section. Specific technical details as well as further analysis can be found in (Nozawa et al., 2023).

8.2.1 Concert experiment

The experiment involved the Portorius String Quartet, who performed movements from Mozart (*String Quartet no. 15 in D Minor K. 421*) and Haydn (*String Quartet Op.76 No.1 in G major, III: Menuetto. Presto*) quartets, as well as improvised work. For the repertoire works, the same piece was performed twice in two performance modes: *Strict* mode (strictly following every textual instruction while aiming for the best and most expressive performance), and *Let-go* mode (with a creative, improvisatory approach, allowing more risk-taking and spontaneous expressive gestures). Relevant performances are shown in Tab. 8.1. Audio-video recordings of the four repertoire pieces are shared on the Open Science Framework server.[1]

Participants

The performance was attended by 50 audience members. After removing subjects with missing data, we ran analysis for the remaining 42 audience members. 13 audience members wore blindfolds in order to identify the effect of visual information on the perception of the music.

Here we must note a diversity of nationalities, in particular 12 different nationalities from Europe, 4 different nationalities from Asia, plus 2 Australians and 1 Mexican. Moreover, unlike the usual distribution of classical music attendees, most of our participants were under 30, and also female. A large proportion were familiar with playing music, but only a subset were formally trained or actively practising.

Table 8.1: Pieces relevant to this experiment from the performance programme

Piece	Type	Composer	Performance mode
1	repertoire	Mozart	*Let-go*
2	repertoire	Mozart	*Strict*
7	repertoire	Haydn	*Strict*
8	repertoire	Haydn	*Let-go*

[1] Available at osf.io/ar64j

Data collection

The performers' head motion was measured with inertial measurement units (IMUs) placed on their their forehead. The audience's body motion fluctuations were measured with IMUs contained in smartphones worn around the neck by each listener (Nozawa et al., 2020). The devices produce time series of three-dimensional acceleration vectors sampled at 100Hz.

After each pair of successive performances, the audience rated their subjective evaluation of each performance on seven items: how they felt each performance to be (1) improvisatory, (2) innovative, (3) emotionally engaging, (4) musically convincing, (5) risk-taking, (6) familiar, and (7) sleepy (Dolan et al., 2018). The rating for each item was given on a six-level Likert scale (0—5).

Ethical approval

This study was approved by the Human Subjects Research Ethics Review Committee, Tokyo Institute of Technology (Approval No. 2019101) and ethical approval was also confirmed by the Imperial College Research Ethics Committee. The study was conducted according to the Declaration of Helsinki. Written informed consent was obtained from all participants.

8.2.2 Wavelet analysis

The wavelet synchrony analysis was conducted to identify frequency ranges where there are significant differences in the audience's synchrony between the performance modes.

First, the Euclidean norm is computed for the triaxial acceleration time series:

$$a(t) = \sqrt{a_x^2(t) + a_y^2(t) + a_z^2(t)} \tag{8.1}$$

Synchrony of each pair of signals is measured using the wavelet transform coherence (WTC) (Grinsted et al., 2004) of their acceleration norm time series. WTC which finds regions in time-frequency space where two time series covary, but do not necessarily have high power. Results were computed using the open-source `wavelet-coherence` Matlab package (Grinsted, 2004), with its default setting of the Morlet wavelet with $\omega_0 = 6$ as the wavelet function, and the scale resolution of 12 scales per octave. See Sec 2.2 for background and more details on the wavelet method.

WTC coefficients were computed between the acceleration norm time series of each performer and each audience member to obtain P-A sync, as well as between all audience members to obtain A-A sync. The WTC coefficients $R^2(t, s)$ were temporally averaged

over the duration of the performance $\langle R^2(s) \rangle$. Then, for each audience member, the coefficients with all performers, or all other audience members were averaged. This provides a measure of how much each audience member was in sync with others on average, at each timescale, for each performance.

Due to the similar duration of the repertoire pieces (between 120 and 140 seconds), the same wavelet scales (or Fourier periods) can be used to discuss all pieces. We choose a range of periods from 0.2s to 30s. The lower bound was chosen as the audience's physical activity in the timescales below it have no musically meaningful counterpart. The upper bound is chosen to minimise the spurious effects of the cone of influence.

8.2.3 Music performance analysis

To quantitatively study the music, a number of techniques for the analysis of performance (Bowen, 1996) are used on the audio data, focusing, in particular, on performance related parameters: tempo, dynamics and timbre.

Qualitative assesments of performance-related parameters were contributed by David Dolan and the quartet members, while David Dolan also contributed the measurement of tempo in Sonic Visualiser (Cannam et al., 2010). From this data, the mean and standard deviation of each bar's duration were computed. These durations were interpreted with respect to the tempo, time signature, and the conducting beat applied by the performers for that performance.

To analyse the dynamics of the performance, first the dual-channel audio was converted to mono, by averaging the two channels, then the loudness curve was computed in loudness units (LUFS) (International Telecommunication Union (ITU), 2023) using the `mzPowerCurve` plugin in Sonic Visualiser (Cannam et al., 2010) at a sample rate of 200, with a moving window of 480 samples.

As this study makes use of complex, often 2 minutes long pieces of music, some techniques for analysis of timbre and pitch, were difficult to interpret. On the other hand, we made use of entropy as a measure of music complexity (Margulis & Beatty, 2008). Entropy of the loudness curve, and spectral entropy, respectively, were computed using `lziv_complexity` and `spectral_entropy` in package `antropy` (Vallat, 2018) applied on the loudness curve and directly on the mono WAV audio data.

8.2.4 Statistical tests

To study differences between performance modes, we use audience ratings and the average synchrony and temporal variability of synchrony at each period. We estimate a three-way mixed-effect multilevel model that includes the performance mode and composition as within-subject factors and blindfolding as a between-group factor with fixed effects, and each subject as random effects. We primarily focused on the main effect of the performance mode, as it directly addresses our hypotheses. The main effect of blindfolding and its interaction with performance mode address the impact of visual information available to audience. The composition was included as a controlling variable, so its effects were of little interest at the stage of experimental design. Using the `lme4` package (Bates et al., 2015) in R statistical software, the multilevel model is expressed as

```
rating ~ Blindfold * Composition * Mode + (1|Subject) +
           (1|Composition:Subject) + (1|Mode:Subject)
  sync ~ Blindfold * Composition * Mode + (1|Subject) +
           (1|Composition:Subject) + (1|Mode:Subject)
```

where the dependent (target) variable can be a subjective audience rating, average or variability of synchrony.

All the fixed-effect independent variables are zero-centered before estimation (Yaremych et al., 2023). Statistical significance of the variables were tested using the `lmerTest` package (Kuznetsova et al., 2017). In the analyses of physical synchrony, to correct for multiple testing over many timescales, false discovery rate (FDR) control via the Benjamini-Hochberg procedure (Benjamini & Hochberg, 1995) was applied to the p-values.

For each subject and performance, the mean physical synchrony values in the timescales with significantly higher sync in *Strict* were averaged into the *'beat-sync'* measure, while those with higher sync in *Let-go* were averaged into the *'music-sync'* measure. Synchrony variability values in the timescales with higher sync in *Let-go* were averaged into the *'music-sync variability'* measure.

To investigate how collective movement is predictive of the subjective evaluations by the audience, models of the form `rating ~ sync + (1|Subject)` were tested. Here, `sync` represents either the *'beat-sync'*, *'music-sync'*, or *'music-sync variability'* after centering-within-cluster. This analysis is equivalent to the within-subject repeated measures correlations (Bakdash & Marusich, 2017), and evaluates how the within-subject variances in the sync and rating are consistently correlated over the four performances (*Let-go* and *Strict* performance mode for the both pieces) or over the two performances with the different modes for each piece, separately.

8.3 Results

8.3.1 Audience's experience

Results reveal that the audience was receptive to the performance mode, rating the *Let-go* performances as significantly more Improvisatory ($p = 0.001$), Innovative ($p = 0.043$), and Risk-taking ($p = 0.004$) than the *Strict*. This is in accordance with our hypothesis 1 and previous work (Dolan et al., 2018). In contrast, no significant differences were found regarding how Musically Convincing and Emotionally Engaging both renditions were.

To quantify to what extent these ratings reflect either a unified factor or different aspects of the audience's experience, we performed a principal component analysis (PCA) to evaluate how much variance in questionnaire scores can be explained as being part of a single factor. Results show that the first principal component (PC1) – mainly consisting of the Improvisatory, Innovative, Risk-taking, and Emotionally Engaging items – accounts for 43.9% of the variance (see Fig. 8.1). Furthermore, the value of PC1 is significantly higher for the *Let-go* than the *Strict* mode ($p = 0.018$), supporting the idea that it captures a principal axis that differentiates between performance modes.

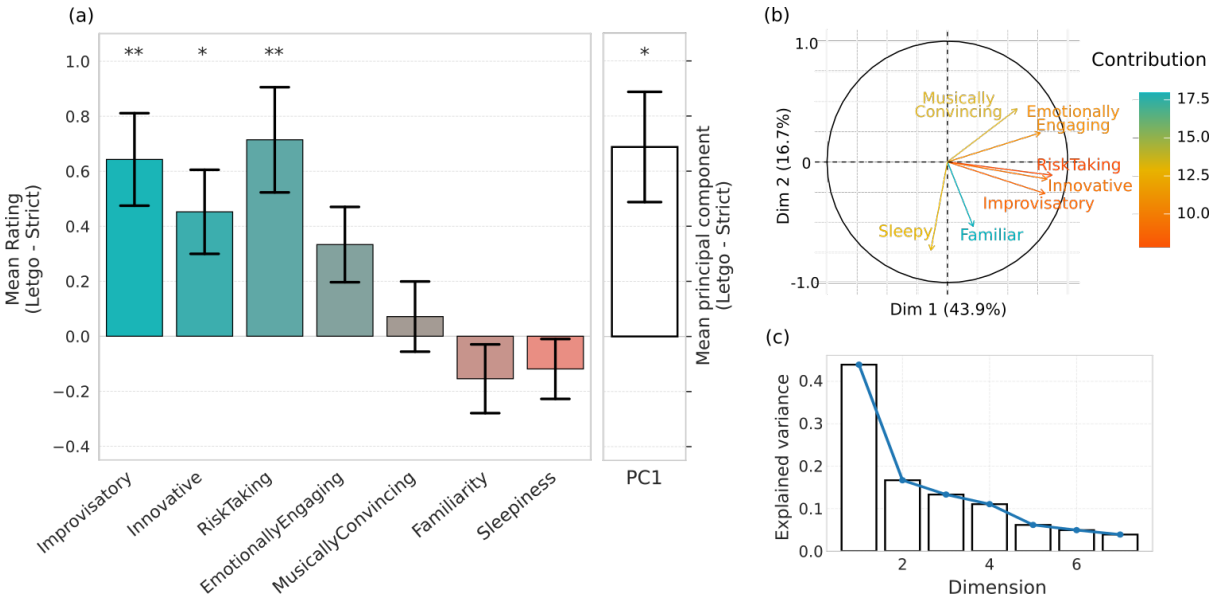


Figure 8.1: **Results for the listeners' qualitative ratings of the performances. (a)** Differences in the audience's perception of the two repertoire works between the *Let-go* and *Strict* modes of performance, showing all performance ratings and the first principal component (PC1). Error bars show standard error of the mean individual differences between the two performance modes. Listeners perceived the *Let-go* mode of performance as significantly more Improvisatory, Innovative, and Risk-Taking. **(b)** Biplot of the contributions of the first two principal components towards the 7 ratings. **(c)** Scree plot showing the amount of explained variance by the 7 principal components.

To explore the relationship between quantitative and qualitative aspects of musical performance, we also gathered subjective accounts of the performance from the musicians. All members of the quartet recognised that during the first pair of performances (of Mozart's piece), the discomfort they felt initially due to the experimental equipment affected their state of flow, causing their first performance to be more rigid than intended for a *Let-go* performance. In the second pair of performances (of Haydn's piece), they felt more together and more emotionally connected during *Let-go*, and also recognised many more moments of significant emotional expression in the *Let-go* mode.

Interestingly, looking into the effect of compositions on the audience's ratings, we find that the differences in PC1 and the Improvisatory, Innovative and Risk-taking ratings between the two performances of the piece by Mozart are weaker than those for the piece by Haydn, as revealed by significant interactions between the performance mode and composition factors by the multilevel models. These results indicate that the audience perceived the differences between the *Let-go* and *Strict* performances of Haydn's composition, but they were not as sensitive to the difference between *Let-go* and *Strict* performances of Mozart's composition. Importantly, this is in accordance with the musicians' subjective reports on their own performance.

8.3.2 Multiscale movement synchrony

The second step in our analysis is to investigate collective motion in audience members, particular movement synchrony among listeners and with the performers, and how they are affected by the performance modes.

For this purpose, we analysed accelerometer data collected from the audience and performers. Synchronisation was computed by the the wavelet transform coherence (WTC) (Grinsted et al., 2004) across the entire spectrum of physical movement, considering the motion sync between audience members (A-A sync) and between performers and audience (P-A sync) over a wide range of timescales or periods.

Results show that in both repertoire pieces, the audience exhibits higher synchrony in the *Strict* mode only on shorter timescales, while during the *Let-go* performances, higher synchrony is seen at longer timescales (see Fig. 8.2).

Short timescales correspond to rhythmic elements of the piece as well as physiological signals such as breathing, and henceforth we refer to synchrony that dominates in *Strict* as *'beat-sync'*. In contrast, longer timescales above 10 seconds dominate in *Let-go*, corresponding to longer musical gestures related to higher-level semantics and musical expression (Godøy & Leman, 2010), which we therefore describe as *'music-sync'*.

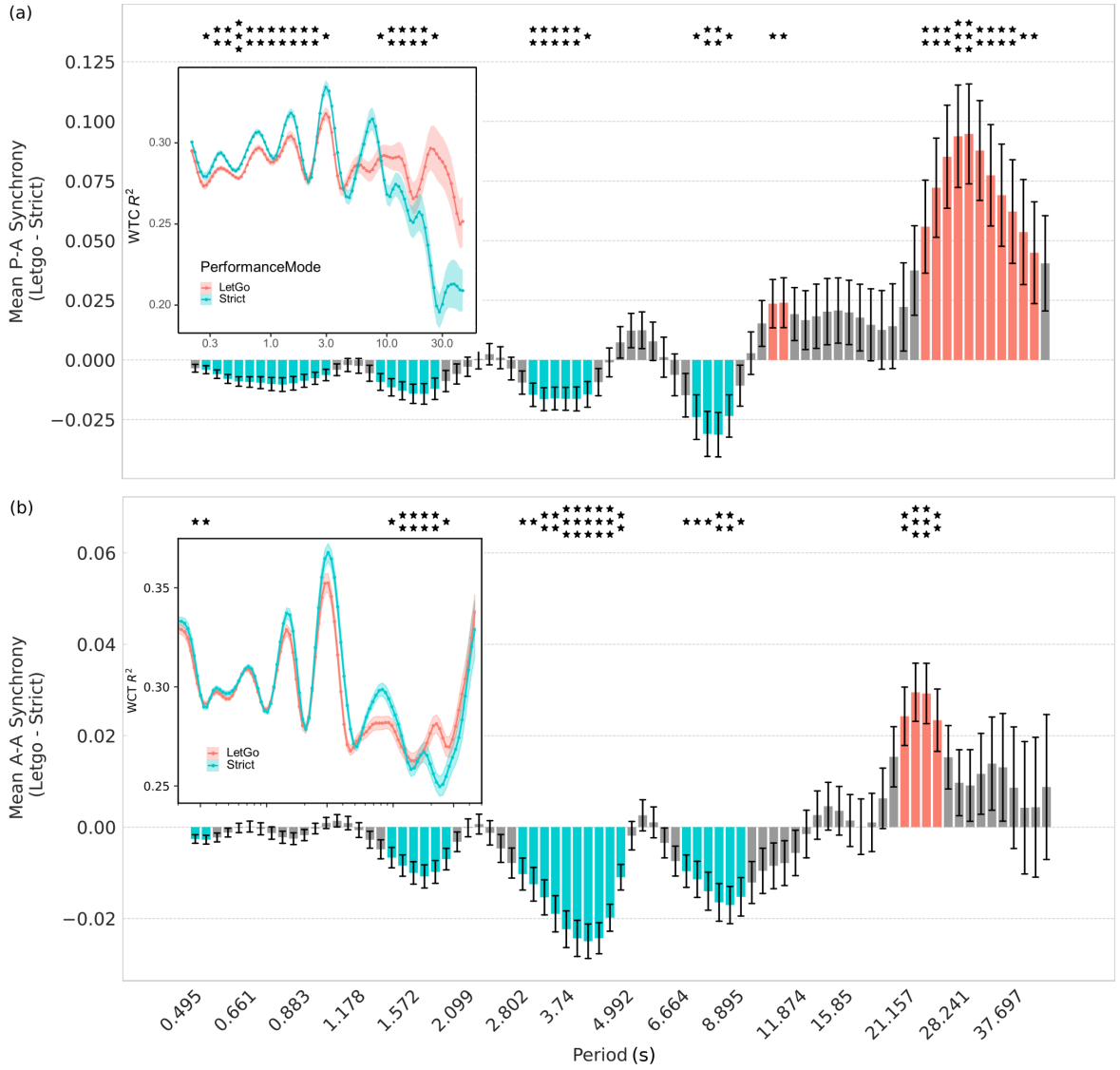


Figure 8.2: **Significant differences between modes of performance in mean synchony at each timescale. (a)** Difference in performer-audience (P-A) synchrony at different timescales (Fourier periods) between the modes of performance, *Let-go* and *Strict*, for both repertoire works. Colours reveal the two synchrony regions: scales with negative differences between *Let-go* and *Strict* in blue (*'beat-sync'*), and scales with positive differences between *Let-go* and *Strict* in red (*'music-sync'*). **(a inset)** Mean P-A sync at different timescales for the two modes for the repertoire works. **(b)** Difference in mean audience-audience (A-A) sync between the two modes for both repertoire works. Colours reveal the two synchrony regions. **(b inset)** Mean A-A sync at different timescales for the two modes for the repertoire works. Error bars in the main plots and shaded areas in the insets indicate standard error of the mean over 42 listeners. Periods with significant differences between modes are marked by asterisks. $*$: $p < .05$; $**$: $p < .01$; $***$: $p < .001$; FDR-corrected.

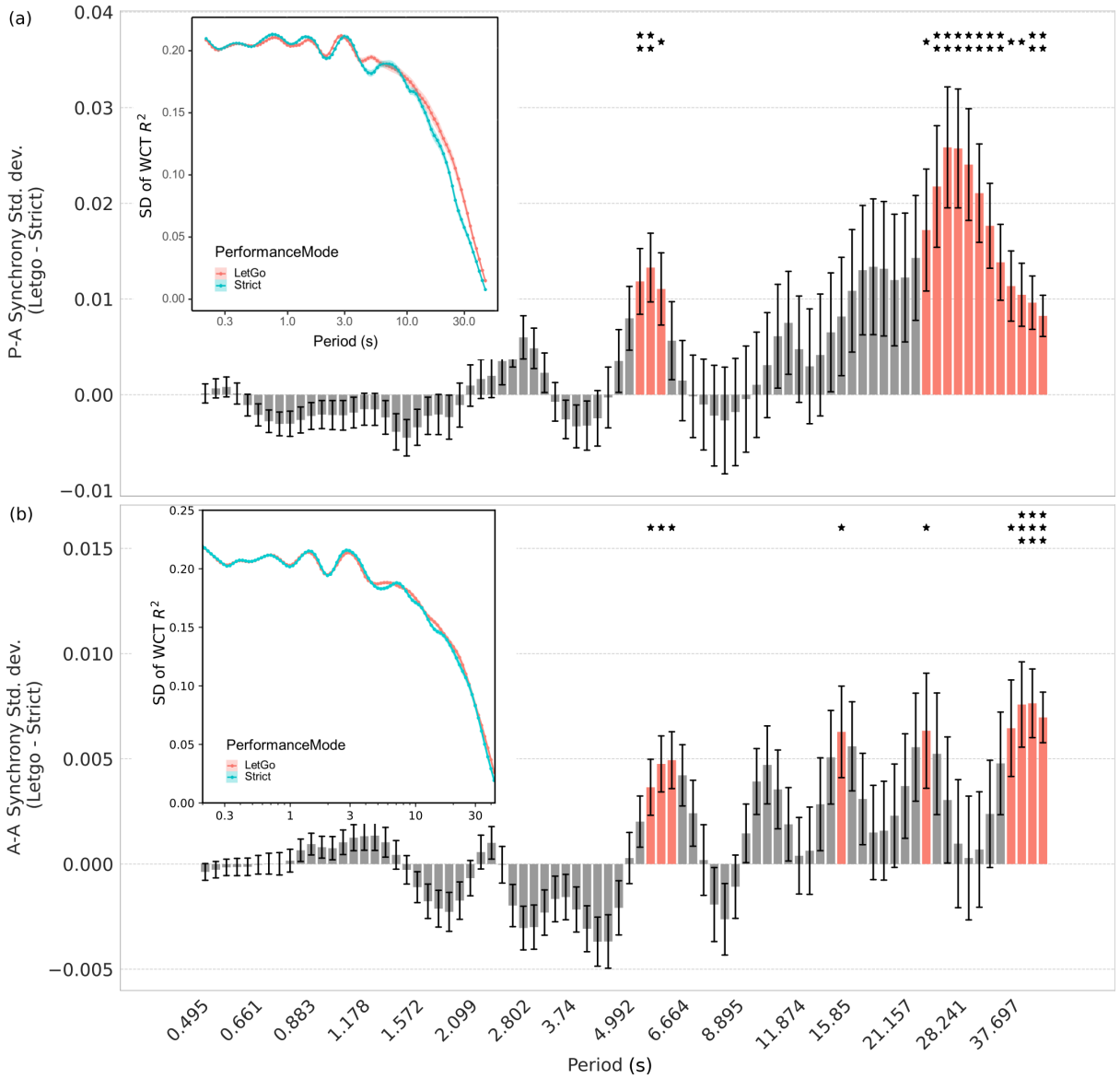


Figure 8.3: **Significant differences between modes of performance in synchony variability at each timescale. (a)** Difference in the temporal variability (standard deviation) of performer-audience synchrony at different timescales between the two modes of performance, *Let-go* and *Strict*, for the two repertoire works. Scales with significantly higher variability in *Let-go* than *Strict* mode (*'music-sync variability'*) are shown in red. **(a inset)** Temporal variability of P-A sync at different timescales for the *Let-go* and *Strict* performances of the two repertoire works. **(b)** Difference in the temporal variability of A-A sync between the two modes of performance for both repertoire works. Scales with significantly higher variability in *Let-go* than *Strict* mode (*'music-sync variability'*) are shown in red. **(b inset)** Temporal variability of A-A sync at different timescales for the *Let-go* and *Strict* performances of the two repertoire works. Error bars in the main plots and shaded areas in the insets indicate standard error of the mean over 42 listeners. Periods with significant differences between the two performance modes are marked by asterisks. $*$: $p < 0.05$; $**$: $p < 0.01$; $***$: $p < 0.001$; FDR-corrected.

In addition to the average P-A and A-A sync, we studied temporal variability of the P-A and A-A sync at each timescale. Results show that the audience exhibits significantly more variability of synchronisation at longer timescales during the *Let-go* performances (see Fig. 8.3). We refer to the temporal variability of the synchrony in these longer timescales as *'music-sync variability'*. No significant differences were observed at shorter timescales.

8.3.3 Synchrony predicts collective experience

To explore possible correlations between the amount of collective synchrony and the experience of participants, we studied whether the differences in synchrony found in the previous section were predictive of the subjective experience as reported in the questionnaire ratings. For this, we built multilevel models using the various questionnaire items as dependent variables, and mean synchrony or variability as independent variables, while accounting for subject ID using a random intercept (see Section 8.2 for details).

Results show that higher *'music-sync variability'* is most significantly associated with higher subjective scores (see Table 8.2), in particular the PC1 and items of the audience ratings that constitute perceived innovativeness of the performance.

	Beat-sync			**Music-sync**			**Music-sync variability**		
Rating	r	t_{125}	p	r	t_{125}	p	r	t_{125}	p
				P-A sync					
PC1	**−0.18**	**−2.04**	**0.043**	0.10	1.13	0.260	**0.24**	**2.82**	**0.006**
Improvisatory	**−0.18**	**−2.03**	**0.044**	0.10	1.14	0.256	**0.21**	**2.36**	**0.020**
Innovative	−0.13	−1.42	0.158	0.07	0.75	0.453	**0.25**	**2.86**	**0.005**
RiskTaking	**−0.28**	**−3.21**	**0.002**	0.14	1.52	0.130	**0.25**	**2.93**	**0.004**
Engaging	−0.14	−1.55	0.124	0.08	0.94	0.347	0.09	0.97	0.336
Convincing	0.03	0.32	0.747	−0.02	−0.23	0.821	0.16	1.81	0.072
Familiar	0.08	0.95	0.344	−0.10	−1.17	0.245	−0.15	−1.66	0.099
Sleepy	0.12	1.40	0.164	−0.09	−1.05	0.295	−0.15	−1.71	0.090
				A-A sync					
PC1	−0.08	−0.85	0.396	0.06	0.64	0.525	**0.29**	**3.43**	**<0.001**
Improvisatory	−0.14	−1.58	0.116	0.02	0.28	0.782	**0.34**	**3.98**	**<0.001**
Innovative	−0.09	−1.02	0.307	0.11	1.28	0.202	**0.29**	**3.35**	**0.001**
RiskTaking	−0.16	−1.82	0.071	0.12	1.31	0.191	**0.29**	**3.41**	**<0.001**
Engaging	0.00	−0.04	0.965	0.00	−0.05	0.958	0.05	0.55	0.586
Convincing	0.12	1.36	0.175	0.01	0.12	0.906	**0.23**	**2.63**	**0.010**
Familiar	0.04	0.47	0.637	0.07	0.79	0.432	−0.02	−0.24	0.809
Sleepy	0.08	0.88	0.383	**0.21**	**2.37**	**0.019**	−0.16	−1.85	0.067

Table 8.2: **Statistical relationships between ratings and collective movement**, described by the mean movement synchrony in shorter and longer timescales, and the temporal variability of synchrony in the longer timescale. Values in the r columns represent correlation coefficients, which indicate the strength and direction of the associations. Values in the t_{125} columns represent t test statistics with 125 degrees of freedom, which are obtained by the multilevel models. Significant associations with $p < 0.05$ are marked in bold.

In contrast, increases in the average *'beat-sync'* were negatively associated with PC1 and the Improvisatory and Risk-taking ratings. This indicates that higher synchrony in this timescale was linked to lower audience perception of the performance as Improvisatory. The significant association between *'beat-sync'* and subjective scores were observed only in P-A sync and not in A-A sync. Changes in average *'music-sync'* between audience members or musicians were not significantly linked to differences in the subjective scores.

This suggests that having more dynamic synchrony at the scale of the musical gestures related to higher-level semantics and musical expression is associated with the distinctive experience provided by the *Let-go* performance, while having higher synchrony with musicians in the *'beat-sync'* scale is more characteristic of the less improvisatory experience.

8.3.4 Music performance analysis

Assuming that music serves as the primary driver of the collective behaviour observed in the audience, our findings on movement synchrony and the audience's experience can be better contextualised by examining specific attributes of the musical performance with the aid of music performance parameters: dynamics, timbre and tempo.

A brief study of the piece's dynamics, by using the loudness curve reveals both *Let-go* performances had a larger dynamic range and showed higher pattern complexity, which is in line with higher level of unexpectedness in terms of performed expressive gestures and phrasing, and also in concordance to subjective reports by the musicians. Moreover, we observe that the results related to pattern complexity of the loudness curves are consistent with mode of performance, with higher values in *Let-go*.

Spectral entropy, on the other hand, which relates to the complexity of timbre, seems more consistent with the subjective reports of the musicians themselves, who maintained the modes of performance were not as clearly differentiated in the performances of Mozart. (See Tab. 8.3 as well as Limitations).

Finally, we studied the tempi of the performances using graphs of tempo curves generated in Sonic Visualiser (Cannam et al., 2010). For each performance, the musicians have established a beat of rhythmic reference based on the tempo, time signature and mode of performance.

When analysing tempo curves of the peformances of Mozart's piece, we related to a crotchet $^1/_4$ as a beat of rhythmic reference. Measurements revealed that the average duration of a crochet in the *Strict* mode is 0.74s, and 0.744s in the *Let-go* mode. This makes the mean duration of a half-bar approximately 1.5 seconds, and the mean duration of a bar approximately 3 seconds. When analysing the performances of Haydn's minuet, we studied the tempo in relation to one whole bar of $^3/_4$ as beat of rhythmic reference.

	Mozart *Strict*	Mozart *Let-go*	Haydn *Strict*	Haydn *Let-go*
Tempo variability (s)	**0.083**	**0.088**	**0.175**	**0.227**
Mean Loudness (LUFS)	**-42.99**	**-42.19**	**-45.23**	**-44.16**
Std. Dev. Loudness (LUFS)	6.62	6.74	8.23	7.48
Loudness pattern complexity	**1100**	**1106**	**1419**	**1442**
Spectral entropy	15.57	15.42	16.22	16.36

Table 8.3: **Quantitative comparison of perfromance-related parameters between the two modes of performance.** Results in bold show consistent differences between the two modes in both pieces.

The movement comprises three sections, *minuet-trio-minuet*, each with slightly different tempo, so we computed the average bar duration for each section. The average durations of each bar of three crochets is 0.6, 0.885, 0.551 seconds in *Strict*, and 0.631, 0.958, 0.585 seconds in *Let-go*, which all match to timescales included in *'beat-sync'*. Therefore, in both Haydn and Mozart performances, the mean duration of beats of rhythmic reference and musical gestures comprising of 2 or 4 such beats correspond to timescales within *'beat-sync'*.

On average, tempi were slightly slower in *Let-go* performance modes, and more importantly, we found tempo variability is consistently higher in Let-go than in *Strict* performance mode (see Tab. 8.3). This result agrees with the musicians' observation that the *Strict* performance mode is characterised by more rigidly even short-term beats and higher synchrony at a single, short-term beat level. It is also related to the fact that the audience may find these more rigidly even beats more predictable, likely causing the higher movement synchrony in short *'beat-sync'* timescales during *Strict* performances.

To understand the longer, *'music-sync'* synchrony timescales, we distinguish between the metronomic beat described above, and the deeper pulse of the piece, corresponding to musical phrasing and macrostructures. During the *Let-go* performance mode, in which an improvisational state of mind is applied, the pulse referred to by the quartet members is longer; and can change according to expressive intentions and, therefore, may have different durations. For example, in the Mozart piece, a phrase made of 4 bars would last on average 10-12 seconds, which is within the *'music-sync'* timescale. Longer durations in *'music-sync'* can be associated with even longer phrasing structures.

8.4 Discussion

This study investigated how the improvisational approach to performance, termed the *Let-go* mode, impacts the audience's collective experience in comparison to the *Strict* performance mode, which represents the mainstream approach in Western classical music performance. The analysis focused on three aspects: (1) the audience's ratings of the music as a quantifier of their experience; (2) movement synchrony between the performers and audience, and among audience members, as a quantifier of collective behaviour; and (3) the relationship between the ratings and synchrony to integrate the collective experience and collective movement aspects.

Consistently with previous studies (Dolan et al., 2018), audience rated *Let-go* performance higher than *Strict* counterparts in multiple experiential dimensions, suggesting that the experiment was successful in inducing differentiated musical experiences on the audience, as hypothesised.

Wavelet analysis revealed that an improvisatory approach to performance affects movement synchrony in the audience in opposite directions, depending on the timescale. In effect, *Let-go* performances reduce synchrony comparing with *Strict* in shorter timescales, while they enhance synchrony on longer timescales. Short timescales can be associated with the rhythmic pulse and physiological responses to it, which are more clear in the *Strict* rendition of the music, and longer timescales with longer musical macrostructures and musical phrases (Godøy & Leman, 2010).

Our findings, therefore, suggest that collective music experience is embodied in a multi-scale adaptive interaction between the performers and their audience, with these spanning a longer temporal horizon in *Let-go* renditions than in *Strict* ones. Similar time-scale dependency in movement synchrony has been observed in different forms of social interactions, including collaborative problem solving (Wiltshire et al., 2019) and joke telling (Schmidt et al., 2014).

Results show that *Let-go* performances increase the temporal variability of synchronisation on longer timescales, suggesting *Let-go* performances increase longer-timescale synchrony at specific timings rather than evenly throughout the performances. In other words, *Let-go* enhances the dynamical transition between a convergent (in-sync) phase, where the movements of audience members and performers are well-coordinated, and a divergent (out-of-sync) phase, where their movements are less coordinated.

From a dynamical systems perspective, this temporal variability in synchrony could be interpreted in terms of meta-stability, which captures the temporal dynamics between a high-synchrony ordered phase where the involving elements are coordinated and integrated into quasi-stable low-dimensional states, and low-synchrony disordered phase

where the elements are segregated leading to transient uncoordinated states (Hancock et al., 2023). In our musical context, *Let-go* performance makes the music less predictable for the audience at certain moments, which could lead to the higher degree of temporal variability in the degree of synchrony. Interestingly, in the context of dyadic interpersonal coordination, it has been suggested that meta-stability is a characteristic of well-functioning interactions (Mayo & Gordon, 2020). Along this thought, we speculate that the temporal variability of synchrony could signify how much the musical interaction between performers and audience is functioning in an adaptive and flexible manner.

The statistical associations found between psychological ratings and patterns of collective movement suggest that both may be reflecting different manifestations of the same underlying process. Higher synchrony in the shorter timescale was negatively associated with the audience's perception of the innovativeness of performances, which further supports the idea that the shorter-scale synchrony may reflect rather automatic and unconscious alignment to low-level structural or syntactic aspects of the music. That is, the more predictable a performance was, the easier it may have been for the audience to automatically get entrained into its rhythm. At the same time, the high predictability may have led to below the optimal zone of uncertainty for music pleasure (Gold et al., 2019; Stupacher et al., 2022; Vuust et al., 2022), giving the audience the impression the performance was less innovative. On the contrary, higher synchrony and its temporal variability in the longer timescale was positively associated with the audience's innovative experience.

8.4.1 Limitations

A major limitation of the current study is the sample size. Although the number of audience members participated in the study is almost double the number of our previous study (Dolan et al., 2018), the concert was held only once. It will be important to check whether the findings can be reproduced.

This limitation is even more important as we also attempted experimental manipulations including blindfolding, and collecting data about the participants' psychological absorption (Tellegen, 1974). As the results were not strongly significant due to small sample size, they are not reported in this chapter. Please see our publication for details.

We collected no information about social relationships between participants, and very little details on personality traits. For example, a recent study has shown that people's neural responses to viewing naturalistic stimuli are generally more synchronised with peers who have higher personality similarity (Matz et al., 2022). Another study indicated that pairs of strangers, friends, and lovers viewing a series of video clips show different physiological synchrony patterns depending on the emotion elicited by the videos, with a general tendency for higher synchrony between stranger pairs (Bizzego et al., 2020). While

the current study did not probe into these aspects, it would be interesting to explore how the social relations of audience members might enhance objective synchronisation and subjective musical experience in response to different types of performance approaches.

A final limitation comes from the difficulties of organising naturalistic concert-experiments and balancing between a realistic improvisational state of mind experience within the performers, and robust collection of experimental data. The experimental equipment has had effects on the state of flow of the musicians, causing the first performance of Mozart to be more constrained and less innovative, even though the performers were aiming to play in a *Let-go*, improvisational state of mind. This has resulted in a diminshed effect of the mode of performance in the first pair of pieces. Allowing the musicians to get used to the experimental equipment and context will help improve robustness of future experiments.

8.4.2 Future work

The findings in this study have not only scientific significance in and of themselves but also potential applications. Since verbalising and sharing collective creative experiences is very difficult, designing such experiences and evaluating their success is a particularly challenging task. Usually, this endeavor heavily relies on intuitive judgement from domain experts in the target field, such as music directors or concert organisers.

The current results involving the objective movement synchrony provide a first step towards the quantification of some aspects of these ephemeral experiences, opening the possibility for sensing technologies to evaluate their elusive yet important aspects. This evaluative information could help the design process by accelerating the try-and-evaluate loop and facilitating knowledge sharing.

Furthermore, real-time utilisation of the synchrony information could be used to enhance the experience of participants. For example, performers may be able to monitor the extent to which the audience is engaged and adjust their performance accordingly. It may be also possible, in some specific artistic contexts, to enrich the audience's musical experience by converting the synchronisation state into dynamic visual effects or sensations for other modalities, and presenting them along with the music.

8.4.3 Conclusion

In conclusion, this research uncovers the relevance of the often-neglected multiscale coordination between audience and performers, and reveals its deep connections with the quality of the collective subjective experience. Our results provide quantitative evidence that illuminates how a collective music experience is embodied in a multiscale dynamical

interaction which expands the group flow aspects of the relationships between the improvising musicians (Csikszentmihalyi, 1990; Noy et al., 2015) to a complex dialogue with the audience that is enhanced by the innovative, risk-taking and unexpected qualities of improvisatory performance. The current results provide a first step towards the quantification of some aspects of these ephemeral experiences, opening the possibility for sensing technologies to evaluate their elusive yet important aspects.

Last but not least, the reported results highlight the importance of regarding creative group activities as physically embodied collective experiences, suggesting that a rich tapestry of physical behaviour is underlying the shared experience even in audiences that are often regarded as passive. The contribution of multiscale synchrony to the positive experience of both performers and listeners is an exciting avenue for exploration in collective psychology and studies of group flow.

Chapter 9

Conclusions

Chapter Summary

The study of complex systems can provide many beneficial insights to better understand human behaviour, experience and society. In this chapter, we briefly review all the findings of the thesis and relate them to collective intelligence and shared experience. Finally, we outline some philosophical interpretations and some ideas for future work.

9.1 Summary of findings

At the beginning of this thesis, we set out to meet three objectives: identify candidate measures of emergence that can quantify collective behaviour; test them on different examples of collective motion across different characteristic scales and systems of interest; and finally, use them to foster (possibly self-organising) collective activities and prosocial outcomes in human groups.

Complexity science provides excellent tools to pursue this inquiry. Through research on swarm intelligence in animals and collective intelligence in neural systems on one hand, and the study of coordination dynamics and joint action on the other, we identified two candidate substrate-independent methods of analysis: information-theoretic measures of causal emergence $\Psi - \Gamma - \Delta$ introduced by (Rosas et al., 2020a) and inspired by developments in consciousness science, and wavelet coherence analysis used in interpersonal coordination studies (Issartel et al., 2015; Xu et al., 2013).

First, the Ψ measure was used to quantify emergence in random walks (Chapter 4), self-propelled particle systems (Chapter 4), multi-agent systems (Chapters 4 and 6) and experimental data of group movement (Chapters 5 and 7). We found that the measure detects collective motion in synthetic and experimental trajectory data, yet it is much more difficult to interpret when used to quantify coupled behaviour in Gaussian random walks. These findings, while conflicting, can be explained by an important distinction in the study of emergence: namely the difference between statistical dependencies among variables, and actual causal or mechanistic interdependencies between components or agents represented by those variables (Rosas et al., 2022). More specifically, we should note the measures used to construct the criteria, namely MMI-PID, have specific shortcomings in particular on Gaussian data (Barrett, 2015), as independent Gaussians have been found to show net synergy under MMI-PID. Moreover, MMI-PID has also been found to show that some systems become more synergetic when they are not behaving collectively (Varley, 2024), which may explain some of our findings in the null case.

Then in Chapter 6, we used the measures of emergence on *Megabike* (Scott et al., 2024a) a self-organising multi-agent system devised to study collective action and cooperation in various social structures. In the scenario employed for our experiment, emergence measures are used to quantify effectiveness of elected leaders in a situation characterised by voluntary association. We find both causal emergence and downwards causation describe all surviving groups, with the emergence criterion Ψ showing more variance in groups who were allowed more flexibility in knowledge alignment. To our knowledge, this work provides the first quantitative attempt to measure causal feedback loops in social systems, and opens up new possibilities of using emergence measures as quantitative indices of political systems.

In Chapter 7, we introduced `Synch.Live`, a participatory collective artistic experience in the spirit of social sculpture, which doubles as a behavioural science experiment. Framed as a game with an unspecified task and a group feedback mechanism, `Synch.Live` requires solving a spatial multi-agent problem through cooperation by 10 participants moving together in flock-like motion. We showed that solving an unspecified group challenge in response to group feedback is possible, and moreover, that flock-like collective movement has the potential to yield social benefits and well-being, such an increased sense of connectedness to others that has also been seen in group rituals and psychedelic therapy (Kettner et al., 2021). Furthermore, individuals with an awareness of working strategies were more likely to be part of winning groups, suggesting the importance of individual contributions to the group task.

Finally in Chapter 8, we presented a study of collective motion in humans with an alternative measure of emergence focusing on temporal synchronisaton. Since the audience was seated, and the study involved music, frequency domain methods are better suited in this case. In this experiment, we found that improvisatory music performance affects the collective motion and collective experience of the audience in different ways, at different temporal scales. And more specifically, that longer-period synchronisation and *metastable* synchronous states, which are characterised by flexibility and adaptability (Hancock et al., 2023), correlate with an innovative collective experience.

Studying the same measure accross multiple systems and use-cases allows us to get a better understanding of the methods and measures used. We confirmed the shortcomings of MMI-PID when used to construct the $\Psi - \Gamma - \Delta$ measures by testing the measures on Gaussian random walks, finding emergence false positives, where non-interactive systems are considered emergent by the criteria. Nonetheless, when used in non-Gaussian data and especially in two dimensions, we found it is strongly affected by redundant information accross components. A different PID may yield different results, depending of the redundancy function chosen. In the future, we should aim to find a measure that quantifies the same information, not only the same *amount* of information being shared.

9.2 Philosophical interpretations

From the multiple ideas of emergence proposed by philosophers and scientists alike, this thesis focuses on self-organisation and synergy, and is most concerned with emergent phenomena that arise from mechanistic or causal interactions between components, such as forms of coordination. Nonetheless, the studies in Gaussian random walkers have revealed very clearly that measures of causal emergence can also detect statistical interdependencies between time series that exist in spite of no interactions between components.

As such, researchers should always be mindful of assumptions and experimental paradigms, and whenever possible, introduce null cases where the agents do not interact for comparison. It is as important to focus on conceptual and philosophical frameworks which emphasise the interactions between agents, especially when considering animals or humans with physicality and agency. This makes it important to study experience and emotions, which are in turn intrinsically linked to action. Some of these ideas are briefly outlined below:

Embodiment and enactivism In Parts II and III, we suggested that movement is a transparent, observable phenomenon that can act as a proxy for the more ephemeral aspects of individual experience and agency, and can even be related to social interactions and coordination with others (Zhang et al., 2018). The philosophical frameworks of enactivism and embodied cognition emphasise the strong relations between body, mind, and environment, and argue that cognitive processes are shaped by physical, embodied interactions with the environment (Varela et al., 2016). Enactivism has been extended to include social aspects, more specifically the interplay between individuals and the processes of their interactions (De Jaegher & Di Paolo, 2007). These ideas are aligned with our findings in Part III, where collective motion was associated to various indicators of group experience, and success in a group task was predicted by individual awareness.

Agency versus structure In social philosophy, the agency-structure problem refers to whether human agency or social structure is the primary causal force in society. Our findings in Chapter 6 agree with the ideas of emergentist sociologists (Elder-Vass, 2010), who posit that social structures are causally emergent from individual actions and social interactions between agents, but also manifest downwards causation in how they affect the behaviour of individuals in turn, creating causal feedback loops. These ideas can also be related to embodiment and enactivism: agent behaviour is shaped by interactions with extrinsic forces – in this case social norms and structures –, but also, in turn, actions undertaken by agents can also shape social norms and structures.

Improvisation, adaptation, self-organisation Self-organization is often linked to learning processes within social systems. Communication channels and feedback mechanisms facilitate adaptation, allowing systems to respond constructively to environmental changes (Comfort, 1994). Furthermore, we may speak even of collective adaptation, when a group behaves intelligently as one and adapts in ways impossible to individual agents alone (Galesic et al., 2023). Studies of collective co-creation, such as musical and dance improvisation, have emphasised practically that improvisation is a crucial aspect of self-organisation in social agents. For example, improvisation requires musicians to spontaneously coordinate their actions with each other, and this is facilitated by achieving

an expert level as an individual. This coordination is not merely a result of individual cognitive structures but is better understood as a continuous self-organization of perception and action processes (Keller, 2008; Walton et al., 2015), and the interplay between rule-following and novel actions.

A similar finding has been reported in the human brain, where synergy is associated with cognition and redundancy with perception, as such balancing between varying degrees of adaptation and robustness required by each process (Luppi et al., 2022).

Shared experience and group flow An important aspect to discuss, especially with respect to the experience related to group activities, is phenomenology. Philosopher Thomas Nagel defines phenomenology as 'the subjective character of experience', claiming that 'an organism has conscious mental states if an only if there is something it is like to be that organism.' (Nagel, 1974). In the last part of the thesis, we found that collective motion changes, and is changed by, the subjective character of collective experience.

One kind of collective experience related to collective action is team or group flow (Walker, 2010). This state is marked by a deep sense of engagement where individuals experience a loss of self-consciousness and a merging of action and awareness with the group. Group flow can be seen in sports, teamwork, or co-creation, where participants not only share goals but also synchronise emotions and physical movements (Pels et al., 2018). In other words, group members not only act as one, but feel as one too. The work of philosopher Elisabeth Pacherie also emphasizes the role of collective emotions in shared experiences, highlighting how these emotions can emerge, for example, through perception-action matching as individuals try to predict each other's actions, and through joint attention, which provides mechanisms to share representations of objects and actions. This phenomenon has been called 'collective effervescence': where shared emotional states enhance social bonding and group identity (Chung et al., 2023, 2024).

Group flow was confirmed by subjective reports of `Synch.Live` participants, as well as subjective reports of ensemble musicians, who felt like they were 'reading each other's minds' in their most intense moments of togetherness during musical improvisation. In previous studies, these states have also been associated with increased brain complexity and information processing (Dolan et al., 2018; Wan et al., 2014)

9.3 Practical applications and future work

A number of practical applications and avenues for future work have been teased throughout this thesis. Here, we outline the most immediate directions where the quantitative research in this thesis can be applied, as well as some ideas for further research:

Traffic and evacuation Developments in swarm intelligence have already contributed to logistics and safety: natural computing by slime mould was used to optimise the Tokyo railway system (Tero et al., 2010), while ant colony algorithms have been used to optimise search and rescue operations (Morin et al., 2022). Combined with the prevalence of CCTV in public spaces and improved availability of drone cameras, the $\Psi - \Gamma - \Delta$ criteria for emergence could be applied directly to trajectories of human movement in cities. The criteria could provide a real-time quantifier of safe and efficient transport in busy areas, during search and rescue operations, or when evacuating buildings. Such real-time quantification of crowd behaviour could also indicate areas for immediate emergency response. Alternatively, the criteria could also be used on data from crowd simulations, in order to select from various alternative evacuation routes, for example.

Team sports science Many team sports manifest as complex forms of spatial movement and have been linked to self-organising group dynamics, even where the teams do have a pre-established leadership structure (Gréhaigne et al., 2011). Football, rugby, basketball etc. could be investigated directly with criteria of emergence, even with the same methods and technology used by `Synch.Live`. Already, indices of metastability and entropy have been used successfully to study diversity, adaptability and flexibility in group tactics when playing football, for example (Ric et al., 2016). Instantaneous Ψ computed on the movement trajectories of players could provide an index of how synergetic, flexible, adaptive or efficient various strategic configurations of the players are. Moreover, average Ψ computed for a specific team against different adversaries, in different conditions or with variations on team roles could provide a general index of team performance in various situations and optimise team configuration and player choices.

Team cohesion and performance Synchronization is known to enhance feelings of unity and efficacy, leading to improved group performance and satisfaction (Salanova et al., 2014). We also found that success in the group task of `Synch.Live` is associated to connectedness to others and predicted by individual awareness. As such, flock-like motion and physical and physiological synchrony may be used to facilitate improved team performance. First of all, since the multi-agent spatial task in `Synch.Live` requires situational awareness, metacognition, and improvising new strategies, it can be used as a control task in quantitative studies of team performance, by comparing various indices of performance between groups who have succeeded in `Synch.Live` and those who did not. The same kind of experiment could be undertaken but with inducing physical synchrony in a team before a group task (Jackson et al., 2018). Conversely, we may separately devise exercises that improve situational awareness, communication, or ability to improvise of team members, and test their success using the collective task in `Synch.Live`.

Quantifying ephemeral creative phenomena The methodology of our study of movement synchrony in concert audiences can be generally applied to many other instances of seated audiences, for example, audiences in the cinema and theatre, or students sitting in lectures. Multiscale synchronisation can be seen as a quantitative marker of the audence's enjoyment of a performance, lecture or film. In the performance arts, group synchrony could provide feedback towards improving the experience of both performers and audience, as well as the artistic artifact itself, thus creating an adaptive, co-creative process between audiences and performers. But it can also prove useful for screen tests of new films or during rehearsals.

Indices of team organisation or political systems As teased in Chapter 6, the *Megabike* multi-agent simulation could implement many different social structures in small teams. These can be tested comparatively using measures of emergence: for example, comparing an elected effective leader with an authoritarian one. In a similar fashion, we may devise methodologies based on measures of emergence which can be used to compare meta-aspects of team or organisation performance, such as different team hierarchical structures or lack thereof.

Relationship between flocking motion and synchrony In this thesis, we have focused on spatial and temporal emergence in collective movement. This was motivated on a case-by-case basis. Nonetheless, we did not investigate the relationship between the two methods. Recently, such an attempt was made in unifying findings from coordination dynamics and dynamical systems and findings in swarm intelligence (Zhang et al., 2019). More specifically, we may wish to investigate the emergence of so-called collective effervescence in `Synch.Live` through measures of synchrony applied to movement, breathing rate, heart rate variability, and arousal, and even study the neural activity and inter-brain synchrony of the players (Dumas et al., 2010). And more generally, we may wish to investigate the relationships between spatial measures of emergence and temporal measures of synchrony in collective behaviour in flocks, for example.

Emergence in space and time More generally, the methods explored in this thesis suggest two important aspects of emergence which were mostly investigated separately: structure forming in space, and patterns evolving in time. In general, the emergence of collective behaviour does not only manifest as a reduction in uncertainty when components are taken together, but also by observing reduced fluctuations in time. In other words, the emergent properties manifest as if the whole has a "life of its own". When agents work together, a small deviation in time is easily averaged into the collective behaviour. As such, temporal synchrony at a longer scale in general should be indicative of collective behaviour, including spatial pattern formation as well.

Most information-theoretic accounts of emergence do not formally discuss this issue. In contrast, in statistical physics, correlation functions can be computed both over space and time to give a more complete account of emergent behaviour. Findind a measure that has such advantages, and does not require prior knowledge of the collective behaviour like order parameters do, is an important direction for future work.

A possible such measure is the dynamical independence recently introduced by (Barnett & Seth, 2023), which depends on transfer entropy rather than PID. Dynamical independence allows a more mechanistic description of emergence: through modelling the dynamical systems underlying the phenomena under scrutiny and quantifying their state space with information theory, it allows for the discovery of emergent properties in both the time and frequency domain, and, moreover, across both spatial and temporal scales.

9.4 Closing thoughts

We are living in a time of social alienation and political division, where many people feel disconnected from their peers and the leadership structures who fail to represent their interests. But we have seen how but in the natural world of eusocial insects and social animals, social structures are created spontaneously from the interactions of individuals. Communication and attention to others are crucial here, as is rule-following, while at the same time encouraging diversity and agency.

We hope that this thesis provides an interesting interdisciplinary exploration which emphasises the importance of emergence and self-organisation in efficient group behaviour, in animals as well as humans, as a result of the conflicting tendencies between individual and collective drives, improvisation and rule-following, disorder and order.

Finally, we hope our findings will inspire people to both have confidence in their own agency and to cooperate with others, such that we may create the fine balance between synergy and redundancy which characterises some of the most adaptive, egalitarian, and efficient behaviours in nature.

In other words, so that we may be *together, but not the same.*

Image credits

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Fig 2.3: Lizier, J. (2015). *Kraskov (KSG) technique* [Figure]. Reproduced from (Lizier, 2015).

Fig 2.5: Williams, P. L. & Beer, R. D. (2010). *Fig. 2. Redundancy lattice for (A) 3 and (B) 4 variables* [Figure]. Free to use. Reproduced from (Williams & Beer, 2010).

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