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A minimal realization technique for the dynamical structure function of a class of LTI systems

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***Abstract*—The Dynamical Structure Function of a Linear Time Invariant (LTI) system reveals causal dependencies among manifest variables without specifying any particular relationships among the unmeasured states of the system. As such, it is a useful representation for complex networks where a coarse description of global system structure is desired without detailing the intricacies of a full state realization. In this paper, we consider the problem of finding a minimal state realization for a given dynamical structure function. Interestingly, some Dynamical Structure Functions require uncontrollable modes in their state realizations to deliver the desired input-output behavior while respecting a specified system structure. As a result, the minimal order necessary to realize a particular Dynamical Structure Function may be greater than that necessary to realize its associated transfer function. Although finding a minimal realization for a given dynamical structure function is difficult in general, we present a straightforward procedure here that works for a simplified class of systems.**

I. Introduction

In this paper, we address the problem of constructing a minimal state-space realization of a system represented by a specific Dynamical Structure Function. The Dynamical Structure Function (DSF), introduced by Goncalves and Warnick in [1] and [11], is a representation of linear time invariant (LTI) systems that encodes more detail about a system's structure than its transfer function (TF), but less than its state-space realization [3]. As a result, the DSF is a useful modeling tool for complex networks where some information about the network's global structure is desired without engaging the full complexity of a complete state-space realization [2], [5], [6], [12]–[14]. Examples of applications that have effectively leveraged the DSF as a modeling technology include system biology, in the reconstruction of biochemical reaction networks [4], [10], [17], [18]; computer science, in the vulnerability analysis and design of secure architectures for cyber-physical systems [26], [27]; and distributed systems, in the design of distributed and decentralized control systems [28]–[30] and structure-preserving model-reduction [15].

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Underlying all of these applications, however, is the theoretical question relating a Dynamical Structure Function to its minimal state realizations. The problem of characterizing the minimal state realizations of a given transfer function was considered by Kalman [7] and leads to many important insights about the nature of these distinct representations of an LTI system. In particular, these results reveal that a TF-minimal realization has no uncontrollable or unobservable modes, and that its order is characterized by the transfer function's Smith-McMillian degree. However, as will be shown here, a DSF-minimal realization may necessarily contain uncontrollable modes (but not unobservable modes) and that its order is bounded below by the Smith-McMillian degree of its associated transfer function. The implications of this result are profound, indicating that a particular number of uncontrollable modes may be necessary to realize a system with a particular structure e.g. a ring or a completely decoupled system.

Moreover, a surprising consequence of this fact is that a Dynamical Structure Function may have both stable and unstable realizations, including both stable and unstable minimal realizations. This disconnection between the stability properties of representations is not present with transfer functions and their minimal state realizations, making the minimal realization question considered here absolutely necessary to characterize the stability properties of a Dynamical Structure Function. Thus, for example, we can determine, using the techniques in this paper, that if the minimal realization of a given Dynamical Structure Function has no uncontrollable modes, then we know that its stability properties are the same as its associated transfer function. On the other hand, if we discover that uncontrollable modes are necessary to realize a given Dynamical Structure Function, then both stable and unstable minimal realizations may be possible.

The next section reviews the theory of Dynamical Structure Functions and relates them to both transfer functions and state-space realizations as representations of causal LTI systems. Section III then presents the main result, an algorithm for finding a minimal realization of a given Dynamical Structure Function for systems with no zeros and simple poles; results for finding the minimal realization of the DSF of a general system are in preparation for publication and can be found in [21]. Section IV then discusses the implications of these results, including the fact that DSFs can, in general, have both stable and unstable realizations.

II. Background: Dynamical Structure Functions

This section introduces the required definitions of causal dynamical network structures, commonly known as dynamical

structure functions (Section II-A). An example of dynamical structure functions can be found in the next subsection (Section II-B).

In network theory and applications, the most important step is defining what is actually meant by a network. This is a step that is typically ignored but fundamental to obtain well-defined networks. Just like state-space and transfer functions, networks are not well defined until system variables are fixed. For example, for a transfer function to be well-defined, we need to specify what the inputs and outputs are. These inputs and outputs are chosen carefully for particular objectives (for example to model or control the system). Similarly, for a network to be well defined, we need to specify what the nodes represent. In an electrical circuit that could be the current across active devices or voltages across them. In a mass-spring system it could be position and/or velocity of masses. In cell biology, the states could represent concentrations of molecules inside a cell. In addition, the relationship between non-measured (or hidden) and measured states also needs to be specified and fixed. Different choices of states lead to different networks, and it is up to users to define what network representation is useful to them. Once the state variables are defined (e.g. concentrations of molecules inside cells), then the state space is fixed and the DSF are also well define and unique. The remainder of this paper assumes that such a choice of states has been taken. Moreover, to simplify notation, the paper assumes that the first states are the measurements (outputs), followed by unmeasured or hidden states.

A. Definitions

$$\begin{array}{rcl} \dot{x} & = & A^o x + B^o u \\ y & = & C^o x \end{array} \tag{1}$$

where $x \in \mathbb{R}^n$, $u \in \mathbb{R}^m$, and $y \in \mathbb{R}^p$, and (A^o, B^o, C^o) are real matrices of the appropriate dimension. As discussed above, the choice of states is fixed, which results in unique matrices (A^o, B^o, C^o). Here we restrict our attention to the case where $p < n$, $C^o = [I_p \ 0]$ (where I_p is the $p \times p$ identity matrix) and $x(0) = 0$. The choice of $C^o = [I_p \ 0]$ reflects the fact that, after some reordering, the first states are the measurements, as explained above.

To define dynamical structure functions, we separate the state variables in two parts: $x^T = [y^T \ z^T]^T \in \mathbb{R}^n$ is the full state vector, $y \in \mathbb{R}^p$ are partial measurements of the state, and z are the $n-p$ "hidden" (unmeasured) states. Taking the Laplace transforms of the signals in (1) yields

$$\begin{bmatrix} sY \\ sZ \end{bmatrix} = \begin{bmatrix} A^o_{11} & A^o_{12} \\ A^o_{21} & A^o_{22} \end{bmatrix} \begin{bmatrix} Y \\ Z \end{bmatrix} + \begin{bmatrix} B^o_1 \\ B^o_2 \end{bmatrix} U \tag{2}$$

where Y, Z, and U are the Laplace transforms of y, z, and u, respectively. Solving for Z gives

$$Z = (sI - A^o_{22})^{-1} A^o_{21} Y + (sI - A^o_{22})^{-1} B^o_2 U$$

Substituting this last expression of Z into (2) then yields

$$sY = W^o Y + V^o U \tag{3}$$

where $W^o = A^o_{11} + A^o_{12}(sI - A^o_{22})^{-1} A^o_{21}$ and $V = B^o_1 + A^o_{12}(sI - A^o_{22})^{-1} B^o_2$. Now, let R^o be a diagonal matrix formed of the diagonal terms of W^o on its diagonal, i.e. $R^o = \text{diag}\{W^o\} = \text{diag}(W^o_{11}, W^o_{22}, ..., W^o_{pp})$. Subtracting $R^o Y$ from both sides of (3) gives:

$$(sI - R^o) Y = (W^o - R^o) Y + V^o U$$

Inverting $(sI - R^o)$ (which is always invertible since R^o is proper) leads to:

$$Y = QY + PU \tag{4}$$

where

$$Q = (sI - R^o)^{-1} (W^o - R^o) \tag{5}$$

and

$$P = (sI - R^o)^{-1} V^o \tag{6}$$

Definition 1: Given a causal LTI system described by its state space realization as in (1), define the *Transfer Function* as $G = C^o(sI - A^o)^{-1}B^o$.

Definition 2: Given a causal LTI system described by its state space realization as in (1), define its *Dynamical Structure Function* as the pair of transfer function matrices, (Q, P), as derived in Equations (2)-(6).

Definition 3: A dynamical structure function, (Q, P), is defined to be *consistent* with a particular transfer function, G, if there exists a state-space realization of G, of some order, and of the form (1), such that (Q, P) are specified by (5) and (6). Likewise, a state-space realization is consistent with (Q, P) if that state-space realization gives (Q, P) from (5) and (6).

Definition 4: A state-space realization is G-minimal if this state-space realization corresponds to a minimal state-space realization of G. A state-space realization is (Q, P)-minimal if this state-space realization is consistent with (Q, P) and its order is smaller than or equal to that of all state-space realizations consistent with (Q, P).

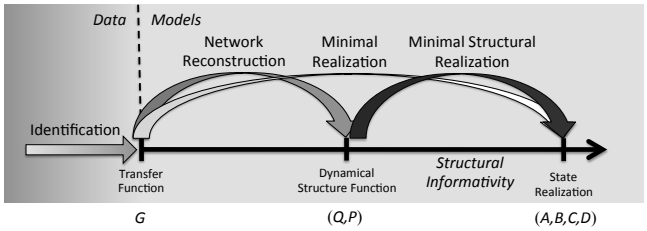

Fig. 1: Different types of representations for the same system describe different amounts of structural information. The Dynamical Structure Function captures more structural information than the transfer function, but less than the state-space realization. Identification, Network Reconstruction, and Minimal Realization are all problems of translating one, less structurally informative description of the system to another, more structurally informative description. This paper addresses the *Minimal Structural Realization* problem (dark arrow), translating a Dynamical Structure Function to a minimal state-space realization.

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B. Interpretation and properties

DSF have several important properties. For example, the diagonal elements of Q are zero and all other entries in (Q, P) are strictly proper.

Consider the following example to complement Figure 1 and better understand the differences between the state-space, the DSF and the transfer function.

Proposition 1: [21] Given a dynamical system (1) and the associated dynamical structure functions $[Q, P]$ with R^o constructed as explained above (see (1)-(6)), the following conditions must hold

$$\text{diag}\{A^o_{11}\} = \lim_{|s|\to\infty} R^o(s); \tag{7}$$

$$A^o_{11} - \text{diag}\{A^o_{11}\} = \lim_{|s|\to\infty} sQ(s); \tag{8}$$

$$B^o_1 = \lim_{|s|\to\infty} sP(s). \tag{9}$$

Proof: Eq. (7) is directly obtained from the definition of $R^o(s)$:

$$\begin{aligned}\lim_{|s|\to\infty} R^o(s) &= \lim_{|s|\to\infty} \text{diag}\{W^o(s)\} \\ &= \text{diag}\{\lim_{|s|\to\infty} W^o(s)\} = \text{diag}\{A^o_{11}\}\end{aligned}$$

Since the proofs of eq. (8) and (9) are very similar, we focus on eq. (8) only. In the following, we use the fact that for any square matrix M, if $M^n \to 0$ when $n \to +\infty$, then

$$(I - M)^{-1} = \sum_{i=0}^{\infty} M^i.$$

From the definition of Q in (5),

$$Q(s) = \sum_{i=1}^{\infty} s^{-i} {R^o}^{\,i-1}(s)\,(W^o(s) - R^o(s))$$

and

$$W^o(s) = A^o_{11} + \sum_{i=1}^{\infty} s^{-i} A^o_{12} {A^o_{22}}^{\,i-1} A^o_{21},$$

when $|s|$ has been chosen large enough so that $\left\|\frac{R^o}{s}\right\| < 1$ and $\left\|\frac{A^o_{22}}{s}\right\| < 1$.

Hence, $Q(s) = (A^o_{11} - R^o(s))s^{-1} + L(s)$, in which $L(s)$ is a matrix polynomial of s, whose largest degree is -2. Finally, multiplying by s on both sides and taking the limit as $|s|$ goes to ∞ results in eq. (8). A similar argument can be used to prove eq. (9). ∎

Remark 1: This proposition reveals an important property of dynamical structure functions: they encode the direct causal relations between observed variables, i.e., $A^o_{11}[i, j]$, $\forall i \neq j$. These relations cannot be encoded by transfer functions.

Example 1: Consider the following structured state-space system with its associated transfer function:

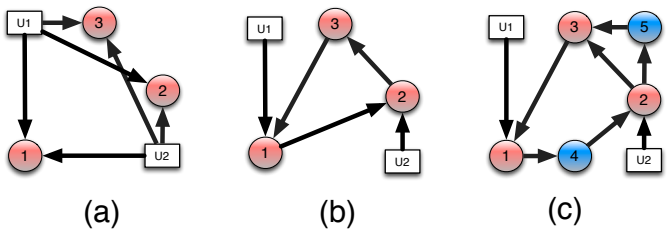

Fig. 2: The nodes represents states, square inputs and edges the directed interactions. Red nodes are measured states and blue hidden. **(a)** The graph topology of the transfer function, **(b)** corresponding graph topology given by the Dynamical Structure Function, and **(c)** graph topology of a system with two inputs, three measured states (states 1, 2, and 3) and two hidden states (states 4 and 5).

$$\begin{aligned}\dot{x} &= \begin{bmatrix} a_{11} & 0 & a_{13} & 0 & 0 \\ 0 & a_{22} & 0 & a_{24} & 0 \\ 0 & a_{32} & a_{33} & 0 & a_{35} \\ a_{41} & 0 & 0 & a_{44} & 0 \\ 0 & a_{52} & 0 & 0 & a_{55} \end{bmatrix} x + \begin{bmatrix} b_{11} & 0 \\ 0 & b_{22} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} u \\ y &= \begin{bmatrix} I_3 & 0 \end{bmatrix} x\end{aligned}$$

$$Y = G(s)U,\ G(s) = \begin{pmatrix} G_{11}(s) & G_{12}(s) \\ G_{21}(s) & G_{22}(s) \\ G_{31}(s) & G_{32}(s) \end{pmatrix},$$

where G_{ij} is generally not identically zero, that is, the transfer function matrix is typically full even though the state realization has a very particular sparsity structure. For this particular example, the underlying network for transfer matrix is very different from that for state-space as shown in Fig. 2.

According to the definition, the corresponding Dynamical Structure Function is then given by

$$Q = \begin{pmatrix} 0 & 0 & \frac{a_{13}}{s-a_{11}} \\ \frac{a_{24}a_{41}}{(s-a_{22})(s-a_{44})} & 0 & 0 \\ 0 & \frac{a_{35}a_{52}+a_{32}(s-a_{55})}{(s-a_{33})(s-a_{55})} & 0 \end{pmatrix},$$

$$P = \begin{pmatrix} \frac{b_{11}}{s-a_{11}} & 0 \\ 0 & \frac{b_{22}}{s-a_{22}} \\ 0 & 0 \end{pmatrix}.$$

Figure 2 illustrates the different notions of structure associated with each representation of this system. Comparing with Fig. 1, the DSF has more information than the transfer function, and less than the state-space representation [1].

The results in Proposition 1 give

$$\lim_{|s|\to\infty} sQ(s) = \begin{pmatrix} 0 & 0 & a_{13} \\ 0 & 0 & 0 \\ 0 & a_{32} & 0 \end{pmatrix};$$

$$\lim_{|s|\to\infty} sP(s) = s \begin{pmatrix} \frac{b_{11}}{s-a_{11}} & 0 \\ 0 & \frac{b_{22}}{s-a_{22}} \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} b_{11} & 0 \\ 0 & b_{22} \\ 0 & 0 \end{pmatrix}.$$

which are consistent with respective entries of the state-space representation.

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C. Problem formulation

Similar to transfer functions, there are two important theoretical problems for dynamical structure functions (as shown in Fig. 1). One is identification, i.e. how to obtain dynamical structure functions from input-output data, which was addressed in [17]. The other problem is minimal realization, i.e. how to find a state-space realization with minimal order that is consistent with a given dynamical structure function.

Obtaining a minimal realization is at the core of systems biology identification problems as it helps understand the minimum number of unmeasured molecular species needed to explain observed input-output data. A low number of hidden states means that most molecule species in that pathway have been identified and measured, showing a good understanding of the system; while a large number shows that there are still many unmeasured variables, suggesting that new experiments should be carried out to better characterise the biological system or pathway of interest.

Motivated by this, we aim to solve the following problem in the rest of this paper.

Problem 1: ***[Minimal structural realization]*** Given a dynamical structure function $[Q,\ P]$, from all realizations $\Sigma \triangleq (A,\ B,\ C = [I,\ 0])$ consistent with $[Q,\ P]$ find one where A has the smallest dimension among all such realizations.

III. Algorithm to find a (Q,P)-minimal realization

The Minimal Structural Realization problem considers how to generate a state-space realization of minimal order that is consistent with a given Dynamical Structure Function. Note that if we knew $W^o(s)$ and $V^o(s)$, given by Equation (3), then the problem would be straightforward, as we could minimally realize the transfer function given by the combined matrix $[W^o(s)\ V^o(s)]$, yielding matrices $(\bar{A},\bar{B},\bar{C},\bar{D})$ such that $[W^o(s)\ V^o(s)] = \bar{C}(sI-\bar{A})^{-1}\bar{B}+\bar{D}$. Partitioning the resulting $\bar{B} = [\bar{B}_1\ \bar{B}_2]$ and $\bar{D} = [\bar{D}_1\ \bar{D}_2]$ matrices commensurate with the sizes of W and V, we could then construct the desired realization from $(\bar{A},\bar{B},\bar{C},\bar{D})$ directly from the definitions of W and V:

$$\begin{aligned}\begin{bmatrix}\dot{y}\\ \dot{z}\end{bmatrix} &= \begin{bmatrix}\bar{D}_1 & \bar{C}\\ \bar{B}_1 & \bar{A}\end{bmatrix}\begin{bmatrix}y\\ z\end{bmatrix}+\begin{bmatrix}\bar{D}_2\\ \bar{B}_2\end{bmatrix}u\\ y &= \begin{bmatrix} I_p & 0\end{bmatrix}\begin{bmatrix}y\\ z\end{bmatrix}\end{aligned} \tag{10}$$

The challenge in minimally realizing a system's DSF arises from the fact that we do not know W and V, but instead only know Q and P. Recall from Equations (5) and (6) that we could construct W^o and V^o from Q and P, and subsequently could then use the realization procedure outlined above for $(W^o,\ V^o)$, if we also knew $R^o(s)$. As a result, the key to minimally realizing the DSF is finding a $R(s)$ that, when combined with the given (Q,P) pair, results in a (W,V) pair that has minimum Smith-McMillian degree.

This problem is formulated precisely as:

$$R^* = \mathbf{argmin}_R\ \deg\{[W\ V]\} \tag{11}$$

$$= \mathbf{argmin}_R\ \deg\{(sI-R)[Q\ P]+[R\ 0]\} \tag{12}$$

$$= \mathbf{argmin}_R\ \deg\left\{(sI-R)s^{-1}[sQ\ sP]+[R\ 0]\right\}, \tag{13}$$

where deg is the Smith-McMillan degree (see [9] for details) and R is chosen over the set of proper diagonal transfer matrices. Note that the reformulation to Equation (13) is useful in the subsequent results because both $(sI-R)s^{-1}$ and $[sQ\ sP]$ are proper transfer functions, which admit state-space realizations. Furthermore, note that, since there are many choices for R^* that minimize the order of minimal realizations of $[W\ \ V]$, a chosen R^* may be different from the system's actual value of R. Future work may consider precisely what extra information about the system is needed to reconstruct its actual R^o, or realize the actual state-space representation of the system given only its DSF, but this paper considers how to find *some* minimal realization that is consistent with the given DSF, not necessarily how to recover the system's actual state space description.

In general, the problem posed in eq. (13) is difficult. Nevertheless, for a particular class of systems we can characterize the optimal solution R^* and use the result to drive an algorithm for constructing minimal realizations of Dynamical Structure Functions. The following theorem makes these ideas precise.

Theorem 1: Assume $[I-Q\ \ P]$ only has simple poles and does not have any zeros[1]. A minimal order realization of $[W\ \ V]$ in (13) can be achieved using a constant diagonal matrix R^*.

Proof: From the definition, we have the prior knowledge that R^* should be a diagonal matrix.

Assume R^* has at least one term on the diagonal with the degree of the numerator greater or equal to 1, e.g., suppose the i^{th} term in $(sI-R^*)s^{-1} = \frac{(s+b)\epsilon_i(s)}{s\phi_i(s)}$ with any $b\in\mathbb{R}$ and $deg(\epsilon_i(s)) = deg(\phi_i(s)) \geq 1$, where $deg(\cdot)$ returns the degree of a polynomial. Hence, the product $(sI-R^*)s^{-1}[sQ\ \ sP]$ will introduce $deg(\phi_i(s))$ new poles, since $[I-Q\ \ P]$ does not have any zeros. Due to the assumption of simple poles, a good choice of R can eliminate at most $deg(\epsilon_i(s)) = deg(\phi_i(s))$ poles. As a consequence, we can change the i^{th} term from $\frac{(s+b)\epsilon_i(s)}{s\phi_i(s)}$ to $\frac{s+a}{s}$ without increasing the order. Doing this along all the elements of R^* proves the result. ∎

If R^* is a constant matrix, the term $[R^*\ \ 0]$ in eq. (11) is also a constant matrix. Therefore, the order of a minimal realization is only determined by $(sI-R^*)s^{-1}[sQ\ \ sP] \triangleq N[sQ\ \ sP]$. Thus, finding the "optimal" R^* which leads to the minimal order in eq. (11) is equivalent to finding a diagonal proper transfer matrix N (N with corresponding minimal realization (A_2,B_2,C_2,I) is restricted to the set of matrices of the form $(sI-R^*)s^{-1}$ with a constant R^* from Theorem 1) such that $N[sQ\ \ sP]$ has as few poles as possible. Based on this idea, the following algorithm is proposed:

Step 1: *Find a Gilbert's realization of the dynamical structure function.*

First, using the results in Lemma 1 of [1], we find a minimal realization (A_1,B_1,C_1,D_1) of $[sQ\ \ sP]$. When $[sQ\ \ sP]$ has l simple poles, using Gilbert's realization [20] gives

$$[sQ\ \ sP] = \sum_{i=1}^{l}\frac{K_i}{s-\lambda_i} + \lim_{s\to\infty}[sQ\ \ sP],$$

[1]These assumptions can be relaxed, see Section 3.6 of [21] for more details.

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where $K_i = \lim_{s\to\lambda_i}(s-\lambda_i)[sQ \quad sP]$ and has rank 1 since we are assuming that $[sQ \quad sP]$ has simple poles.

Consider a matrix decomposition of K_i of the following form:

$$K_i = E_i F_i, \ \forall i,$$

where $E_i \in \mathbb{R}^p$ has full column rank and $F_i = (E_i^T E_i)^{-1} E_i^T K_i$. Then $A_1 = \text{diag}\{\lambda_i\} \in \mathbb{R}^{l\times l}$, $B_1 = \begin{bmatrix} F_1^T & F_2^T & \dots & F_l^T \end{bmatrix}^T$, $C_1 = \begin{bmatrix} E_1 & E_2 & \dots & E_l \end{bmatrix}$ and $D_1 = \lim_{s\to\infty}[sQ \quad sP]$.

Step 2: *Find the maximal number of cancelled poles.*
Let $\mathcal{B}$ be the Boolean operator $\mathbb{R}^p \to \{0,1\}^p$, e.g., $b = \mathcal{B}(a)$ means $b[i] = 0$ if $a[i] = 0$, otherwise $b[i] = 1$ if $a[i] \neq 0$. We define Φ as a largest subset of $\{\mathcal{B}(E_1), \cdots, \mathcal{B}(E_l)\}$ such that all the elements in Φ are mutually orthogonal. We also define ϕ as the cardinality of Φ. Computationally, ϕ can be obtained using the algorithm presented in the Appendix. We claim that ϕ is equal to the maximum number of poles we can eliminate.

Proposition 2: If $[I-Q \quad P]$ only has simple poles and does not have any zeros, then the minimal order of $[W \quad V]$ in eq. (11) is

$$l - \phi.$$

Proof: See Appendix. ■

As a consequence, the order of the minimal reconstruction is the dimension of A_{11} (the constant p) plus the minimal dimension of A_{22} (obtained above): $p + l - \phi$.

Step 3: *Construct R^* to obtain the minimal reconstruction.*
Once we have Φ, using eq. (25) and $N(s) = (sI - R^*)s^{-1}$, we know that $N(\lambda_i)[j,j] = 0$ implies $R^*[j,j] = \lambda_i$. Consequently, each element in the set Φ will determine at least one element in R^*. This last fact can be used to construct R^* element by element. Once R^* is found, we can obtain A and B using eq. (10).

Example 2: Consider a dynamical structure function $[Q,P]$:

$$[Q \mid P] = \left[\begin{array}{ccc|c} 0 & \frac{1}{s+2} & \frac{1}{s+3} & \frac{1}{s+4} \\ \frac{1}{s+1} & 0 & \frac{1}{s+3} & \frac{1}{s+4} \\ \frac{1}{s+1} & \frac{1}{s+2} & 0 & \frac{1}{s+4} \end{array}\right].$$

We first compute the Smith McMillan degree of the corresponding transfer function: $\deg\{G\} = \deg\{(I-Q)^{-1}P)\} = 4$, meaning that a 4^{th} order state-space model is enough to realize the transfer function. It is interesting to look at the minimal order realization consistent with the dynamical structure function. The different steps of the algorithm proposed in the previous section successively yield the following:

Step 1: A minimal Gilbert realization of $s[Q,P]$ is

$$A_1 = \text{diag}\{-1,-2,-3,-4\}, \ B_1 = \text{diag}\{2,2,2,4\},$$
$$C_1 = \begin{bmatrix} 0 & -1 & -1.5 & -1 \\ -0.5 & 0 & -1.5 & -1 \\ -0.5 & -1 & 0 & -1 \end{bmatrix}, \ D_1 = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{bmatrix}.$$

Step 2: By definition, $E_i = C_1 v_i$ where $v_i \in \mathbb{R}^4$ has 1 in its i^{th} position and zero otherwise. Thus,

$$\{\mathcal{B}(E_1), \cdots, \mathcal{B}(E_4)\} = \left\{ \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right\}.$$

Furthermore, ϕ is 1 and the order of a minimal realization of the given dynamical structure function is $p+l-\phi = 3+4-1 = 6$. Hence, the system must contain at least 3 hidden states.

Step 3: R^* can be chosen as $\text{diag}\{a,-1,-1\}$, $\text{diag}\{-2,a,-2\}$, $\text{diag}\{-3,-3,a\}$, or $\text{diag}\{-4,-4,-4\}$ for any $a \in \mathbb{R}$.

The reconstructed networks are represented in Fig. 3. There are three measured (red) nodes, labeled $1,2,3$ and by the analysis above, there are at least three hidden nodes such that the corresponding realization is consistent with the dynamical structure function. The red connections between measured nodes are the same for all candidate networks which is in accordance with Proposition 3.6.1 in [21]. Dashed lines correspond to the connections between hidden and measured nodes.

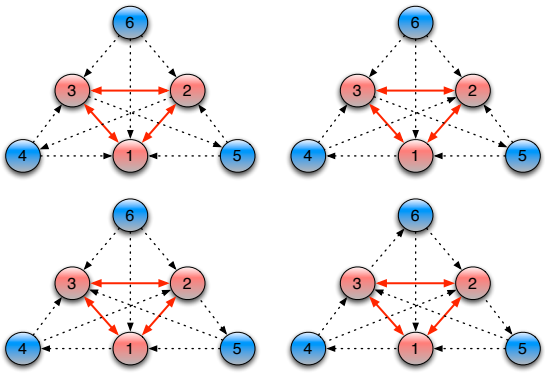

Fig. 3: Topologies corresponding to the four $[Q,P]$ minimal realizations. The measured nodes are colored red, while the hidden ones blue. Red connections between measured nodes are the same for all the networks, indicating the direct interactions among measured states, due to Proposition 3.6.1 in [21]. Each node has a self-loop but we omit it for simplicity.

In the context of biochemical reaction networks, this indicates that there are at least 3 unmeasured species interacting with the measured species. Of course, the "true" biological system might be even more complicated, i.e., it might have more than 6 species. Yet, when more states are measured, the dynamical structure functions can be easily updated and a new search for a minimal realization of the updated system can be performed to reveal the corresponding minimal number of hidden states. Interestingly, however, we discover that since the minimal structural degree is 6, and the Smith McMillian degree is 4, there must be at least two uncontrollable modes in any realization that achieve this structure with the specified dynamics.

Example 3: The Wnt signaling pathway is a highly conserved signaling pathway found in many multi-cellular organisms. It plays a role in the regulation of normal embryonic development, tissue homeostasis, and tissue regeneration. Mutations in the Wnt signaling pathway have been implicated to play a role in cancer dynamics, particularly colorectal cancer and hepatocellular carcinoma [31], [33]. Thus, understanding the components, structure, and function of the Wnt pathway is important and one of the primary focuses of researchers

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studying cell signaling.

The Wnt pathway controls and regulates the amount of β-catenin in the cell, a critical constituent of the cadherin complex. Mutation and over expression of β-catenin is correlated with many forms of cancer, including colon cancer, melanoma, hepatocellular carcinoma, ovarian cancer, endometrial cancer, medulloblastoma pilomatricomas, and prostate cancer [32]. Thus, the mechanisms by which β-catenin levels are regulated via the Wnt pathway are of critical importance. Over the course of two decades, the complexity and various comprising reactions of the Wnt pathway have been slowly unraveled. We show here that by using a minimal dynamical structure realization algorithm, we can quickly infer the underlying complexity of the system required to produce a given dynamical network structure.

To begin, we consider the nonlinear mass action kinetics model of the Wnt signaling system as derived in [33]; it is derived assuming bimolecular, unimolecular, or zeroth order reactions and has fifteen states. In state-space form, it can be written as follows:

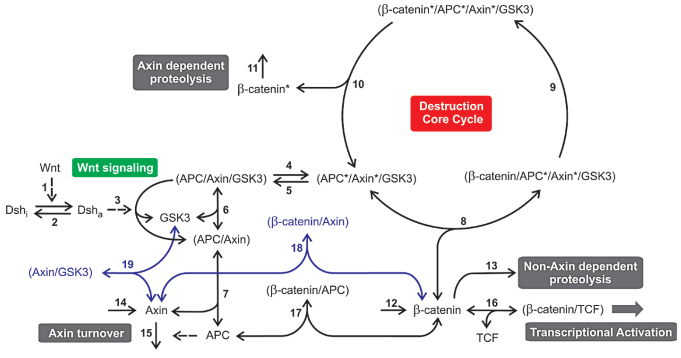

Fig. 4: Reaction diagram of the Wnt signaling pathway, adapted from [33]. Wnt converts inactive Disheveled to an active form, which assists in the breakdown of the dephosphorylated destruction complex (APC/Axin/GSK3). Axin binds with APC to form the APC/Axin complex, which binds in turn to GSK3 to form the unphosphorylated destruction complex. The destruction complex binds to free β-catenin, mediates the phosphorylation of β-catenin and releases it for degradation via ubiquitiniation. In this way, Wnt stimulation results in the destabilization of the destruction complex, which effectively prolongs the lifetime of β-catenin.

$$
\begin{aligned}
\dot{x}_1 &= -k_1\,x_1\,u + k_2\,x_2\\
\dot{x}_2 &= k_1\,x_1\,u - k_2\,x_2\\
\dot{x}_3 &= k_4\,x_4 - k_5\,x_3 - k_{+8}\,x_3\,x_{11} + k_{-8}\,x_8 + k_{10}\,x_9\\
\dot{x}_4 &= -k_3\,x_2\,x_4 - k_4\,x_4 + k_5\,x_3 + k_{+6}\,x_5\,x_6 - k_{-6}\,x_4\\
\dot{x}_5 &= k_3\,x_2\,x_4 - k_{+6}\,x_5\,x_6 + k_{-6}\,x_4\\
\dot{x}_6 &= k_3\,x_2\,x_4 - k_{+6}\,x_5\,x_6 - k_{-6}\,x_4 + k_{+7}\,x_{12}\,x_7 - k_{-7}\,x_6\\
\dot{x}_7 &= -k_{+7}\,x_{12}\,x_7 + k_{-7}\,x_6 - k_{+17}\,x_7\,x_{11} + k_{-17}\,x_{15}\\
\dot{x}_8 &= k_{+8}\,x_3\,x_{11} - k_{-8}\,x_8\\
\dot{x}_9 &= k_9\,x_8 - k_{10}\,x_9\\
\dot{x}_{10} &= k_{10}\,x_9 - k_{11}\,x_{10}\\
\dot{x}_{11} &= -k_{+8}\,x_3\,x_{11} \;+ k_{-8}\,x_8 + v_{12}^o - k_{13}\,x_{11}\\
&\quad - k_{+16}\,x_{11}\,x_{13} + k_{-16}\,x_{14} - k_{+17}\,x_7\,x_{11} + k_{-17}\,x_{15}\\
\dot{x}_{12} &= -k_{+7}\,x_{12}\,x_7 + k_{-7}\,x_6 + v_{14}^o - k_{15}\,x_{12}\\
\dot{x}_{13} &= -k_{+16}\,x_{11}\,x_{13} + k_{-16}\,x_{14}\\
\dot{x}_{14} &= k_{+16}\,x_{11}\,x_{13} - k_{-16}\,x_{14}\\
\dot{x}_{15} &= k_{+17}\,x_7\,x_{11} - k_{-17}\,x_{15}
\end{aligned}
\tag{14}
$$

In these equations, the concentration of Wnt protein is denoted as u since, in practice, Wnt can be viewed as an adjustable or controlled quantity that is introduced exogenously into the system to stimulate β-catenin levels [34]. For clarity, the rest of the system states are listed in Table I with their corresponding biological name. Note that biological names with an asterisk are proteins or complexes that are in their phosphorylated state.

Because of its complexity, the model is difficult to analyze. Thus, the authors in [33] propose a series of time-scale separation assumptions that can systematically eliminate specific states. In particular, it is possible to reduce the model to an eighth order model, given as follows:

$$
\begin{aligned}
\dot{x}_2 &= k_1\,\left(DSH^0 - x_2\right)u - k_2\,x_2\\
\dot{x}_3 &= k_4\,x_4 - k_5\,x_3 + \frac{k_{-8}}{K_8}\,x_3\,x_{11}\\
\dot{x}_4 &= -k_3\,x_2\,x_4 - k_4\,x_4 + k_5\,x_3 + k_{+6}\,x_6\,GSK^0 - k_{-6}\,x_4\\
\dot{x}_6 &= k_3\,x_2\,x_4 - k_{+6}\,x_6\,GSK^0 + k_{-6}\,x_4 + k_{+7}\,x_{12}\\
&\quad \frac{K_{17}\,APC^0}{(K_{17}+x_{11})} - k_{-7}\,x_6\\
\dot{x}_9 &= \frac{k_9}{K_8}\,x_3\,x_{11} - k_{10}\,x_9\\
\dot{x}_{10} &= k_{10}\,x_9 - k_{11}\,x_{10}\\
\dot{x}_{11} &= -k_{+8}\,x_3\,x_{11} + \frac{k_{-8}}{K_8}\,x_3\,x_{11} + v_{12}^o - k_{13}\,x_{11} - k_{+16}\\
&\quad x_{11}\frac{K_{16}TCF^o}{K_{16}+x_{11}} - k_{+17}\,\frac{(K_{17}APC^o)}{(K_{17}+x_{11})\,x_{11}} + k_{-17}\frac{APC^o\,x_{11}}{k_{17}+x_{11}}\\
\dot{x}_{12} &= -k_{+7}\,x_{12}\,\frac{K_{17}\,APC^o}{K_{17}+x_{11}} + k_{-7}\,x_6 + v_{14}^o - k_{15}\,x_{12}
\end{aligned}
\tag{15}
$$

while the states measured are the concentration of dephosphorylated β-catenin, dephosphorylated destruction complex (APC/Axin/GSK3), and APC/Axin. The corresponding output

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State	Protein Name	State	Protein Name	State	Protein Name
x_1	DSH$_i$	x_6	APC/Axin	x_{11}	β_{cat}
x_2	DSH$_a$	x_7	APC	x_{12}	Axin
x_3	APC*/Axin*/GSK3	x_8	β_{cat}/APC*/Axin*/GSK3	x_{13}	TCF
x_4	APC/Axin/GSK3	x_9	$\beta_{cat}*$/APC*/Axin*/GSK3	x_{14}	β_{cat}/TCF
x_5	GSK3	x_{10}	$\beta_{cat}*$	x_{15}	β_{cat}/APC

TABLE I

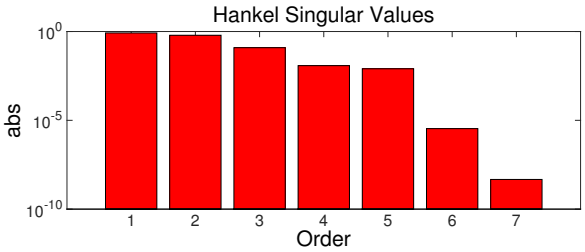

Fig. 5: Hankel singular values of G in logarithmic scale.

equations are given as:

$$\begin{aligned} y_1 &= x_{11} \\ y_2 &= x_4 \\ y_3 &= x_6. \end{aligned} \tag{16}$$

The parameters used in this model are the same as those in [33]. Most of these parameters are measured or inferred experimentally, while the remainder $(k_{+8}, k_{-8}, k_{+17}, k_{-17}, k_{+18},$ and $k_{-18})$ are estimated (see Table II for a complete list). It is important to note that the system (15) is a nonlinear state-space model. However, the nonlinear system converges to a steady state [33], indicating that approximating the dynamics of the nonlinear system with a linearization in a neighborhood of its steady state may be acceptable. After linearizing around the steady state (estimated from numerical simulation), we obtain the following LTI state-space model:

Following the approach in the prequel, it is instructive to first transform the LTI system so that the output matrix $C = \begin{bmatrix} I & 0 \end{bmatrix}$. For this, we define $z = Tx$ where

$$T = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{18}$$

The transformed realization $(\tilde{A}, \tilde{B}, \tilde{C})$ is then given in eq. (19). Based on this state-space realization $(\tilde{A}, \tilde{B}, \tilde{C})$ the corresponding transfer function can be computed in eq. (20) The magnitude of the Hankel singular values of G are provided in Fig. 5. Given that the two smallest Hankel singular values are around four orders of magnitude smaller than the next smallest one, a typical system identification algorithm would likely return at most a 5^{th} order system.

The dynamical structure function $(Q(s), P(s))$ is computed in eq. (21) and (22).

Again, we examine the Hankel singular values of non-zero elements in $[Q, P]$ and also truncate those Hankel singular values that are orders of magnitude smaller than the next smallest ones. Applying the proposed algorithm gives a minimal realization of $[Q, P]$ of 7^{th} order. Furthermore, we can obtain, using Proposition 1 in the paper, the causal relationship between measured states as:

$$\tilde{A}^o_{11} - \text{diag}\{\tilde{A}^o_{11}\} = \lim_{|s|\to\infty} sQ(s) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 4.54 \\ -9.9 * 10^{-9} & 5.45 & 0 \end{bmatrix};$$

$$\tilde{B}^o_1 = \lim_{|s|\to\infty} sP(s) = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

This biologically motivated example illustrates the main features of the paper.

a) In particular, it shows that when there are pole/zero cancellations between $(I - Q)^{-1}$ and P, such canceled poles do not show up in G but can still be seen in (Q, P). In this example, (Q, P) revealed two additional states that could not be seen in G, and, hence, it provided information on the existence of additional complexity, not seen from the transfer function.
b) It also reveals the direct causal relation between measured states, how the three states x_{11}, x_4 and x_6 affect each other, which cannot be seen in G.

IV. Discussion and Implications

Solving the Minimal Structural Realization problem leads to a number of interesting insights about Dynamical Structure Functions as a representation of LTI networks. First, since the minimal structural degree of a particular DSF can be strictly greater than the Smith-McMillian degree of its associated transfer function, we see that *uncontrollable modes may be necessary* to realize systems with a particular dynamic behavior and structure.

This necessity of the presence of uncontrollable modes in systems that require particular dynamics and structure is rather unexpected and surprising. It has especially interesting consequences for the design of controllers that meet particular structural constraints [29], in that these controllers may necessarily contain uncontrollable modes to meet their structural constraints.

Furthermore, this result leads to another important insight about the nature of these representations, namely that Dynamical Structure Functions with structural degree strictly greater than the Smith-McMillian degree of their associated transfer functions may have both stable and unstable realizations. This can happen when, for example, the transfer function is stable

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$$\begin{bmatrix}\dot{x}_2\\ \dot{x}_3\\ \dot{x}_4\\ \dot{x}_6\\ \dot{x}_9\\ \dot{x}_{10}\\ \dot{x}_{11}\\ \dot{x}_{12}\end{bmatrix} = \begin{bmatrix} -18.2 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & -.99 & .27 & 0 & 210 & 0 & -3\times10^{-4} & 0\\ -1.05\times10^{-6} & .13 & -5.72 & 4.55 & 0 & 0 & 0 & 0\\ 0 & 0 & 5.45 & -5.45 & 0 & 0 & 9.92\times10^{-8} & 9.09\\ 0 & 0.07 & 0 & 0 & -210 & 0 & 2.39\times10^{-5} & 0\\ 0 & 0 & 0 & 0 & 210 & -.41 & 0 & 0\\ 0 & -.85 & 0 & 0 & 0 & 0 & -9.92 & 0\\ 0 & 0 & 0 & .91 & 0 & 0 & 9.92\times10^{-8} & -9.26\end{bmatrix}\begin{bmatrix}x_2\\ x_3\\ x_4\\ x_6\\ x_9\\ x_{10}\\ x_{11}\\ x_{12}\end{bmatrix} + \begin{bmatrix}1.65*10^8\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\end{bmatrix} u \tag{17}$$

$$\begin{bmatrix}y_1\\ y_2\\ y_3\end{bmatrix} = \begin{bmatrix}0&0&0&0&0&0&1&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\end{bmatrix}\begin{bmatrix}x_2 & x_3 & x_4 & x_6 & x_9 & x_{10} & x_{11} & x_{12}\end{bmatrix}^T$$

$$\tilde{A} = \begin{bmatrix} -9.92 & 0 & 0 & 0 & -0.85 & 0 & 0 & 0\\ 0 & -5.72 & 4.54 & -1.06\times10^{-6} & 0.13 & 0 & 0 & 0\\ -9.9\times10^{-9} & 5.45 & -5.45 & 1.06\times10^{-6} & 0 & 0 & 0 & 9.09\\ 0 & 0 & 0 & -18.22 & 0 & 0 & 0 & 0\\ -2\times10^{-4} & .27 & 0 & 0 & -.98 & 210.0 & 0 & 0\\ 2.4\times10^{-5} & 0 & 0 & 0 & 7.46\times10^{-3} & -210.0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 210.0 & -0.42 & 0\\ 9.92\times10^{-8} & 0 & 0.91 & 0 & 0 & 0 & 0 & -9.26\end{bmatrix} \tag{19}$$

$$\tilde{B} = \begin{bmatrix}0&0&0&1.65&0&0&0&0\end{bmatrix}^T * 10^8$$

$$\tilde{C} = \begin{bmatrix}1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\end{bmatrix}$$

$$G = \begin{bmatrix}\frac{-2.489e{-}06s^5-0.0005675s^4+40.13s^3+8837s^2+8.573e04s+1304}{s^7+259.6s^6+1.131e04s^5+1.973e05s^4+1.578e06s^3+5.285e06s^2+4.258e06s+3.954e05}\\ \frac{-174.9s^5-4.041e04s^4-7.947e05s^3-4.446e06s^2-3.666e06s-5.482e04}{s^7+259.6s^6+1.131e04s^5+1.973e05s^4+1.578e06s^3+5.285e06s^2+4.258e06s+3.954e05}\\ \frac{174.9s^5+4.03e04s^4+7.704e05s^3+4.278e06s^2+4.356e06s+7.675e05}{s^7+259.6s^6+1.131e04s^5+1.973e05s^4+1.578e06s^3+5.285e06s^2+4.258e06s+3.954e05}\end{bmatrix}. \tag{20}$$

$$Q = \begin{bmatrix}0 & Q_{12} & 0\\ Q_{21} & 0 & \frac{4.54s+4.415}{s^2+6.693s+5.528}\\ \frac{-9.9e{-}09s^2+7.184e{-}07s+7.501e{-}06}{s^3+23.97s^2+178.4s+390.7} & \frac{5.45s+50.47}{s^2+14.71s+42.2} & 0\end{bmatrix} \tag{21}$$

$$P = \begin{bmatrix}0\\ \frac{-174.9s-170.1}{s^3+24.91s^2+127.5s+100.7}\\ \frac{174.9s+1620}{s^3+32.93s^2+310.2s+768.8}\end{bmatrix}. \tag{22}$$

$$Q_{12} = \frac{-0.2295s^5-145s^4-3.065e04s^3-2.185e06s^2-4.163e06s-2.01e06}{s^7+642.9s^6+1.404e05s^5+1.098e07s^4+1.231e08s^3+2.982e08s^2+2.704e08s+8.451e07}, \tag{23}$$

$$Q_{21} = \frac{-2.6e-05s^5-0.01578s^4-3.195s^3-218.1s^2-415.2s-200.4}{s^7+638.7s^6+1.378e05s^5+1.042e07s^4+8.259e07s^3+1.828e08s^2+1.589e08s+4.842e07} \tag{24}$$

but the uncontrollable modes necessary to realize the DSF can be either stable or unstable. Future work lies in the application of the developed theory to real-world applications emerging in complex dynamical network research.

V. Acknowledgement

Ye Yuan, Guy-Bart Stan and Jorge Gonçalves gratefully acknowledge the support of EPSRC under the projects EP/E02761X/1, EP/I03210X/1 and EP/I032223/1. Sean Warnick gratefully acknowledges the support of grants AFRL FA8750-09-2-0219, FA8750-11-1-0236, DHS contract number HSHQDC-13-C-B0052, and useful conversations with Nicola Elia and Russ Howes. Guy-Bart Stan also gratefully acknowledges the support of the EPSRC Centre for Synthetic Biology and Innovation at Imperial College, London.

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Parameter Name	Value	Parameter Name	Value
Dsh^o	100 nM	k_{-6}	0.909 min $^{-1}$
APC^o	100 nM	k_{+8}	20 min $^{-1}$
TCF^o	15 nM	k_{-8}	2 min $^{-1}$
GSK^o	50 nM	k_9	206 min^{-1}
K_7	50 nM	k_{10}	206 min^{-1}
K_8	120 nM	k_{11}	206 min^{-1}
K_{16}	30 nM	k_{13}	2.57×10^{-4} min^{-1}
K_{17}	1200 nM	k_{15}	0.167 min^{-1}
k_1	0.182 min^{-1}	k_{+16}	9.09×10^{-2} min^{-1}
k_2	1.82×10^{-2} min^{-1}	k_{-16}	9.09×10^{-1} min^{-1}
k_3	5.00×10^{-2} min^{-1}	k_{+17}	9.09×10^{-2} min^{-1}
k_4	0.267 min^{-1}	k_{-17}	9.09×10^{-1} min^{-1}
k_5	0.133 min^{-1}	v_{12}	0.423 nmol^{-1} min^{-1}
k_{+6}	9.09×10^{-2} nmol^{-1} min^{-1}	v_{14}	8.22×10^{-5} nmol^{-1} min^{-1}

TABLE II

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APPENDIX

Proof to Proposition 2:

This article has been accepted for publication in a future issue of this journal, but has not been fully edited. Content may change prior to final publication. Citation information: DOI 10.1109/TCNS.2015.2498468, IEEE Transactions on Control of Network Systems

Proof: Using results from Section 4 of [19], if a pole of $[sQ \;\; sP]$, say λ_i, is cancelled by $N = (sI - R^*)s^{-1} \triangleq C_2(A_2 - sI)^{-1}B_2 + I$, then the realization of the cascade $(sI - R)s^{-1}[sQ \;\; sP]$ loses observability.

In this case, it follows that there exists a nonzero vector $w_i = [w_{1,i}^T, w_{2,i}^T]^T$ such that

$$\begin{bmatrix} A_1 - \lambda_i I & 0 \\ B_2C_1 & A_2 - \lambda_i I \\ C_1 & C_2 \end{bmatrix} \begin{bmatrix} w_{1,i} \\ w_{2,i} \end{bmatrix} = 0.$$

The first equation shows that $w_{1,i}$ is an eigenvector of A_1 corresponding to λ_i. Since A_1 is diagonal, $w_{1,i}^T = \begin{bmatrix} 0 & \dots & 0 & 1_{i^{th}} & 0 & \dots & 0 \end{bmatrix} \in \mathbb{R}^{1\times l}$. Therefore, we have

$$\begin{bmatrix} A_2 - \lambda_i I & B_2 \\ C_2 & I \end{bmatrix} \begin{bmatrix} w_{2,i} \\ C_1 w_{1,i} \end{bmatrix} = 0.$$

Noticing that $C_1 w_{1,i} = E_i$ and that

$$\begin{bmatrix} I & 0 \\ -C_2(A_2 - sI)^{-1} & I \end{bmatrix} \begin{bmatrix} A_2 - sI & B_2 \\ C_2 & I \end{bmatrix} = \begin{bmatrix} A_2 - sI & B_2 \\ 0 & N(s) \end{bmatrix},$$

we obtain, since $\lambda_i \neq 0$ is not a pole of N,

$$N(\lambda_i)E_i = 0. \tag{25}$$

In summary, designing R^* to cancel any pole λ_i of $[sQ \;\; sP]$ is equivalent to imposing that eq. (25) holds. The next question is: given $[sQ \;\; sP]$ what is the maximal number of poles that can be cancelled by N, i.e., what is the largest number of poles for which eq. (25) is satisfied?

To answer this, notice that $E_i[j]$ being nonzero for some j, implies that there exists at least one nonzero element in the j^{th} row of E_i. In this case, satisfying eq. (25) imposes that the j^{th} diagonal element of $N(\lambda_i)$ is 0, i.e., the j^{th} diagonal element of R^* is λ_i. In other words, a nonzero element in E_i corresponds to a fixed value in the corresponding diagonal position in R^*. Since R^* is a constant diagonal matrix then any pair of orthogonal vectors in $\{\mathcal{B}(E_1), \cdots, \mathcal{B}(E_l)\}$ does not intervene in the choice of an element on the diagonal of R^*.

Therefore, the minimal order of $[W \;\; V]$ in eq. (11) is $l - \phi$. ■

Algorithm to find ϕ and Φ:

As is presented in [23], an undirected graph is denoted by $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where $\mathcal{V} = \{\nu_1, \dots, \nu_l\}$ is the set of nodes and $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$ is the set of edges.

For our purposes, we construct an undirected graph $\mathcal{G}_a$ using the following rules:

- A node is associated with each boolean vector in the set $\{\mathcal{B}(E_1), \cdots, \mathcal{B}(E_l)\}$. There are thus l nodes in the considered graph.
- An undirected edge (i, j) is drawn between node i and node j if the equality $\mathcal{B}(E_i)^T\mathcal{B}(E_j) = 0$ is satisfied.

It is easy to see that the maximum cardinality of the set Φ corresponds to the maximum number of nodes in a complete subgraph K_n of the graph $\mathcal{G}_a$.

Although the problem of finding a largest complete subgraph in an undirected graph is an NP-hard problem, methods to this end have been well-studied in [24][2]. To our best knowledge, for an arbitrary graph, the fastest algorithm has a complexity of $\mathcal{O}(2^{n/4})$ [25]. Therefore, we can use these methods to obtain a largest complete subgraph and consequently compute the corresponding set Φ and its corresponding cardinality ϕ.

[2]Some corresponding MATLAB code can be downloaded from http://www.mathworks.com/matlabcentral/fileexchange/19889.