The isocurvature fraction after WMAP 3-yr data

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ABSTRACT
I revisit the question of the adiabaticity of initial conditions for cosmological perturbations in view of the 3-yr Wilkinson Microwave Anisotropy Probe (WMAP) data. I focus on the simplest alternative to purely adiabatic conditions, namely a superposition of the adiabatic mode and one of the three possible isocurvature modes, with the same spectral index as the adiabatic component.

I discuss findings in terms of posterior bounds on the isocurvature fraction and Bayesian model selection. The Bayes factor (models likelihood ratio) and the effective Bayesian complexity are computed for several prior ranges for the isocurvature content. I find that the cold dark matter isocurvature fraction is now constrained to be less than about 10 per cent, while the fraction in either the neutrino entropy or velocity mode is below about 20 per cent. Model comparison strongly disfavours mixed models that allow for isocurvature fractions larger than unity, while current data do not allow one to distinguish between a purely adiabatic model and models with a moderate (i.e. below about 10 per cent) isocurvature contribution.

The conclusion is that purely adiabatic conditions are strongly favoured from a model selection perspective. This is expected to apply in even stronger terms to more complicated superpositions of isocurvature contributions.

Key words: methods: statistical – cosmological parameters – cosmology: theory.

1 INTRODUCTION
The detailed nature of the initial conditions for cosmological perturbations is one of the open questions in cosmology. The exquisite precision of the Wilkinson Microwave Anisotropy Probe (WMAP) measurement of the first acoustic peak location in the cosmic microwave background (CMB) temperature power spectrum ($\ell = 220.7 \pm 0.7$, see Hinshaw et al. 2006) is a strong indication in favour of adiabatic initial conditions, which predict for the first peak $\ell \approx 220$. The alternative possibility of cold dark matter (CDM) isocurvature initial conditions excites a sine wave (rather than the cosine excited by adiabatic conditions) in the photon–baryon plasma, resulting in a first acoustic peak displaced by half a period to $\ell \approx 330$, see e.g. Trotta (2004), Durrer (2004). Furthermore, the ratio of the Sachs–Wolfe plateau for $\ell \lesssim 50$ to the height of the peak is very different for the two modes.

A few years ago, Bucher and collaborators introduced two new isocurvature modes, called ‘neutrino density’ (or, more appropriately, ‘neutrino entropy’) and ‘neutrino velocity’ modes (Bucher, Moodley & Turok 2000). They are characterized by a non-vanishing initial entropy perturbation in the neutrino sector and by a non-vanishing difference in the neutrino to photon velocity, respectively. A superposition of the adiabatic and the three isocurvature modes (cold dark matter, neutrino entropy and neutrino velocity) constitutes the most general initial conditions for the perturbations, at least if the Universe is radiation-dominated in its early phase (Trotta 2004). A baryon isocurvature mode is observationally indistinguishable from a CDM isocurvature one (Bucher, Moodley & Turok 2001; Gordon & Lewis 2003) and can thus be neglected without loss of generality.

Allowing for the most general type of initial conditions has two effects on cosmological parameter extraction from CMB measurements. First, the extra parameters associated with the initial conditions introduce severe degeneracies which limit our ability to reconstruct the cosmology (Trotta, Riazuelo & Durrer 2001, 2003), even though this can fortunately be remedied by using polarization information (Bucher et al. 2001; Trotta & Durrer 2004). Secondly, it becomes difficult to constrain the type of initial conditions, i.e. the amount of isocurvature contributions allowed on top of the predominantly adiabatic mode (Moodley et al. 2004).

Recent works have investigated general isocurvature admixtures in the initial conditions (Beltran et al. 2005b; Moodley et al. 2004; Bean, Dunkley & Pierpaoli 2006). In this work I focus on the simplest alternative to a purely adiabatic power spectrum, namely a superposition with one totally (anti)correlated isocurvature mode at the time with the same spectral index as the adiabatic one. This is partly motivated by models for the generation of initial conditions such as the curvaton (see e.g. Gordon & Lewis 2003; Lyth & Wands 2002 and references therein), where this kind of scenario arises as a...
generic prediction. A second justification comes from the model selection approach used in the second part of this work. In comparing the simplest (i.e., purely adiabatic) scenario with a more complex one, it makes sense to start by adding a minimal number of extra parameters, and then see whether the extended model is justified by the data. This model selection perspective has been recently advocated by Beltran et al. (2005a), Trotta (2005).

This Letter is organized as follows: in Section 2 I introduce the parametrization of the initial condition parameters space I am considering, while in Section 3 I review some concepts of Bayesian statistics and in particular the model selection approach. I present my results in terms of parameters constraint and model comparison outcome in Section 4 and offer my conclusions in 5.

2 THE ISOCURVATURE FRACTION

The most general initial conditions for cosmological perturbations are described by a symmetric $4 \times 4$ matrix, $M$, with 10 free parameters representing the amplitudes of the pure modes (along the diagonal) and their correlations (off-diagonal elements). From a phenomenological point of view, there are also 10 more parameters describing the spectral tilt of each mode and correlator. If one is phenomenological in nature, there are also 10 more parameters (diagonal) and their correlations (off-diagonal elements). From a phenomenological point of view, there are also 10 more parameters describing the spectral tilt of each mode and correlator. If one is phenomenological in nature, there are also 10 more parameters representing the amplitudes of the pure modes (along the diagonal) and their correlations (off-diagonal elements). Hence, the number of parameters needed to describe the spectral density of each mode is 10, and the number of parameters needed to describe the spectral correlation between different modes is also 10. Therefore, the total number of free parameters is 20.

One observes that this approach allows for a very general description of the initial conditions, as the available parameter space under the prior is very large. For instance, it can be argued that the choice of priors affects the results of the parameter estimation. However, it is important to note that the choice of priors is not unique, and different choices can lead to different conclusions because the Occam’s razor effect is not invariant under non-linear transformations of variables.

Once a fundamental model for the generation of the initial conditions is specified, one can select the appropriate physical variable over which to impose a prior that reflects the state of knowledge before the data is seen. For instance, it can be argued that the choice of the $f_s$ parametrization is closer to the curvaton set-up, while the choice of the $f_s$ parametrization is not.

A flat prior on $\alpha_s$ gives equal prior accessibility volume to adiabatic-dominated ($|\alpha_s| \leq 0.5$) and isocurvature-dominated ($|\alpha_s| > 0.5$) models. The prior on $f_s$ is very much dependent on what one thinks the available parameter space is under the extended model. Therefore I discuss below the results of model selection as a function of the prior width $\Delta f_s$, taking a flat prior in the range $-\Delta f_s < f_s < \Delta f_s$. This allows an easy comparison once a prior range under a specific model is given. I postpone to a future work a detailed analysis of prior selection based on first principles.

3 PARAMETER ESTIMATION, MODEL SELECTION AND MODEL COMPLEXITY

Bounds on the isocurvature fraction are derived in terms of high probability regions in the posterior probability density function (pdf) for the parameters $\theta$ given the data vector $d$, $p(\theta \mid d)$. This is obtained through Bayes’ theorem,

$$p(\theta \mid d) = \frac{p(d \mid \theta) \pi(\theta)}{p(d)},$$

where $p(d \mid \theta)$ is the likelihood function, $\pi(\theta)$ is the prior pdf and $p(d)$ is the model likelihood (sometimes called ‘the evidence’) of the data under the model. The model likelihood is a normalization constant that is independent of the parameters of the model, and it can be ignored as far as the parameter estimation step is concerned. It becomes the key quantity for model selection, and in particular I am interested in the relative odds between the simplest, purely adiabatic model $M_\theta$ and a model augmented by an extra isocurvature contribution, $I_s = (M_\theta, f_s)$, with $x = \alpha_s, \nu$ as above. The change in the degree of belief in the two models after having seen the data is described by the Bayes factor

$$B = \frac{p(d \mid M_\theta)}{p(d \mid I_s)},$$

which is the ratio of the normalization constants for the two models in Bayes’ theorem, equation (4). Because the two models are nested (i.e. one obtains $M_\theta$ from $I_s$ by setting the isocurvature fraction to zero, $f_s = 0$), the Bayes factor can be conveniently computed using the Savage–Dickey density ratio (SDDR) (see Trotta and references therein)

$$B = \left. \frac{p(f_s \mid d, I_s)}{\pi(f_s \mid I_s)} \right|_{f_s=0}.$$

This is easy to compute from a Monte Carlo Markov Chain (MCMC), requiring only knowledge of the properly normalized posterior over the extra variable $f_s$ of the extended model. Furthermore, using the SDDR has the advantage that the impact of a change of prior can usually be evaluated by simply post-processing a chain including the new prior. This is the approach used below in Section 4. If the posterior pdf is well approximated by a Gaussian distribution with mean $\mu$ and standard deviation $\sigma$, and for a flat
prior in the range $-\Delta f \le f_s \le \Delta f$, the Bayes factor of equation (5) becomes
\[ B = \sqrt{\frac{8}{\pi}} \frac{\Delta f}{\sigma} \left[ \text{erfc} \left( -\frac{|\mu| - \Delta f}{\sqrt{2}\sigma} \right) - \text{erfc} \left( \frac{|\mu| + \Delta f}{\sqrt{2}\sigma} \right) \right]^{-1}. \] (7)

For $\ln B > 0$, model $M_s$ is favoured over $I_s$ because the extra complexity (in terms of wasted parameter space) of $I_s$ is not warranted by the data, while for $\ln B < 0$, $I_s$ is favoured because the data require the extra parameter. A useful rule of thumb (Kass & Raftery 1995) is that a positive (stronger) preference requires $|\ln B| \gtrsim 1$ ($\gtrsim 3$). A model likelihood ratio $|\ln B| > 5$ (corresponding to odds $>150:1$) is deemed to constitute ‘decisive’ evidence.

Finally, the last relevant quantity for this analysis is the Bayesian model complexity, which measures the number of parameters the data can support, regardless of whether the parameters in question are actually detected or not (for more details, see Kunz, Trotta & Parkinson 2006). The Bayesian complexity is defined as
\[ C_0 = \chi^2(\bar{\theta}) - \chi^2(\bar{\theta}), \] (8)
where the effective $\chi^2(\bar{\theta})$ is derived from the likelihood as $\chi^2(\bar{\theta}) = -2 \ln p(d|\bar{\theta})$. The bar denotes an average over the posterior pdf, while the hat denotes a point-estimator which in this case I take to be the mean under the posterior, i.e. $\bar{\theta} = \bar{\theta}$. I will use $C_0$ to quantify the number of supported parameters in the extended models $I_s$, in order to verify whether the isocurvature fraction is a variable that could have been detected using current data. A detailed discussion of the meaning and interpretation of the Bayesian complexity can be found in Kunz et al. (2006).

It is important to stress that both the model likelihood and the Bayesian complexity depend not only on the data but also on the model description one chooses to adopt, i.e. on the prior choices one makes for $\pi(f_s)$ (see Trotta 2006 for an example applied to the case of dark energy models). This is an irreducible feature of the Bayesian model selection approach. It seems that there cannot be an absolute notion of ‘a best model’, but only relative statements about the support the data give to different models when compared to each other. Furthermore, the very concept of Bayesian complexity is only meaningful when the constraining power of the data is compared to the scale of the problem at hand, which again must be defined by specifying the prior.

The simplest model $M_0$ is a flat $\Lambda$CDM universe with purely adiabatic conditions, described by following set of six parameters
\[ \theta = (\zeta, \omega_0, \omega_\gamma, \Theta_s, n_s, \tau) \] (9)
where $\zeta$ is the curvature perturbation, $\omega_0$ and $\omega_\gamma$ are the physical densities of baryons and the CDM, respectively, $\Theta_s$ is the ratio of the sound horizon to the angular diameter distance to last scattering, $n_s$ is the spectral tilt and $\tau$ is the optical depth to reionization. An extra bias parameter $b$ for the matter power spectrum is treated as a nuisance parameter and marginalized over, hence I do not count it as an additional parameter. I do not consider tensor modes nor extra neutrino species nor running of the spectral index. I take the three neutrino families to be massless and I fix the dark energy equation of state to $w = -1$ at all redshifts. All of those choices are motivated by the fact that inclusion of any of the above extra parameters is presently not required by the data. This means that a comparison between a model including both the isocurvature fraction and one of the above extra parameters against the simple adiabatic model would favour even more strongly the latter, as a consequence of the extra Occam’s factor effect coming from the extra parameter. In this sense, the model selection is basically conservative.

The situation is different for parameter constraints, because in this case strong degeneracies between the isocurvature fraction and other extra parameters might change the posterior bounds on $f_s$. In particular, one can expect a strong degeneracy between the CDM isocurvature mode and the presence of a tensor mode from gravity waves, when considering temperature power spectrum information alone. The extra power contributed by the CDM isocurvature to the Sachs–Wolfe plateau for small $\ell$ values is strongly anticorrelated with the tensor mode amplitude. However, inclusion of polarization data would help in breaking this degeneracy, at least partially. The impact of allowing a tensor mode contribution is very mild for the neutrino modes, as the Sachs–Wolfe plateau is lower than the first acoustic peak for these modes, and as a consequence constraints on their amplitudes are dominated by the height of the peak, not by the height of the plateau. Similar considerations also apply for a possible running of the spectral index. Other parameters that mainly affect the angular diameter distance to last scattering and therefore the position of the acoustic peaks in the spectrum (such as the dark energy equation of state, the curvature of spatial sections or an extra background of relativistic particles) present only weak degeneracies with the isocurvature fractions, because the position of the peaks is strongly constrained by the data.

In the following, I therefore limit my analysis to the six-parameter model $M_s$ described above, complemented in the extended models by the isocurvature fractions as follows. The extended models, $I_s$, contain a non-vanishing isocurvature fraction
\[ I_s = (\theta, f_s) \] (10)
where $f_s$ is defined in equation (2) and $x = ci, ne, or nd$. The spectral index of the isocurvature mode is the same as the adiabatic one, $n_s$. The correlation coefficient between the adiabatic and the isocurvature mode is $\pm 1$, depending on the sign of $f_s$.

4 RESULTS AND DISCUSSION

In this section I present my results about the isocurvature fraction in terms of posterior bounds, Bayesian model selection and effective model complexity.

I use the WMAP 3-yr temperature and polarization data (Hinshaw et al. 2006; Page et al. 2006) supplemented by small–scale CMB measurements (Readhead et al. 2004; Kuo et al. 2004). I add the Hubble Space Telescope measurement of the Hubble constant $H_0 = 72 \pm 8$ km s$^{-1}$ Mpc$^{-1}$ (Freedman et al. 2001) and the Sloan Digital Sky Survey (SDSS) data on the matter power spectrum on linear scales (Tegmark et al. 2004).

In Fig. 1 I plot the one-dimensional, marginalized posterior pdf on the isocurvature fraction parameter $f_s$. I have adopted a flat prior of $f_s$, with width much larger than the posterior, so that the range of the prior does not influence the result. The isocurvature fraction is compatible with zero for all three isocurvature modes, with a slight shift of the peak of the pdf to negative values. This corresponds to a negative correlation, in which case the contribution to the large-scale CMB power due to the isocurvature autocorrelation spectrum is largely compensated by the negative correlator. The posterior mean and standard deviation for $f_s$ are given in Table 1, as well as one-dimensional marginalized intervals encompassing 95 per cent of probability. I find that the isocurvature fraction for the CDM mode is constrained to be $-0.10 < f_s < 0.06$ (95 per cent probability), while for the two neutrino modes I obtain $-0.20 < f_s < 0.12$ (neutrino entropy) and $-0.18 < f_s < 0.22$ (neutrino velocity). It is noticed that the tightest constrained mode is the CDM isocurvature one. This is because with the definition of $f_s$, for a given value of $f_s$, the CDM
One can see that for models with poor predictivity, i.e. large prior, i.e. the number of parameters effectively constrained by the data.

The isocurvature fraction is compatible with 0. This is consistent with the conclusion that current data are not strong enough to select among the three isocurvature modes. I also plot the Gaussian approximation to the SDDR for the Bayes factor, equation (7), for the CDM isocurvature mode, and find a very good match with the value computed numerically from the Monte Carlo chain.

For a prior choice $\Delta f = 1$, the Bayesian complexity is close to 7, indicating that all of the 7 parameters of the extended model have been measured. I therefore conclude that models predicting up to the same amount of isocurvature to adiabatic power (the case $\Delta f = 1$) are strongly disfavoured for the CDM mode, and mildly disfavoured in the case of the two neutrino modes. However, if the prior range is reduced below $\Delta f = 1$, i.e. for models predicting predominantly adiabatic initial conditions with subdominant isocurvature contribution, the Bayes factor gives an inconclusive result, with about equal odds for the purely adiabatic and the mixed models. At the same time, the Bayesian complexity decreases, indicating that $f_s$ is only poorly constrained with respect to the scale of the prior, especially for the neutrino density and velocity modes. This reinforces the conclusion that current data are not strong enough to select among a purely adiabatic model and one which predicts up to 10 per cent isocurvature to adiabatic power (the case $\Delta f = 1$), indicating that the data require an isocurvature component, as the Occam’s razor effect, while models predicting an isocurvature fraction below about 10 per cent in any of the three modes cannot presently be ruled out (ln $B < 1$). The dotted line gives the Gaussian approximation to the Bayes factor, equation (7), for the CDM isocurvature mode. Bottom panel: the Bayesian complexity gives the effective number of parameters the data can support. For $\Delta f \lesssim 1$ the isocurvature component in the neutrino entropy and velocity modes is not supported by the data. The errors have been computed as the variance of 10 random subchains, and the neutrino entropy and velocity modes have been shifted horizontally to the left and to the right, respectively, for clarity.

5 CONCLUSIONS

I have submitted the question of the type of initial conditions for cosmological perturbations to renewed scrutiny in the light of WMAP 3-yr data. I have focused on the simplest and well motivated alternative to a purely adiabatic model, namely an admixture of one

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totally (anti)correlated isocurvature mode at the time, with the same spectral tilt as the adiabatic one.

Posterior bounds on the isocurvature fraction from WMAP 3-yr data combined with other CMB measurements and SDSS have been derived. The isocurvature fraction in the CDM mode is constrained to be less than about 10 per cent, while the maximum allowed neutrino isocurvature contribution (either density or velocity) is about 20 per cent.

Bayesian model selection tends to favour purely adiabatic initial conditions with strong odds (>20:1) when compared to models predicting isocurvature fractions larger than unity. For such models – having a large prior range on the isocurvature fraction – it has been shown that the data can support 7 parameters, but that only 6 of them are required, with no need to include isocurvature modes from a model selection point of view. These findings confirm the conclusions of Kunz et al. (2006). However, mixed models that limit the isocurvature contribution to less than about 10 per cent cannot presently be ruled out. I have shown that the constraining power of the data for this class of models is insufficient, and therefore we must hold our judgement until better data becomes available. These findings are however dependent on the parametrization chosen for the isocurvature fraction, that in this work is motivated by the curvaton scenario. The question of prior selection will be further addressed in a future publication.

It is reasonable to expect that the same conclusion would apply in even stronger terms to the case of more complicated models, e.g. those involving a superposition of different isocurvature modes at the same time, or with arbitrary correlations among them. In fact, more complicated models (such as the class considered by Bean et al. 2006) ought to be even more disfavoured because of their larger volume of wasted parameter space. At present, Occam’s razor is perfectly compatible with the simplest possibility, namely purely adiabatic initial conditions.

I think that this model comparison approach can be a useful complement to parameter constraints analysis, and that it can offer valuable guidance in building models for the generation of primordial perturbations.

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