Assumptions of the primordial spectrum and cosmological parameter estimation

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Abstract. The observables of the perturbed universe, cosmic microwave background (CMB) anisotropy and large structures depend on a set of cosmological parameters, as well as the assumed nature of primordial perturbations. In particular, the shape of the primordial power spectrum (PPS) is, at best, a well-motivated assumption. It is known that the assumed functional form of the PPS in cosmological parameter estimation can affect the best-fit parameters and their relative confidence limits. In this paper, we demonstrate that a specific assumed form actually drives the best-fit parameters into distinct basins of likelihood in the space of cosmological parameters where the likelihood resists improvement via modifications to the PPS. The regions where considerably better likelihoods are obtained allowing free-form PPS lie outside these basins. In the absence of a preferred model of inflation, this raises a concern that current cosmological parameter estimates are strongly prejudiced by the assumed form of PPS. Our results strongly motivate approaches toward simultaneous estimation of the cosmological parameters and the shape of the primordial spectrum from upcoming cosmological data. It is equally important for theorists to keep an open mind towards early universe scenarios that produce features in the PPS.
1. Introduction

Precision measurements of anisotropy and polarization in the cosmic microwave background (CMB), in conjunction with observations of the large-scale structure, suggest that the primordial density perturbation is dominantly adiabatic and has a nearly scale-invariant spectrum \[1, 2\]. This is in good agreement with most simple inflationary scenarios which predict nearly power law (PL) or scale-invariant forms of the primordial perturbation \[3−5\]. However, despite the strong theoretical appeal and simplicity of a featureless primordial spectrum, our results highlight that the determination of the shape of the primordial power spectrum (PPS) directly from observations with minimal theoretical bias would be a critical requirement in cosmology.

The observables of the perturbed universe, such as CMB anisotropy galaxy surveys and weak lensing, all depend on a set of cosmological parameters describing the current universe, as well as the parameters characterizing the presumed nature of the initial perturbations. While certain characteristics of the initial perturbations, such as the adiabatic nature and tensor contribution, can and are being tested independently, the shape of the PPS remains, at best, a well-motivated assumption.

It is important to distinguish between the cosmological parameters that describe the present universe from that characterizing the initial conditions, specifically the PPS, \[P(k)\]. However, it is customary in cosmological parameter estimation to treat the two sets identically. Based on sampling on a coarse grid in the cosmological parameter space, we have already shown that the CMB data are sensitive to the PPS \[6\]. The best-fit cosmological parameters with free form PPS have much enhanced likelihoods and the preferred regions significantly separated from the best-fit parameters obtained with assumed PL PPS. It is also known that specific features in the PPS can dramatically improve the fit to data (see e.g. \[7\] and references therein).

In this paper, we present another important issue introduced by our prior ignorance about the PPS. While known correlations between cosmological parameters are always folded into parameter estimation, the analogous situation for \[P(k)\] is not as widely appreciated. An assumed functional form for the PPS is equivalent to an analysis with a free-form PPS, where, say, \[P(k)\], is estimated in separate \(k\) bins, but then one imposes a strong correlation between the power in different bins. As we show in this paper, the assumed form (equivalently, the implied correlations in \(P(k)\) at different \(k\)) drives a significant number of degrees of freedom available in the cosmological parameters to adjust into suitable specific combinations. Hence, the assumed form of PPS could be dominant in selecting the best-fit regions (see e.g. \[8\], where features in the PPS lead to very different best-fit cosmological parameters). For specific functional forms, the corresponding best-fit models lie entrenched in distinct basins in the parameter space. Our results show that in these basins, the likelihood is remarkably robust to variations in the PPS. We
conclude that there are sufficient degrees of freedom in the cosmological parameters to mould the fit around the constraints imposed by the assumed form of the PPS.

In this paper, we elucidate this issue in the context of CMB data from WMAP for three different well-known assumed forms of the primordial spectrum, \( P(k) \), (i) scale-invariant Harrison–Zeldovich (HZ) with \( P(k) = A_s \), (ii) scale-free PL with \( P(k) = A_s k^{-
 -1} \) and (iii) running PL (RN) with \( P(k) = A_s k^{-n_0} \exp(-1.45 \ln(k/k_*)/n_{\text{run}}) \) where \( k_* \) is a pivot point.

The methodology and analysis are described in section 2. The results are given in section 3 and the conclusion of our work in section 4.

2. Method and analysis

The angular power spectrum of CMB anisotropy, \( C_l \), is a convolution of the PPS, \( P(k) \), generated in the early universe with a radiative transport kernel, \( G(l, k) \), determined by the current values of the cosmological parameters. The precision measurements of \( C_l \) and the concordance of cosmological parameters measured from other cosmological observations allow a possibility of direct recovery of \( P(k) \) from the observations. In our analysis we use an improved (error-sensitive) Richardson–Lucy (RL) method of deconvolution to reconstruct the optimized PPS at each point in the parameter space [6, 9–12]. The RL-based method has been demonstrated to be an effective method of recovering \( P(k) \) from \( C_l \) measurements [6, 11, 12] (see [13] for some other reconstruction methods).

In this paper, we study the improvement in likelihood allowed by an ‘optimal’ free-form PPS at points in the cosmological parameter space around the best-fit region for the three different assumed forms of PPS, namely HZ, PL and RN. We apply our deconvolution method to reconstruct an ‘optimal’ form of the PPS at each point [6].

Markov-chain Monte-Carlo (MCMC) samples of parameters provide a fair sampling of the parameter space around the best-fit point. We use the MCMC chains generated based on 3 year data by the WMAP team for parameter estimation with HZ, PL and RN forms of the PPS. We reconstruct the optimized PPS for each point of these chains and obtain the ‘optimal’ PPS likelihood based on the reconstructed spectrum.

We limit our attention to the flat \( \Lambda \)CDM cosmological model and consider the four dimensional (4D) parameter space, \( \Omega_m h^2, \Omega_b h^2, h \) and \( \tau \). This corresponds to a minimalistic ‘vanilla model’, a flat \( \Lambda \)CDM parameterized by six parameters \( (n_s, A_s, H_0, \tau, \Omega_b, \Omega_{dm}) \). In the case of the HZ PPS assumption, \( n_s = 1 \), leaving only five parameters. The case of assuming a constant running in the spectral index (RN), \( n_{\text{run}} \), leads to seven parameters. The dimensionality in the three models is different solely due to the parameters of the assumed PPS. Hence, in our analysis we always have a 4D space of cosmological parameters (since we recover the optimal PPS).

In order to represent the likelihood in a 4D parameter space, we find it convenient to define a normalized distance, \( \rho \), between two points:

\[
\rho(a, b) = \sqrt{\frac{\sum \epsilon_i (P_i^a - P_i^b)^2}{\sum \sigma_i^2}},
\]

where \( P_i^a \) and \( P_i^b \) are the values of \( i \)th cosmological parameter at point ‘a’ and point ‘b’, respectively. To ensure that equal separations along different parameters have a similar meaning, we divide \( P_i^a - P_i^b \) by the standard deviation \( \sigma_i^b \) at point ‘b’. We assign point ‘b’ to be a best-fit point where \( \sigma_i^b \) are the 1\( \sigma \) confidence limits derived by the WMAP team from the corresponding
MCMC chains. Since we are primarily interested in studying the region around the best-fit point, $\rho$ provides a convenient definition of distances to other points with respect to it. (Note the ‘distance’ $\rho$ is ‘asymmetric’ in ‘a’ and ‘b’ when $\sigma_i^b \neq \sigma_i^a$ and should be interpreted accordingly.)

3. Results

The simplest characterization of the likelihood landscape, $L(P_i)$, around the best-fit point is to study its behavior as $\rho$ increases with separation from the best-fit point. The trend in the likelihood can then be compared for two cases—assuming a form of the primordial spectrum or allowing an optimal free form. (We use the effective chi-square, $\chi^2 \equiv -2 \ln L$ instead of $L$.)

We now define $\rho_c$ as the distance from each point in the given MCMC samples to the best-fit point. For each point, we compute the effective $\chi^2$ difference, $\Delta \chi^2$ (i.e. twice the relative log-likelihood), with respect to this best-fit point, both for the likelihood obtained under the assumed PPS and with a free-form PPS (the optimal PPS recovery in our deconvolution). Figure 1 shows scatter-plots of $\Delta \chi^2$ versus $\rho_c$ for the case of PL and RN assumptions of the primordial spectrum. Green crosses show the expected behavior that locally the likelihoods worsen with $\rho_c$ as points depart from the best-fit parameters. On the other hand, the red pluses mark the same points in the cosmological parameter space, but for the $\Delta \chi^2$ obtained under free-form optimal PPS. It is clear from figure 1 that a free-form optimal PPS can very markedly improve the likelihood relative to that in the assumed form PPS. What is more remarkable is that the improvement through optimal free-form PPS is suppressed in a basin around $\rho_c < 1$. This is apparent in the absence of red plus marks near the lower left corners of the plots.

It is also interesting to mention that the basins for the three assumed forms of the PPS are very distinct and non-overlapping. The parameter distances between the best-fit points assuming HZ, PL and RN forms of the primordial spectrum are quite large. We have $\rho_{(PL,HZ)} = 14.56$, $\rho_{(RN,HZ)} = 43.79$, $\rho_{(HZ,PL)} = 6.89$, $\rho_{(RN,PL)} = 4.85$, $\rho_{(HZ,RN)} = 11.09$ and $\rho_{(PL,RN)} = 2.44$. It is important to also note that the best-fit point obtained under one assumed form of PPS may be disfavored with high confidence by another assumption.

As mentioned above, in the basins around the best-fit points it is very difficult to get a significantly better likelihood allowing for a free-form PPS. It is instructive to explore the nature of these basins and the trends of likelihood assuming the free-form PPS for each of the parameters $\Omega_m h^2$, $\Omega_{w} h^2$, $h$ and $\tau$. To do so, for each parameter, $i$, we split the separation, $\rho$, between points, $a$ and $b$, in the parameters into a separation $\Delta P_i = (P_i^a - P_i^b)/\sigma_i^b$ along the parameter and the ‘perpendicular’ distance $\rho_{\perp} = \sqrt{\sum_{j \neq i} (P_j^a - P_j^b)^2/(\sigma_j^b)^2}$ measuring the separation in the other three parameters.

Figure 2 shows, for the PL PPS case, a 2D surface representation of the optimized $\Delta \chi^2$ around the best-fit point plotted against $\Delta P_i$ and $\rho_{\perp}$ for each of the parameters. We have weighted the neighboring sample points by their Euclidean distance in the parameter space to assign an average likelihood at each point. The color palette is chosen such that red (blue) regions have poorer (better) likelihood than the reference value of the best-fit model. The white regions have a likelihood comparable to the best-fit value. In this representation, the figures clearly show that in all cases, there is a plateau in the parameter space (the red regions) enclosing the best-fit point where a free-form PPS does not improve the likelihood. The location of the best-fit points are marked by red arrows. Outside these basins, there are blue regions where optimal free-form PPS leads to very significant improvement in the likelihood. (However,
Figure 1. The panels show the comparative scatter plots of relative $\chi^2$, with and without optimal $P(k)$, versus the normalized distance $\rho_c$, (equation (1)) in parameter space of the sample points for sub-samples of the MCMC chains generated by the WMAP team. Green crosses show $\Delta \chi^2$ relative to the best-fit value. Red pluses mark the same points in the parameter space but with $\chi^2$ derived after ‘optimization’ of the primordial power spectrum. The top and bottom panels correspond to MCMC chains assuming PL form and RN form PPS, respectively. The obvious absence of red points with significantly negative $\Delta \chi^2$ for $\rho_c < 1$ marks the basins for each assumed PPS where no (or minor) improvement in likelihood is seen even invoking a free-form ‘optimal’ PPS. The basins for the three assumed PPS are non-overlapping. For comparison, in the PL case (upper panel), the distances to the best-fit HZ model $\rho_{(HZ,PL)} = 6.89$ and the RN model $\rho_{(RN,PL)} = 4.85$, respectively. In the RN case (lower panel), the distances to best-fit HZ and PL models are $\rho_{(HZ,RN)} = 11.09$ and $\rho_{(PL,RN)} = 2.44$, respectively.
Figure 2. A 2D surface representation of the optimized $\Delta \chi^2$ around the best-fit point for the PL PPS case for the four parameters. For each parameter, $i$, $\Delta P_i$ measures separation along the parameter and $\rho_{i\perp}$ measures the separation in three other parameters. Regions in the parameter space with $\Delta \chi^2 > 0$ are shown in red and are separated by a white band (representing $\Delta \chi^2 \approx 0$) from the regions with $\Delta \chi^2 < 0$ shown in blue. Red plateaus represent the regions where allowing the free-form primordial spectrum does not improve the likelihood. Red arrows show the position of the best-fit point assuming the PL form of PPS.

note that these are far from being the global minima for optimal PPS cosmological parameter estimates—as shown in [6], there are models with much higher likelihood.)

The plots in figure 2 also supplement the PL plot in figure 1 (top), by indicating the direction in the parameter space from the best-fit models where likelihood resists improvement against modifications to the PPS.

We should note that a correlation between the cosmological parameters can be seen from our results. The likelihood surfaces in figure 2 show at which points in the parameter space we may have a similar likelihood that is somehow representing the correlation between the parameters. The four cosmological parameters used in our analysis are the basic parameters in CMB analysis and although there might be some correlations between them (in the derivation of likelihood) they are fundamentally independent parameters. However, this has not been our main concern in this paper, so we have not gone into much detail. Our main point is to show
how we may end up with other corners of the parameter space by assuming different forms (or a free form) of the primordial spectrum. We should also clarify that the choice of $\rho$ used in this paper is somehow arbitrary in the sense that we want to have an estimation of the distance between different points in the parameter space. One could use another form of $\rho$ but the results could not be significantly different.

Another important point to mention regards the degrees of freedom in our likelihood analysis. One should note that it is not justifiable to define the degrees of freedom for our non-parametric reconstructed free form of the primordial spectrum. This issue has been discussed earlier in [6, 11, 12]. It has been shown, however, that one cannot derive a very good likelihood at any point in the parameter space having this freedom to choose the form of the primordial spectrum. This fact is the basis of this work in which we try to optimize the form of the primordial spectrum to derive the best likelihood at each point. One should realize that this freedom is for all points in the parameter space so if we cannot improve the likelihood in part of the parameter space even allowing the free form of the primordial spectrum; this shows the strong setting of the other parameters (cosmological parameters). Our analysis is clearly a non-Bayesian analysis and we show that setting the strong priors on the form of the primordial spectrum can result in ambiguities in the derivation of the cosmological parameters and can be potentially misleading.

4. Conclusion

In this paper, we have shown that the assumed form of the PPS plays a key role in the determination of cosmological parameters. In fact, the functional form of the PPS forces the best-fit cosmological parameters to specific preferred basins of high likelihood to the data. These estimated cosmological parameters are then significantly biased. It is similar to the case in an $N$-dimensional parameter space of a model, when we fix the values of $m$ parameters ($m < N$) and vary the other $N - m$ parameters to fit an observation. The resultant best-fit values of these $N - m$ parameters can be very different, depending on the values assigned to the fixed $m$ parameters. If there is no good reason to select a particular set of fixed values, the determination of the rest of the parameters remains under question. Assumption of the assumed (say, PL) form of the primordial spectrum can also be interpreted as a very strong, specific correlation between $P(k)$ at different $k$. This assumption is similar to setting values for the $m$ parameters with specific correlations. We surmise that the assumed form of the PPS could be the dominant reason that in the basins for each assumed form it was not possible to achieve a marked improvement in $\chi^2$ by allowing optimal free-form PPS (see figure 2). It is very important to note that despite allowing a free form for the primordial spectrum, not all cosmological models (i.e. all points in the parameter space) can be fitted equally well to the data. We clearly show that some points in the cosmological parameter space fit the WMAP CMB data significantly better than the other points, by ‘optimizing’ the likelihood over a free form of the primordial spectrum. We conjecture that the positive definiteness of the primordial spectrum does not allow us to fit all the points in the parameter space to the data equally well, and some points will have a better fit to the data. Hence, the result that we do not get a good likelihood for some points in the parameter space has nothing to do with being trapped in a local minima. We do not employ any global minimization (or sampling) algorithm/technique where this could be an issue. We should also clarify that our analysis in this paper is not meant to be a consistency check of the standard PL form of the primordial spectrum (or any form of $P(k)$). It is known that the PL form of
the primordial spectrum is very consistent with the data [14–16]. Our main point in this paper is to emphasize the fact that in the process of cosmological parameter estimation, assumptions regarding the functional form of the primordial spectrum can be extremely critical. In other words, the preferentially selected best fit values from the distinct basin in the cosmological parameter space can result in a particular form of $P(k)$, and this causes apparent robustness in the variations of $P(k)$ within these basins, which can potentially be misleading as we may think we have found the actual form of $P(k)$ with high certainty.

In summary, we show that the apparently ‘robust’ determination of cosmological parameters under an assumed form of $P(k)$ may be misleading and may well largely reflect the inherent correlations in the power at different $k$ implied by the assumed form of the PPS. We conclude that it is very important to allow for deviations from scale-invariant, scale-free or simple phenomenological extensions of the same in the PPS while estimating cosmological parameters. This provides a strong motivation to pursue approaches that simultaneously determine both the cosmological parameters and the PPS from observations. The rapid improvement in cosmological observations, such as the CMB polarization spectra, holds much promise towards this goal. It is not unlikely that early universe scenarios that produce features in PPS could, in fact, be favored by data.

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