Principal Component Analysis of the Cosmic Microwave Background Anisotropies: Revealing The Tensor Degeneracy

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ABSTRACT
A principal component analysis of cosmic microwave background (CMB) anisotropy measurements is used to investigate degeneracies among cosmological parameters. The results show that a degeneracy with tensor modes – the ‘tensor degeneracy’ – dominates uncertainties in estimates of the baryon and cold dark matter densities, $\omega_b = \Omega_b h^2$, $\omega_c = \Omega_c h^2$, from an analysis of CMB anisotropies alone. The principal component analysis agrees well with a maximum likelihood analysis of the observations, identifying the main degeneracy directions and providing an impression of the effective dimensionality of the parameter space.

Key words: cosmic microwave background- cosmology:miscellaneous.

1 INTRODUCTION
Since the discovery of CMB anisotropies by the COBE team (Smoot et al. 1992) there has been rapid progress on the observational front, culminating with publication earlier this year of evidence for multiple acoustic peaks in the CMB power spectrum (Netterfield et al. 2001; Lee et al. 2001; Halverson et al. 2001). It has long been known that accurate measurements of the CMB anisotropies can be used to estimate parameters characterising the primordial fluctuations, the geometry of the Universe and its matter content (e.g. Jungman et al. 1996; Bond, Efstathiou & Tegmark 1997; Zaldarriaga, Spergel & Seljak 1997). In fact, the most recent measurements paint a gratifyingly consistent picture compatible with the simplest models of inflation (i.e. a spatially flat Universe with scale-invariant adiabatic fluctuations). Furthermore, the derived value of the baryon density $\omega_b$ appears to be consistent with the value $\omega_b = 0.020 \pm 0.002$ inferred from primordial nucleosynthesis and deuterium abundance measurements from quasar absorption line spectra (Burles, Nollett & Turner 2001, and references therein).

It has also long been known that there are significant degeneracies amongst cosmological parameters estimated from CMB anisotropies, i.e. parameter combinations exist that produce nearly identical CMB power spectra (Bond et al. 1994; Efstathiou & Bond 1999, hereafter EB99). The best known is the geometrical degeneracy between the matter and vacuum energy densities, $\Omega_m$ and $\Omega_\Lambda$, and the curvature $\Omega_k = 1 - \Omega_m - \Omega_\Lambda$. This degeneracy is almost exact and precludes reliable estimates of either $\Omega_\Lambda$ or the Hubble parameter $h$ from measurements of the CMB anisotropies alone. The existence of parameter degeneracies means that the best fitting parameters and their errors can be extremely sensitive to the chosen parameter set (e.g. whether the Universe is assumed to be spatially flat) and to adopted ‘prior distributions’ (e.g. observational constraints on the Hubble constant). This complicates the interpretation of CMB anisotropy parameter studies and the intercomparison of limits determined by different authors.

Almost all CMB parameter analyses (with the notable exception of the work of Tegmark and collaborators, Tegmark 1999; Tegmark, Zaldarriaga & Hamilton, 2001; Wang, Tegmark & Zaldarriaga, 2001) have ignored a tensor component (see for example, Lange et al. 2001; Jaffe et al. 2001; de Bernardis et al. 2001; Pryke et al. 2001; Stompor et al. 2001). This special case is certainly interesting because a wide class of inflationary models predict a negligible contribution from tensor modes. Indeed it has been argued persuasively that the absence of tensor modes is generic to any model in which the inflaton potential is related to the Higgs sector of a grand unified theory (Lyth 1997).

However, so little is known about inflation (if indeed inflation occurred) that it may be dangerous to neglect a tensor mode, particularly if some cosmological parameters of interest are sensitive to tensor modes. In fact, in single-field inflation models the relative amplitudes of the tensor and scalar tensor modes ($r$) and their spectral indices ($n_t$ and $n_s$) are related to the inflaton potential and its first two derivatives (e.g. see Hoffman & Turner 2001 for a recent discussion). In this class of model the relation between

* Here $h$ is Hubble’s constant $H_0$ in units of 100kms$^{-1}$Mpc$^{-1}$
2 PRINCIPAL COMPONENT ANALYSIS

We use the compilation of band power estimates $\Delta T_B^2$ and their covariance matrix $C_{BB'}$ computed by Wang et al. (2001, hereafter WTZ01) from 105 CMB anisotropy measurements. These band power estimates include a model for calibration and beam errors (see WTZ01 for further details). Each band power estimate is related to the power spectrum $C_\ell$ of the CMB anisotropies by

$$\Delta T_B^2 = \frac{T_0^2}{2\pi} \sum_{\ell=1}^{1500} \ell(\ell+1)C_\ell W_B(\ell) \quad (1)$$

where $W_B$ is the window function for each band power (also computed by WTZ01). These band-power estimates are plotted in Fig. 1. Also plotted in this figure is a fiducial model\(^\dagger\) with the following parameters: $\omega_b = 0.020$, $\omega_c = 0.13$, $h = 0.7$ ($\Omega_b = 0.04$, $\Omega_c = 0.26$), $\Omega_k = 0$, $\tau_{\text{opt}} = 0.1$, $n_s = 1$, $n_t = 0$, $\tau_{10} = 0.2$. These parameters provide an extremely good fit to the observations and are very close to the concordance values determined by WTZ01 and the author from a full likelihood analysis. The addition of a small tensor component has little effect on the fit shown in Fig. 1, but is introduced to regularize the Fisher matrix of equation (2).

Given the covariance matrix of the observations, we can form the Fisher matrix for the (mean subtracted) parameter set $\{s_i\}$:

$$F_{ij} = \sum_{BB'} C_{BB'}^{-1} \frac{\partial \Delta T_B^2}{\partial s_i} \frac{\partial \Delta T_{B'}^2}{\partial s_j} \quad (2)$$

In defining the parameter set $s_i$, we use $\ln \omega_b$ and $\ln \omega_c$ rather than $\omega_b$ and $\Omega_c$ and $\Omega_D = \Omega_k = 0.286\Omega_\Lambda$ rather than $\Omega_k$. The latter expresses the geometrical degeneracy (see EB99), since if all parameters other than $\Omega_b$ and $\Omega_\Lambda$ are held fixed, the condition $\delta\Omega_D = 0$ preserves the positions of the acoustic peaks for small variations of the parameters about those of the fiducial model. The normalization parameter $Q$ is defined following EB99 so that $Q^2$ is the mean band power ($\sum_{\ell=1}^{1500} \ell(\ell+1)C_\ell$) of a model relative to that of the fiducial model plotted in Fig. 1. With this definition, $Q$ is observationally well constrained and is largely decoupled from variations in cosmology and the optical depth $\tau_{\text{opt}}$ (unlike measures of the amplitude related to low multipoles). The tensor to scalar ratio $\tau_{10}$ is defined so that $C_{10}^T = \tau_{10}C_{10}^S$. With these definitions, we can compute the Fisher matrix from derivatives of the power spectra $C_\ell^T$ and $C_\ell^S$, as

\(^\dagger\) The CMB power spectra in this paper were computed using the CMBFAST code of Seljak & Zaldarriaga (1996).
in standard analyses of parameter forecasting (Jungman et al. 1996, Bond et al. 1997). Alternatively, we could compute the Hessian matrix by estimating second derivatives of the likelihood function around the maximum likelihood value either directly or by summing over first and second derivatives of $\Delta T^2_k$. In most situations using either the Fisher and Hessian matrixes should give closely similar results, and in fact, the second derivatives of $\Delta T^2_k$ are often ignored in order to stabilise numerical evaluations of the Hessian (see e.g. Press et al. 1992).

Having computed the Fisher matrix, we diagonalise it,

$$
F = \mathbf{U} \Lambda \mathbf{U}^T, \quad \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N).
$$

The matrix $\mathbf{U}$ defines a set of principal components, $\mathbf{X}$, i.e. orthogonal linear combinations of the original parameters,

$$
\mathbf{X} = \mathbf{U}^T \mathbf{s},
$$

such that the variance of the component $X_i$ is equal to $1/\lambda_i$. (See BE99 for an application of principal component analysis to the MAP and Planck satellites.)

The eigenvalues and components of $\mathbf{U}^T$ for our chosen set of variables and fiducial model are listed in Table 1. The principal components have been ordered by their expected variance so that $X_1$ is the best determined parameter and $X_9$ is the worst. The last line in the table lists the predicted variances of the parameters $s_i$, $(\sqrt{F_{ii}})$. As can be seen from Table 1, the present data can be used to constrain three parameter combinations well and three extremely poorly, with the remaining constrained at intermediate levels of accuracy. The best and worst determined principal components have a straightforward interpretation. $X_1$ has a high weight from $\Omega_D$, and so, in effect, measures the positions of the acoustic peaks; $X_2$ has a high weight from the overall amplitude of the spectrum $Q$; $X_3$ has high weights from the scalar spectral index $n_s$ and $\tau_{opt}$ and provides a measure of the shape of the fluctuation spectrum. The component $X_9$ accounts for almost all of the variance of $\Omega_D$, and $\Omega_s$ and $\Omega_{\Lambda}$, and describes the geometrical degeneracy and the extremely poor constraints that the present data place on tensor modes. The component $X_8$ describes the tensor degeneracy and accounts for almost all of the variance of the parameters $\ln \omega_t$, $\ln \omega_c$, $\eta_s$ and $\Omega_D$. Together, the components $X_8$ and $X_9$ accounts for almost all of the variance of all of the parameters with the exception of the amplitude $Q$.

The principal component analysis therefore suggests that acceptable models lie on a plane within the 9 dimensional parameter space. This is illustrated in Fig. 2a which shows likelihood contours in projections chosen to illustrate the geometrical and tensor degeneracies. The upper panels show the geometrical degeneracy in the parameter pairs $\Omega_{\Lambda} - \Omega_s$ and $h - \Omega_{\Lambda}$. The dashed lines show the degeneracy directions defined by the component $X_9$. The solid line in the $\Omega_{\Lambda} - \Omega_s$ plane shows the constraint $\delta \Omega_D = 0$. The solid

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\[\text{Figure 2.} \text{ Various projections of the likelihood functions chosen to illustrate the geometrical and tensor degeneracy. One, two and three-sigma likelihood contours are plotted in each panel. The panels to the left were computed from the Fisher matrix (equation 2) and the panels to the right show 'pseudo-marginalized' contours computed from a full likelihood analysis of the data described by Efstathiou et al. (2001). The solid lines in the upper panel show the approximate locus of the geometrical degeneracy computed from the constraint equation (3). The dashed lines in the upper and lower panels show the degeneracy directions defined by the component $X_9$ and $X_8$ respectively. The filled circles show the parameters of the nearly degenerate models plotted in Fig. 3. The crosses in figures 2b show the positions of the peaks in the likelihood function.}\]
line in the $h - \Omega_{\Lambda}$ plane is computed from the constraint equation

$$h = \frac{(\omega_b + \omega_c)^{1/2}}{(1 - \Omega_b - \Omega_{\Lambda})^{1/2}},$$

with $\omega_b$, $\omega_c$, and $\Omega_{\Lambda}$ set to the values of the target model. The dotted lines in the lower two panels show the degeneracy directions defined by the component $X_s$.

The Fisher matrix and the associated principal component analysis is approximate and it is not obvious a priori how well they describe degeneracies especially for parameter values that are quite a long way from those of the target model. Fig. 2b shows the analogous contours computed from a full likelihood analysis of the data of Fig. 1 (see the companion paper of Efstathiou et al. 2001 for a detailed discussion). The agreement is surprisingly good. The general directions of the geometrical and tensor degeneracies follow those of the Fisher matrix analysis. There are some differences however. The low order CMB multipoles offer some discrimination of models with high values of $\Omega_{\Lambda}$ via the integrated Sachs-Wolfe effect (see EB99), thus models with $\Omega_{\Lambda} \gtrsim 0.88$ are excluded by the data. The maximum likelihood analysis shows that the tensor degeneracy allows high values of $\omega_b$ but that the likelihood function falls sharply for $\omega_b \lesssim 0.018$ (interestingly only just below the value favoured from primordial nucleosynthesis deuterium constraints).

The three filled circles in Fig. 2 show the parameter values for the target model and for two nearly degenerate models with extreme values of $\omega_b$ chosen to lie along the tensor degeneracy direction. (The device used here, of varying low order principal components to produce degenerate pairs of models, was used by EB99 to investigate parameter degeneracies for the MAP and Planck satellites.) One model has $\omega_b = 0.042$ and the other has $\omega_b = 0.012$. The models were intentionally chosen to have similar values of $\Omega_{\Lambda}$, consequently the high baryon density model has a low value of $h$ which one might argue is incompatible with independent measurements of the Hubble constant (Freedman et al. 2001). However, our purpose here is to show how the constraints on $\omega_b$ derived from CMB anisotropies alone are weakened when tensor modes are included. The high and low baryon density models are compared to the data and to the fiducial model in Fig. 3.

Despite the very different parameter values, the models produce almost identical CMB power spectra by construction. The exact likelihood analysis (Fig. 2b) shows that the model with the high baryon density is compatible with the data at about the 2$\sigma$ level. The low baryon density model is formally excluded by the data at a high level of significance (> 3$\sigma$) because it fails to match the height of the first acoustic peak. This is a characteristic feature of models with a low baryon density. Nevertheless, the diagram is interesting because it shows that that the lower limits on $\omega_b$ are extremely sensitive to any residual systematic errors that might affect the peak heights (see e.g. de Bernardis et al. 2001, figure 1).

### Table 1: Principal components for data of Fig. 1

| $\lambda_i^{1/2}$ | $\lambda_{nb}$ | $\ln \omega_b$ | $\ln \omega_c$ | $\sigma_p$ | $\sigma_{\omega_b}$ | $\sigma_{\omega_c}$ | $\sigma_{\Omega_{\Lambda}}$ | $\sigma_{\Omega_b}$ | $\sigma_{\Omega_{r_{10}}}$ |
|------------------|----------------|---------------|---------------|-------------|---------------------|------------------|----------------------|------------------|---------------------|
| 1                | 8.492E-03      | 8.006E-02     | -1.813E-01    | 2.083E-02   | -1.564E-01          | -6.389E-03       | -3.049E-03          | 9.631E-01       | 3.110E-01           |
| 2                | 4.243E-02      | 2.907E-02     | -3.167E-02    | 9.036E-01   | 1.092E-01           | 6.335E-02        | 6.335E-02           | 1.473E-01       | 4.500E-02           |
| 3                | 3.626E-02      | -1.594E-01    | 1.038E-01     | 8.064E-01   | 3.934E-01           | 2.935E-01        | -1.804E-01          | 3.592E-01       | 1.132E-01           |
| 4                | 7.134E-02      | -2.707E-01    | 1.719E-01     | 1.786E-03   | -1.171E-02          | 4.286E-01        | 3.402E-01           | 9.385E-02       | 2.190E-01           |
| 5                | 1.303E-01      | 5.401E-01     | 6.827E-01     | 7.021E-02   | 2.468E-01           | 2.137E-01        | 9.979E-02           | 9.107E-01       | 6.951E-02           |
| 6                | 3.827E-01      | -2.104E-01    | 4.213E-01     | 1.719E-01   | 1.523E-01           | 9.087E-01        | 3.116E-03           | 5.643E-01       | 1.250E-01           |
| 7                | 8.900E-01      | 2.102E-01     | -3.877E-01    | 1.425E-01   | -2.171E-03          | 3.737E-01        | 9.385E-02           | 5.118E-01       | 1.121E-01           |
| 8                | 1.572E+00      | 1.949E-01     | -3.544E-01    | 1.425E-01   | -2.171E-03          | 3.737E-01        | 9.385E-02           | 5.118E-01       | 1.121E-01           |
| $s_1^2$          | 0.41           | 0.75          | 0.38          | 0.023       | 1.3                | 1.8              | 0.17                 | 3.1             | 1.4                 |

3 DISCUSSION

The reader might question the usefulness of the results presented in the previous section. Firstly, the principal component analysis provides only an approximate description of the parameter degeneracies, whereas they emerge precisely from a brute force maximum likelihood analysis. Secondly, models at the extreme ends of the ranges allowed by the tensor degeneracy have unusual parameters (for example, the model with $\omega_b = 0.042$ in Fig. 3b has a low Hubble constant and a high value of the scalar spectral index) and so are surely excluded by other observational constraints. We discuss each of these points in turn.

(i) Effective dimensionality: The main use of the principal component analysis is to assess the effective dimensionality of the space of acceptable models within the multidimensional space defined by the physical parameters $s_1$ and to assess whether this effective dimensionality is sensitive to changes of the parameter set. For example, let us assume that we are interested in the values of the parameters $\omega_b$ and $\omega_c$. The principal component analysis tells us that most of the variance of these parameters is contributed by only two poorly constrained principal components. The values of these parameters are therefore affected by major parameter degeneracies which can only be removed by imposing external constraints or by performing a fundamentally different type of CMB experiment. For example, the effects of the tensor degeneracy on $\omega_b$ and $\omega_c$ can be broken by extending the CMB measurements to much higher multipoles (see EB99) and/or by setting limits on a tensor component from an analysis of a B-type polarization pattern in the CMB (see e.g. Kamionkowski & Jaffe, 2000, and references therein).

(ii) Complementary information: CMB parameter degeneracies can be broken by invoking complementary information. A well known example is the combination of Type Ia supernovae measurements with the CMB to break the geometrical degeneracy (see e.g. de Bernardis et al. 2001 for a recent...
analysis). WTZ01 break the tensor degeneracy by combining the CMB data with a number of constraints including estimates of the power spectrum on small scales from observations of the Lyα forest (Croft et al. 2001) and limits on the Hubble constant from HST Hubble Key Project (Freedman et al. 2001). The problem here is that it becomes progressively more difficult to assess whether parameter values are affected by systematic errors as more external constraints are applied, particularly if the external constraints involve complex observations and assumptions. (For example, how can we test empirically whether density fluctuations in the inter-galactic medium as traced by the Lyα forest match those of the dark matter?). Even if the parameter values are shown to remain consistent as external constraints are applied, there is no guarantee that the final combined likelihood distribution will be accurate. Ideally, we would like to apply as small a number of external constraints as possible using data sets with well controlled errors. The Fisher matrix analysis of the previous section offers a guide as to which external constraints will be most effective at breaking degeneracies. The effects of external constraints can easily be assessed using the Fisher matrix: let $P_{ij}$ be the covariance matrix of the parameters $s_i$ from external constraints, then the covariance matrix after combining with the CMB is

$$C_{ij} = (F_{ij} + P_{ij}^{-1})^{-1}.$$  

As mentioned in Section 2, the models plotted in Fig. 3 were chosen by construction to have similar values of $\Omega_\Lambda$, so it is clear that combining the CMB results with constraints on $\Omega_\Lambda$ from Type Ia supernovae observations will have little effect on the parameters $\omega_b$ and $\omega_c$. Constraints on the Hubble constant will be more effective in narrowing the range of allowed values of $\omega_b$ and $\omega_c$. However, from Fig. 2 we can see that the tensor degeneracy exhibits a strong correlation between $\omega_b$, $\omega_c$, and the scalar spectral index $n_s$. Even a relatively poor constraint on the scalar spectral index will lead to a sharp tightening of the $\omega_b$ and $\omega_c$ error contours. (A constraint $\Delta n_s$ on the spectral index will narrow the error on the baryon density to $\Delta \ln \omega_b \approx (U_{18}/U_{38}) \Delta n_s$, i.e. $\Delta \ln \omega_b \approx 1.04 \Delta n_s$.) This suggests that the recent estimates of the galaxy power spectrum from the 2dF Galaxy Redshift Survey (Percival et al. 2001) will be highly effective at breaking the tensor degeneracy, leading to tight constraints on the matter content of the Universe. This is borne out by a detailed analysis presented in a companion paper (Efstathiou et al. 2001).

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