Maximum-Likelihood Analysis of the COBE Angular Correlation Function

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ABSTRACT

We have used maximum-likelihood estimation to determine the quadrupole amplitude $Q_{\text{rms}}$ and the spectral index $n$ of the density fluctuation power spectrum at recombination from the COBE DMR data. We find a strong correlation between the two parameters of the form $Q_{\text{rms}} = (15.7 \pm 2.6) \exp[0.46(1 - n)] \mu\text{K}$ for fixed $n$. Our result is slightly smaller than and has a smaller statistical uncertainty than the 1992 estimate of Smoot et al.

\textit{Subject headings:} cosmic microwave background — cosmology: observations — large-scale structure of universe

1. Introduction

The search for the cosmic microwave background radiation (CMBR) anisotropies finally yielded positive results with the detection made with the Differential Microwave Radiometers (DMRs) on the \textit{Cosmic Background Explorer} (COBE) satellite (Smoot et al. 1992; Bennett et al. 1992; Wright et al. 1992). These authors analyzed sky maps based on the first year of COBE data and presented quantitative results for the quadrupole moment, the angular correlation function, and power spectrum parameters characterizing the large
angular scale fluctuations. In simple cosmological models the CMBR anisotropy is related directly to the gravitational potential fluctuations present during recombination on large length scales (Sachs & Wolfe 1967). The COBE data thus enable quantitative testing of cosmological theories, free from the complications of galaxy formation.

Perhaps the most important measure of CMBR anisotropy is provided by the angular correlation function of the temperature anisotropy $\Delta T$, $C(\alpha) = \langle \Delta T(\vec{n}_1)\Delta T(\vec{n}_2) \rangle$. The average is taken over the sky for all pairs of directions separated by angle $\alpha = \cos^{-1}(\vec{n}_1 \cdot \vec{n}_2)$. Smoot et al. (1992, Fig. 3) and Wright et al. (1992, Fig. 2) presented estimates for $C(\alpha)$ with the monopole and dipole contributions removed; Smoot et al. (but not Wright et al.) also removed the quadrupole.

Smoot et al. (1992) used a least-squares fit to the measured values $C(\alpha_i)$ to estimate the amplitude (represented by the rms CMBR quadrupole, $Q_{\text{rms-PS}}$) and the spectral index $n$ of the density power spectrum, obtaining $n = 1.1 \pm 0.5$ and $Q_{\text{rms-PS}} = 17 \pm 5 \mu$K for $n = 1$, corresponding to the scale-invariant Peebles-Harrison-Zel’dovich spectrum. In order to make these estimates one needs the covariance matrix for $C(\alpha_i)$. There are two sources of uncertainty contributing to this covariance matrix: measurement errors (chiefly receiver noise) and cosmic variance (the intrinsic statistical fluctuations expected because the CMBR temperature is measured on a surface of finite extent). The cosmic variance, and therefore the full covariance matrix of the measurements, depends on the power spectrum parameters one is trying to determine. Smoot et al. presented least-squares estimates with and without the cosmic variance. The estimated values changed very little but the $\chi^2$ decreased from 79 to 53 for 68 degrees of freedom when the cosmic variance was included. We find that the inclusion of cosmic variance is even more important for the correlation function of Wright et al. (1992, Fig. 2), as it causes $\chi^2$ to decrease from 155 to 52 for 64 degrees of freedom if $n = 1$ and $Q_{\text{rms-PS}} = 17 \mu$K.

Recently, Scaramella & Vittorio (1993) emphasized the importance of cosmic variance. Including this, they reanalyzed the angular correlation function of Smoot et al. (1992) using $\chi^2$ minimization and Monte Carlo simulations. They concluded that the best-fit amplitude is $Q_{\text{rms-PS}} = (14.5 \pm 1.7)(1 \pm 0.06) \mu$K for $n = 1$, where the first error bar is due to cosmic variance and the second one to measurement uncertainties. However, they did not simulate the actual sky sampling and data reduction procedure applied to the data.

There are several shortcomings of the previous statistical analyses. First, the least-squares method is inappropriate when the covariance matrix depends on the parameters one is trying to estimate. In this case least-squares estimators are often biased and in general they do not have minimum variance. The standard least squares error estimates are also biased, and the sum of squares of residuals does not have a $\chi^2$ distribution. Correlations
between different lag angles $\alpha_i$ are not taken into account because the least-squares method (and also the minimum $\chi^2$ method) uses only the diagonal part of the covariance matrix of $C(\alpha_i)$. As we show below, this covariance matrix has three contributions, two of which involve cosmic variance and are nondiagonal. Although the biases can be corrected using Monte Carlo simulations, least-squares estimators do not make the most efficient use of the data because they are not minimum-variance.

Wright et al. (1993) reexamined the COBE data using the rms variance on the $10^\circ$ scale and the Boughn-Cottingham statistic (Boughn et al. 1992). They confirm their earlier results for the quadrupole amplitude, concluding that the amplitude is consistent with $Q_{\text{rms-PS}} = 17 \pm 5 \, \mu\text{K}$ for $n = 1$.

We have chosen instead to estimate the power spectrum parameters using the maximum-likelihood method. This method has the advantage of providing estimates that are asymptotically unbiased and of minimum variance (Eadie 1971). This Letter presents our approximate maximum-likelihood determination of $Q_{\text{rms-PS}}$ and $n$ using realistic Monte Carlo simulations of the COBE sampling and data reduction procedures. We will show that the uncertainties of these two parameters are strongly correlated and that the optimal value of $Q_{\text{rms-PS}}(n)$ for the correlation functions of Smoot et al. (1992) and Wright et al. (1992) is slightly lower and has smaller uncertainty than estimated by those authors.

2. Statistical Method

The measured correlation function $C(\alpha_i)$ was given in $m$ ($= 70$ for Smoot et al. 1992 and 65 for Wright et al. 1992) equidistant points $\alpha_i$ between $0^\circ$ and $180^\circ$. Approximating the $m$-dimensional distribution as a multivariate normal distribution one can write the likelihood function as

$$L(Q_{\text{rms-PS}}, n) = \exp\left[-\frac{1}{2}(\Delta C)^T M^{-1} (\Delta C)\right] \frac{1}{(2\pi)^m \det(M)^{1/2}}. \tag{1}$$

Here $(\Delta C)^T$ and $(\Delta C)$ are $m$-dimensional row and column vectors with entries $(\Delta C)_i = C(\alpha_i) - \langle C(\alpha_i) \rangle$, while $M = \langle (\Delta C) (\Delta C)^T \rangle$ is an $m \times m$ matrix. The angle brackets here denote averages over both measurement errors and the statistical ensemble of temperature fluctuation fields for given $Q_{\text{rms-PS}}$ and $n$. Both $\langle C(\alpha) \rangle$ and $M$ depend on these parameters. Maximum-likelihood estimates $\hat{Q}_{\text{rms-PS}}$ and $\hat{n}$ are obtained by maximizing $L(Q_{\text{rms-PS}}, n)$, keeping $C(\alpha_i)$ fixed at the measured values. The curvature of the likelihood
function around the maximum provides an estimate of the covariance matrix of errors of the estimated values (Eadie 1971).

In assuming a multivariate normal distribution we are maximizing the wrong likelihood function because the actual distribution of $C(\alpha_i)$ involves products of normally distributed variables (the raw temperature measurements) and in general is not normally distributed. However, the assumption of a normal distribution is not crucial to the success of our method when there are small departures from normality. Although the asymptotic property of the smallest variance among all estimation methods is no longer valid, the increase in variance should be small. One could appeal to the central limit theorem and assume that the average over many products of pairs is nearly normally distributed even when the individual products themselves are not. We have tested this possibility by making Monte Carlo realizations of pixel maps and calculating from them the distributions of $C(\alpha_i)$. They are close to normal away from the tails. The extended tails increase the variance of the estimated values, but the effect is small and does not significantly affect the overall efficiency of the maximum-likelihood method. We will use Monte Carlo simulations with the correct distributions to estimate the bias and variance of $\hat{Q}_{\text{rms-PS}}$ and $\hat{n}$.

The DMR instrument measured, for two independent channels at each of three frequencies, the differences in CMBR temperature $T_i - T_j$ between two directions $\vec{n}_i$ and $\vec{n}_j$ separated by 60° (Smoot et al. 1990). These differences were then fitted to give estimates of $\Delta T_i$ (with the monopole, dipole, and possibly quadrupole contributions removed) at 6144 points of an equal area sky map (Torres et al. 1989; Janssen & Gulkis 1992). The correlation function was then calculated by Smoot et al. (1992) and Wright et al. (1992) using

$$C(\alpha_k) = \frac{\sum_i N_i \sum_j N_j \Delta T_i \Delta T_j \delta(\vec{n}_i \cdot \vec{n}_j - \cos \alpha_k)}{\sum_i N_i \sum_j N_j \delta(\vec{n}_i \cdot \vec{n}_j - \cos \alpha_k)},$$

(2)

where $N_i$ is the number of measurements in each pixel $i$ and the $\delta$-function indicates that the sum is performed over all different pairs $\Delta T_i$ and $\Delta T_j$ such that $\cos^{-1}(\vec{n}_i \cdot \vec{n}_j)$ is in a given bin $k$ of $\alpha$. The weighting by $N_i$ gives a minimum-variance estimate for $C(\alpha_k)$. The temperature anisotropies $\Delta T_i$ and $\Delta T_j$ can be drawn either from the same map (autocorrelation) or from two different maps (cross-correlation). Smoot et al. cross-correlated the 53A+B and 90A+B GHz channels, while Wright et al. combined cross-correlations of 53A, 53B, and 90B channels in a manner equivalent to the autocorrelation of a single weighted map.

Evaluating the mean and covariance matrix of $C(\alpha_k)$ requires knowing the $N_i$ and the covariance matrix of temperature measurement errors. These quantities depend in a complex way on the COBE sky scan pattern and on the detailed properties of the DMR instrumentation (Boggess et al. 1992; Smoot et al. 1990). We used a simulation program,
kindly provided by Ned Wright, to simulate the spacecraft operation for the first year of operation, including the correct orbit, spacecraft spin, tracking of the Sun, Moon, and planets, with data rejection if the instrument pointed too close to the Earth and Moon, etc. (Smoot et al. 1992). The simulated measurements were gathered into 6144 equal area pixels using the quad-cube routines provide to us by Wright.

In addition, we calculated the covariance matrix of temperature measurement errors for the sky maps. The main source of measurement error is receiver noise (Smoot et al. 1990). Because the raw DMR measurements are temperature differences for two beams separated by 60°, the errors in the temperature maps (obtained by fitting to the differences) are correlated. We estimated that the off-diagonal elements of the covariance matrix are nearly all much smaller than 1% of the diagonal elements (rising to 6% for a few elements) so that to a good approximation one can safely neglect the noise correlations for different pixels. One can then write \( \Delta T_i = \Delta T^0_i + \epsilon_i \), where \( \Delta T_i \) is the measured value for pixel \( i \), \( \Delta T^0_i \) the true value and \( \epsilon_i \) the noise contribution. The pixel noise is normally distributed with \( \langle \epsilon_i \rangle = 0 \) and \( \langle \epsilon_i \epsilon_j \rangle = (\sigma^2/N_i)\delta_{ij} \), where \( \sigma \) is the noise contribution from a single measurement (Janssen & Gulkis 1992).

The true values \( \Delta T^0_i \) are also stochastic variables in theories of large-scale structure. The ensemble averages are \( \langle \Delta T^0_i \rangle = 0 \) and \( \langle \Delta T^0_i \Delta T^0_j \rangle = C^0(\alpha_k) \), where \( C^0(\alpha_k) \) is a theoretical correlation function (including beam smearing and pixelization). This function is most conveniently characterized by its expansion in Legendre polynomials, \( C^0(\alpha_k) = \sum_l C_l G^2_l P_l(\cos \alpha_k) \), where \( G_l \) is the window function of the DMR beam, for which we used the values given by Wright et al. (1993) with a slight correction for beam smearing and pixelization. The angular power spectrum on large angular scales for primeval adiabatic density fluctuations with \( \Omega = 1 \) is (Bond & Efstathiou 1987)

\[
C_l = \frac{(2l + 1) \Gamma[l + (n - 1)/2] \Gamma[(9 - n)/2]}{5 \Gamma[l + (5 - n)/2] \Gamma[(3 + n)/2]} Q_{\text{rms PS}}^2.
\]

This expression is accurate for the angular scales probed by COBE. To test it we replaced it with the more accurate angular correlation function obtained with a full integration of the coupled Boltzmann and Einstein equations for \( n = 1 \) by Bond & Efstathiou (1987) and found negligible change in our estimates.

Averaging over measurement errors and an ensemble of true sky maps we can now calculate the mean and covariance matrix of \( C(\alpha_k) \) neglecting the fitting and removal of low-order multipoles. For the cross-correlation case we get \( \langle C(\alpha_k) \rangle = C^0(\alpha_k) \); for autocorrelations there is an additional term at \( \alpha_k = 0 \) due to noise. The covariance matrix for the cross-correlation case is the sum of three terms, \( M = NN + SN + SS \), which we denote as noise-noise (NN), signal-noise (SN) and signal-signal (SS) terms. The NN term depends
only on the measurement errors, the SN term scales as $Q^{2}_{\text{rms--PS}}$ and the measurement variance, and SS scales as $Q^{4}_{\text{rms--PS}}$. The contributions to the matrix elements $M_{k_1 k_2}$ are given by the following expressions:

\[ NN = \frac{\sigma_A^2 \sigma_B^2}{N_{\text{tot}}} \sum_{i_1} N_{i_1} \sum_{j_1} N_{j_1} \delta(\vec{n}_{i_1} \cdot \vec{n}_{j_1} - \cos \alpha_{k_1}) , \]

\[ SN = \frac{1}{N_{\text{tot}}} \sum_{i_1} N_{i_1} \sum_{j_1} N_{j_1} \delta(\vec{n}_{i_1} \cdot \vec{n}_{j_1} - \cos \alpha_{k_1}) \]
\[ \times \left\{ \sigma_A^2 \sum_{j_2} N_{j_2} \delta(\vec{n}_{i_1} \cdot \vec{n}_{j_2} - \cos \alpha_{k_2}) C^0(\cos^{-1}[\vec{n}_{j_1} \cdot \vec{n}_{j_2}]) \right\} , \]

\[ SS = \frac{1}{N_{\text{tot}}} \sum_{i_1} N_{i_1} \sum_{j_1} N_{j_1} \sum_{i_2} N_{i_2} \sum_{j_2} N_{j_2} \delta(\vec{n}_{i_1} \cdot \vec{n}_{j_1} - \cos \alpha_{k_1}) \delta(\vec{n}_{i_2} \cdot \vec{n}_{j_2} - \cos \alpha_{k_2}) \]
\[ \times \left\{ C^0(\cos^{-1}[\vec{n}_{i_1} \cdot \vec{n}_{i_2}]) C^0(\cos^{-1}[\vec{n}_{j_1} \cdot \vec{n}_{j_2}]) + C^0(\cos^{-1}[\vec{n}_{i_1} \cdot \vec{n}_{j_2}]) C^0(\cos^{-1}[\vec{n}_{j_1} \cdot \vec{n}_{i_2}]) \right\} , \]

where

\[ N_{\text{tot}} = \sum_{i_1} N_{i_1} \sum_{j_1} N_{j_1} \sum_{i_2} N_{i_2} \sum_{j_2} N_{j_2} \delta(\vec{n}_{i_1} \cdot \vec{n}_{j_1} - \cos \alpha_{k_1}) \delta(\vec{n}_{i_2} \cdot \vec{n}_{j_2} - \cos \alpha_{k_2}) \]

and the indices range over all map pixels. Pixels labeled with $i$ correspond to map $A$, for which the measurement variance of $\Delta T_i$ is $\sigma_A^2/N_i$, while $j$ corresponds to map $B$. For cross-correlations $\sigma_A \neq \sigma_B$ in general. For autocorrelations one sets $\sigma_A = \sigma_B$ and the NN and SN terms are increased by a factor of 2.

We see that the NN term involves double summation over sky maps, the SN term involves triple summation, and the SS term quadruple summation. Even after the galactic latitude cuts made by Smoot et al. (1992, $|b| > 20^\circ$) and Wright et al. (1992, $|b| > 30^\circ$), one is still left with several thousand pixels. While the NN and SN terms can be summed exactly, the direct calculation of SS becomes computationally too expensive. Instead, we evaluated it using Monte Carlo simulations. We generated 10,000 maps for a gaussian random field $\Delta T(\vec{n})$ on the sphere having each theoretical angular power spectrum (i.e., value of $n$) to be tested. For each realization the angular correlation function was measured using equation (2) and the ensemble average was made over the 10,000 samples. Note that by adding the noise to the Monte Carlo samples one could similarly calculate the total covariance matrix (as we did for testing). The advantage of dividing the whole covariance
matrix into three terms is that once we calculate the expression for one value of $Q_{\text{rms-PS}}^2$ we can simply scale it to obtain the results for all different values of $Q_{\text{rms-PS}}^2$ for a given $n$. The $n$-dependence of $C^0(\alpha)$ is sufficiently smooth so that we interpolated the matrix elements of SN and SS evaluated on a grid of values of $n$. To test the whole procedure including the values of $N_i$, we have compared the NN term with the measurement errors for $C(\alpha_i)$ obtained by Smoot et al. (1992, Fig. 3) and Wright et al. (1992, Fig. 2). For both data sets our results agree with the correct values within a few percent.

Given the full covariance matrix it is now straightforward to obtain maximum-likelihood estimates $\hat{Q}_{\text{rms-PS}}$ and $\hat{n}$ for a given set of data $C(\alpha_k)$. The covariance matrix of errors in the parameters may be estimated in the usual way by taking $\Delta \ln L = 0.5$ for one standard deviation. However, we should not trust these asymptotic results because of the small numbers of independent data points given the COBE beam and the intrinsic correlations as well as our assumption of a normal likelihood function.

There is another reason why our estimator may give biased results. Our procedure so far does not correctly simulate the data reduction procedure used by Smoot et al. (1992) and Wright et al. (1992) because we have not accounted for the fitting and removal of low-order multipole moments from the maps before the angular correlation function is computed. If the sky sampling were uniform and complete, this could be accounted for simply by limiting the range of $l$ used to compute $C^0(\alpha_k)$. However, incomplete sky coverage couples different multipoles so that the actual $\langle C(\alpha_k) \rangle$ and covariance matrix differ from what we give above, resulting in a bias in our maximum-likelihood estimator.

To correct for this and other biases and to determine the variance of our estimator we resort again to Monte Carlo simulations. We generate 5000 random sky maps including signal and noise using the estimated values of $Q_{\text{rms-PS}}$ and $n$ for the COBE data as the input parameters. We fit and remove monopole, dipole, and (optionally) quadrupole using the correct galactic latitude cut and then compute the angular correlation function. These samples are used as the input data in the maximum-likelihood estimation described above. The distribution of Monte Carlo estimates around the true value yields the variance and bias of the estimate. We use this bias estimate to correct our results given below.

3. Results

Using the Smoot et al. (1992, Fig. 3) data we obtain maximum-likelihood estimates, before bias correction, of $\hat{n} = 1.2$ and $\hat{Q}_{\text{rms-PS}} = 12.2 \, \mu K$. Using the Wright et al. (1992,
Fig. 2) data the corresponding values are $\hat{n} = 0.9$ and $\hat{Q}_{\text{rms-PS}} = 13.9 \, \mu K$. As indicated above, our estimator is expected to be biased. To compensate for this bias we analyze Monte Carlo simulations of the data that are made with different choices for the true $(n, Q_{\text{rms-PS}})$ and we try to determine those parameters for which the mean estimated values equal the ones we obtain from the real data. We find that the bias in $n$ is less than 0.1, but the bias in $Q_{\text{rms-PS}}$ is significant. In the Smoot et al. case our bias for true values $n = 1$ and $Q_{\text{rms-PS}} = 15.0 \, \mu K$ is $\Delta \hat{Q}_{\text{rms-PS}} = -2.6 \, \mu K$ (the mean estimate is $\langle \hat{Q}_{\text{rms-PS}} \rangle = 12.4 \, \mu K$) while in the Wright et al. case it is $\Delta \hat{Q}_{\text{rms-PS}} = -2.2$. The bias is larger for the Smoot et al. analysis because of the additional quadrupole subtraction applied to the data. The bias is only weakly dependent on $n$ and $Q_{\text{rms-PS}}$. Thus, the bias-corrected estimates are $(n, Q_{\text{rms-PS}}) = (1.2, 14.8 \, \mu K)$ for Smoot et al. and $(0.9, 16.1 \, \mu K)$ for Wright et al.

In general one is interested in the amplitude of fluctuations for a fixed value of $n$. Assuming the scale-invariant slope $n = 1$ and combining the two data sets we obtain $Q_{\text{rms-PS}} = 15.7 \pm 2.6 \, \mu K$, where the uncertainty is taken from our fit to the Wright et al. sample. There is a strong anticorrelation between our estimates of $n$ and $Q_{\text{rms-PS}}$ and they cannot be independently determined with high precision. We find that the approximate relation between the two parameters is of the form

$$\hat{Q}_{\text{rms-PS}} = (15.7 \pm 2.6) \exp[0.46(1 - n)] \, \mu K \, .$$

(7)

Our mean value is slightly higher than that obtained by Adams et al. (1993) using the $\sigma_{\text{sky}}(10^\circ)$ normalization, $Q_{\text{rms-PS}} = 15(1 \pm 0.2) \exp[0.31(1 - n)] \, \mu K$. It is also higher than that obtained by Scaramella & Vittorio (1993). The main reason for these differences is that the fitting and removal of the dipole and quadrupole applied to the real data also subtracted some of the higher-order multipole moments because of nonuniform sky coverage.

Our results for $n = 1.0$ agree within the errors with the results reported by Smoot et al. ($\hat{Q}_{\text{rms-PS}} = 16.7 \pm 4.7 \, \mu K$), with a slightly lower amplitude and a smaller error bar. The change in the amplitude, when combined with the smaller error bar, may not be enough to significantly improve the consistency of the COBE results with the low upper limit on smaller angular scales obtained recently by Gaier et al. (1992).

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