A Fast Method For Bounding The CMB Power Spectrum Likelihood Function

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Abstract

As the Cosmic Microwave Background (CMB) radiation is observed to higher and higher angular resolution the size of the resulting datasets becomes a serious constraint on their analysis. In particular current algorithms to determine the location of, and curvature at, the peak of the power spectrum likelihood function from a general $N_p$-pixel CMB sky map scale as $O(N_p^3)$. Moreover the current best algorithm — the quadratic estimator — is a Newton-Raphson iterative scheme and so requires a ‘sufficiently good’ starting point to guarantee convergence to the true maximum. Here we present an algorithm to calculate bounds on the likelihood function at any point in parameter space using Gaussian quadrature and show that, judiciously applied, it scales as only $O(N_p^{7/3})$. Although it provides no direct curvature information we show how this approach is well-suited both to estimating cosmological parameters directly and to providing a coarse map of the power spectrum likelihood function from which to select the starting point for more refined techniques.

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# 1 Introduction

Planned observations of the Cosmic Microwave Background (CMB) will have sufficient angular resolution to probe the CMB power spectrum up to multipoles $l \sim 1000$ or more (for a general review of forthcoming observations see [1]). If we are able to extract the multipole amplitudes $C_l$ from the data sufficiently accurately we will be able to obtain the values of the fundamental cosmological parameters to unprecedented accuracy. The CMB will then have lived up to its promise of being the most powerful discriminant between cosmological models [2, 3, 4].

Extracting the power spectrum is conceptually simple — the raw data is cleaned and converted into a time-ordered dataset. This is then converted to a sky temperature map, which in turn is analysed to find the location of, and curvature at, the maximum of the likelihood function of the power spectrum. In practice as the size of the dataset increases the problem rapidly becomes intractable by conventional methods. This is particularly true of the final step — the likelihood analysis of any reasonably general sky temperature map.

An observation of the CMB contains both signal and noise
\[ \Delta_i = s_i + n_i \]  

at each of $N_p$ pixels. For independent, zero-mean, signal and noise the covariance matrix of the data
\[ M \equiv \langle \Delta \Delta^T \rangle = \langle ss^T \rangle + \langle nn^T \rangle \equiv S + N \]  
is symmetric, positive definite and dense. For any theoretical power spectrum $C_l$ we can construct the corresponding signal covariance matrix $S(C_l)$; knowing the noise covariance matrix $N$ for the experiment we now know the observation covariance matrix for that power spectrum $M(C_l)$. The probability of the observation given the assumed power spectrum is then
\[ P(\Delta | C_l) = \frac{e^{-\frac{1}{2} \Delta^T M^{-1} \Delta}}{(2\pi)^{N_p/2} |M|^{1/2}} \]  

Assuming a uniform prior, so that\[ P(C_l | \Delta) \propto P(\Delta | C_l) \]  
we can restrict our attention to evaluating the right hand side of equation (3). Unfortunately unless the noise covariance matrix is unrealistically simple (eg. diagonal) both direct evaluation [5, 6] and quadratic estimation [7, 8] of the likelihood function scale as at best $O(N_p^3)$ [9], making them impractical for the forthcoming $10^4 - 10^6$ pixel datasets.

# 2 Bounding The Likelihood Function

Instead of the expensive exact evaluation of the likelihood function, here we implement a much cheaper bounding algorithm due to Golub et al [10, 11]. This method determines bounds
\[ L \leq u^T f(A) u \leq U \]  
for an $n$-vector $u$, symmetric positive definite $n \times n$ matrix $A$ and smooth function $f$ defined on the spectrum of $A$. The underlying idea is to rewrite the problem as a Riemann-Stieltjes integral
which is then approximated using Gaussian quadrature. Since $A$ is symmetric it can be written in eigendecomposition as

$$A = Q^T \Lambda Q$$

(6)

where $Q$ is the orthogonal matrix of normalised eigenvectors and $\Lambda$ is the diagonal matrix of increasing eigenvalues $\Lambda_{ii} = \lambda_i$. Writing $\tilde{u} \equiv Q u$ we have

$$u^T f(A) u = \tilde{u}^T f(\Lambda) \tilde{u}$$

$$= \sum_{i=1}^{n} f(\lambda_i) \tilde{u}_i^2$$

$$= \int_{\lambda_1}^{\lambda_n} f(\lambda) \, d\mu(\lambda) \equiv I(f)$$

(7)

where the measure $\mu(\lambda)$ is a piecewise constant function defined by

$$\mu(\lambda) = \begin{cases} 0 & \lambda < \lambda_1 \\ \sum_{j=1}^{j} \tilde{u}_j^2 & \lambda_j \leq \lambda < \lambda_{j+1} \\ \sum_{i=1}^{n} \tilde{u}_i^2 & \lambda_n \leq \lambda \end{cases}$$

(8)

The integral $I(f)$ can now be bounded above and below using Gauss-Radau quadrature [12]

$$I(f) = \sum_{i=1}^{m} \omega_i f(\theta_i) + \nu_1 f(\lambda_1) + R_1$$

$$I(f) = \sum_{i=1}^{m} \omega_i f(\theta_i) + \nu_n f(\lambda_n) + R_n$$

(9)

with weights $\omega_i$ and $\nu_{1,n}$, nodes $\theta_i$ and $\lambda_{1,n}$, with opposite-signed remainders $R_{1,n}$. Given the resulting bounds on $I(f)$ we can increase the number of nodes $m$ until some convergence criterion, such as a maximum relative error,

$$\frac{U - L}{U + L} < \epsilon$$

(10)

is met. Calculating such bounds scales as $O(mn^2)$ due to the $O(n^2)$ matrix-vector multiplication in using the Lanczos algorithm [12] to calculate each of the $m$ nodes and their weights.

Rewriting the likelihood function of equation (3) as

$$P(\Delta | C_t) \propto \exp \left( -\frac{1}{2} \left( \Delta^T M^{-1} \Delta + \text{Tr} [\ln M] \right) \right)$$

(11)

leaves $\Delta^T M^{-1} \Delta$ and $\text{Tr} [\ln M]$ to be evaluated. The former is already in the required form and can be bounded immediately. For the latter we note that

$$\langle v^T f(A) v \rangle = \text{Tr} [f(A)]$$

(12)

where $v$ is a random vector whose elements are $\pm 1$ with equal probability. Generating $r$ realisations of $v$ we can calculate the bounds

$$L_i \leq v_i^T \ln M \, v_i \leq U_i \quad 1 \leq i \leq r$$

(13)
for each, from which we want to derive bounds on the expectation value
\[ \mu \equiv \langle v^T \ln M v \rangle = \text{Tr}[\ln M] \] (14)

For each realisation the estimator
\[ X_i = \frac{1}{2} (\mathcal{U}_i + \mathcal{L}_i) = \mu + \delta_i + \epsilon_i \] (15)

the sum of the expectation value \( \mu \), a random sample error \( \delta_i \), and a systematic bound-width error \( \epsilon_i \), where
\[ |\epsilon_i| \leq \frac{1}{2} (\mathcal{U}_i - \mathcal{L}_i) \equiv a_i \] (16)

(note that this is an absolute, not relative, error measure). Given the variance of the systematic-free data
\[ S^2 = \frac{1}{r-1} \sum_{i=1}^{r} \left( \mu + \delta_i - \bar{\mu} \right)^2 \]

and assuming that \( r \) is large enough for the central limit theorem to apply, our estimator \( \bar{X} \) has student’s t-distribution with \((r - 1)\) degrees of freedom, and we can take bounds
\[ \bar{X} - \frac{1}{\sqrt{r}} \tau_{r-1, \alpha} S - \bar{a} \leq \mu \leq \bar{X} + \frac{1}{\sqrt{r}} \tau_{r-1, \alpha} S + \bar{a} \] (18)

with \( \alpha \) confidence. Although the systematics prevent us from determining \( S \) itself we can calculate a stochastically larger quantity as follows: taking the sample variance of the midpoints
\[ S^2(X) = \frac{1}{r-1} \sum_{i=1}^{r} (\mu + \delta_i + \epsilon_i - \bar{\mu} - \bar{\delta} - \bar{\epsilon})^2 \]
\[ = S^2 + \frac{1}{r-1} \sum_{i=1}^{r} \left( 2(\delta_i - \bar{\delta})(\epsilon_i - \bar{\epsilon}) + (\epsilon_i - \bar{\epsilon})^2 \right) \]
\[ \geq S^2 - 2S \sqrt{\frac{1}{r-1} \sum_{i=1}^{r} a_i^2} \] (19)

where we have used the fact that
\[ \sum_{i=1}^{r} (\epsilon_i - \bar{\epsilon})^2 \leq \sum_{i=1}^{r} (\epsilon_i)^2 \leq \sum_{i=1}^{r} a_i^2 \] (20)

Thus, defining
\[ A = \sqrt{\frac{1}{r-1} \sum_{i=1}^{r} a_i^2} \] (21)

we have
\[ S^2 - 2A S - S^2(X) \leq 0 \] (22)

and hence the bound
\[ S \leq A + \sqrt{A^2 + S^2(X)} \] (23)

If the number of terms \( m \) required to evaluate each of the \( r \) bound pairs is approximately constant, we have a method to bound the likelihood function which scales as \( O(rmn^2) \) overall.
3 Results

The viability of this approach depends crucially on the way that the number of nodes in the Gauss-Radau quadrature ($m$) and the number of trace estimates ($r$) depend on the size of the dataset ($n$) and the required tightness of the bounds ($\epsilon$). To examine these dependencies we have applied the algorithm to subsets of the COBE data and a standard CDM target power spectrum.

The number of nodes required to achieve a given accuracy clearly depends on that accuracy. At the extrema

$$
\begin{align*}
\epsilon = 1 & \rightarrow m = 1 \\
\epsilon = 0 & \rightarrow m = n
\end{align*}
$$

Figure 1 shows the dependence of the number of nodes on size of the dataset for typical useful values $\epsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, \text{and} 10^{-5}$. The points are from numerical experiments, evaluating bounds on $\mathbf{v}^T \ln M \mathbf{v}$ and averaging over 100 realisations of $\mathbf{v}$. The solid lines are power law fits $m \propto n^\beta$ (giving overall scaling as $O(n^{2+\beta})$) with

$$
\beta = \begin{cases}
1/3 & \text{for } 10^{-1} \geq \epsilon \geq 10^{-2} \\
1/2 & \text{for } 10^{-3} \geq \epsilon \geq 10^{-5}
\end{cases}
$$

Figure 2 shows the normalised 99% confidence bounds achieved on $\text{Tr} \ln M$ for a 1000 pixel dataset as the number of estimates $r$ increases, with coverage set at $\epsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$ and $10^{-5}$. Not surprisingly, the 10% bounds on each estimate give a rather poor overall constraint. However with the 1% and tighter bounds we can determine the logarithm of the likelihood function to $2 - 3\%$ with 99% confidence in as few as 20 realisations. Note that below the 1% level the bounds are dominated by sample error, and become essentially independent of the bound width. Figure 3 shows the 99% confidence bounds achieved after 20 realisations at $\epsilon = 10^{-2}$, showing no systematic variation as the size of the dataset increases.

4 Conclusions

We have presented an algorithm to calculate probabilistic bounds on the power spectrum likelihood function from an $N_p$-pixel CMB map using Gaussian quadrature which scales as between $O(N_p^{7/3})$ and $O(N_p^{5/2})$ — a very significant advance on existing algorithms for the exact calculation which scale as $O(N_p^3)$. Since lowering the convergence constraint below the 1% level gains us only marginally tighter final bounds at the expense of increasing the scaling power, it is not recommended for the forthcoming $10^4 - 10^6$ pixel CMB maps. Our final algorithm of choice therefore gives better than 3% bounds on the logarithm of the likelihood function with $O(N_p^{7/3})$ operations with 99% confidence.

Since this algorithm gives no information about the local curvature of the likelihood function it is not as well suited as quadratic estimator techniques for searching a large multi-dimensional parameter space for its likelihood maximum. However for direct estimation of a small set of cosmological parameters this technique is certainly viable and fast. Moreover, even when the parameters are taken to be the multipole moments (individually or in bins), quadratic estimation, being a Newton-Raphson iteration, requires a starting point ‘sufficiently close’ to the maximum to guarantee convergence; the algorithm presented here is then well suited to provide a coarse overall mapping of the likelihood function from which to select a starting point for more refined techniques.
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Figure Captions

**Figure 1**
A log-log plot of the scaling in the number of quadrature nodes \( m \) required to achieve bounds with a given relative error convergence criterion \( \epsilon \) with the size of the CMB dataset \( n \). The points are obtained from numerical experiments; the lines are power law fits \( m \propto n^\beta \). From the bottom of the figure reading upwards the relative errors are \( \epsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4} \) and \( 10^{-5} \), with corresponding power laws \( \beta = 1/3, 1/3, 1/2, 1/2 \) and \( 1/2 \).

**Figure 2**
A plot of the normalised 99% confidence upper and lower bounds achieved on \( \text{Tr}[\ln M] \) for a 1000 pixel dataset against the estimator sample size \( r \). From the outer limits reading inwards the line-pairs correspond to the relative error convergence criterion being set at \( \epsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4} \) and \( 10^{-5} \).

**Figure 3**
A plot of the variation in the normalised 99% confidence upper and lower bounds achieved on \( \text{Tr}[\ln M] \) with the relative error convergence criterion set at \( \epsilon = 10^{-2} \) after \( r = 20 \) estimates as the size of the CMB dataset \( n \) increases.
Figure 2

Normalised 99% Confidence Upper and Lower Bounds
Figure 3

Normalised 99% Confidence Interval

Size of Dataset