Power Spectrum Estimators For Large CMB Datasets

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Abstract

Forthcoming high-resolution observations of the Cosmic Microwave Background (CMB) radiation will generate datasets many orders of magnitude larger than have been obtained to date. The size and complexity of such datasets presents a very serious challenge to analysing them with existing or anticipated computers. Here we present an investigation of the currently favored algorithm for obtaining the power spectrum from a sky-temperature map — the quadratic estimator. We show that, whilst improving on direct evaluation of the likelihood function, current implementations still inherently scale as the equivalent of $O(N_p^3)$ in the number of pixels or worse, and demonstrate the critical importance of choosing the right implementation for a particular dataset.

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1 Introduction

Over the next ten years a number of ground-based, balloon-borne and satellite observations of the Cosmic Microwave Background (CMB) are planned with sufficient resolution to determine the CMB power spectrum up to multipoles $l \sim 1000$ or more (for a general review of forthcoming observations see [1]). According to current theory this will provide us with the locations, amplitudes, and shapes of the Doppler peaks, and hence 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].

In preparation for these datasets considerable effort is being put into developing ways of extracting the information they contain. Typically the raw data is cleaned and converted into a time-ordered dataset. This is then turned into a sky temperature map, and the map analysed to find its power spectrum. Having obtained the power spectrum of the dataset we can compare it with the predictions of any class of cosmological models to determine the most likely values of the parameters associated with that class. Whilst it would also be possible to estimate such cosmological parameters directly from the data, this would require the assumption of a class of models during the data analysis. We therefore choose to provide the more generic result of the power spectrum.

Here we consider the analysis of an $N_p$ pixel map from a simple pointing experiment for multipoles $1 \leq l \leq N_l$ in bins $1 \leq b \leq N_b$ — ie. we determine the location of and the curvature about the peak of the maximum likelihood function of the binned power spectrum coefficients $C^b_l$.

2 Maximum Likelihood Analysis

Any observation of the CMB contains both signal and noise

$$\Delta_i = s_i + n_i \quad (1)$$

at each pixel. For independent, zero-mean, signal and noise the covariance matrix of the data

$$M \equiv \left< \Delta \Delta^T \right> = \left< s s^T \right> + \left< n n^T \right> \quad (2)$$

is a symmetric, positive definite and dense. Given any binned power spectrum $C^b_l$ and a shape parameter $C^s_l$ within each bin such that

$$C_l = C^s_l C^b_l \quad l \in b \quad (3)$$

we can construct the signal covariance matrix; for a simple pointing experiment this is

$$S_{ii'} \equiv \left< s_i s_{i'} \right> = \sum_{l=0}^{N_l} \frac{2l+1}{4\pi} C_l B^2_l P_l(\cos \theta_{ii'})$$

$$= \sum_{b=0}^{N_b} C^b_b \sum_{l \in b} \frac{2l+1}{4\pi} C^s_l B^2_l P_l(\cos \theta_{ii'}) \quad (4)$$
where $B_i$ is the multipole beam map and $\theta_{ii'}$ is the angular separation of pixels $i, i'$. Taking the CMB fluctuations to be Gaussian is not only consistent with the favoured inflationary cosmologies but also has the maximum entropy if we make no assumption about the higher moments of the data predicted to be non-zero in defect-based models. The probability of the observed dataset given the assumed power spectrum is then

$$\mathcal{L}(C) \equiv P(\Delta \mid C) = e^{-\frac{1}{2} \Delta^T M^{-1} \Delta} \left(\frac{2\pi}{N_p/2}\right)^{1/2}$$  \hspace{1cm} (5)

Assuming a uniform prior, so that $P(C \mid \Delta) \propto P(\Delta \mid C)$, the most likely power spectrum will be that which maximizes $\mathcal{L}(C)$, with covariance matrix

$$[Q^{-1}]_{bb'} = -\frac{\partial^2 \mathcal{L}}{\partial C_b \partial C_{b'}} \bigg|_{C=C_{\text{max}}}$$  \hspace{1cm} (6)

### 3 Direct Evaluation

Historically the most likely power spectrum has usually been obtained by evaluating $\mathcal{L}(C)$ directly over the bin parameter space to locate its maximum (for example for the COBE data [5, 6], with the additional refinement of using a complete set of cut-sky basis functions in place of the incomplete spherical harmonics). To date the fastest general solution uses a Cholesky decomposition of the matrix $M$, costing $O(N_b^2)$ in size and $O(N_b^3)$ in time for a single point in parameter space.

Algorithms for searching the $N_b$-dimensional parameter space — such as maximum gradient ascent — typically require $O(N_b)$ evaluations at each of many steps. Moreover, calculating the covariance matrix at the maximum by discrete differencing requires a further $O(N_b^2)$ evaluations. Overall therefore current implementations of this algorithm scale as $O(N_b^2)$ in size and $O(N_b^2 N_p^2)$ in time, and become hopelessly intractable for any of the anticipated datasets.

Although there have been some attempts to improve on this scaling — for example by transforming to the signal-to-noise eigenbasis [7], using approximations for the determinant [8], or assuming azimuthally symmetric noise [9] — none has provided a fast way to search a high dimensional multipole bin parameter space under an arbitrarily complex dataset.

### 4 Quadratic Estimators

Since we are interested both in a rapid search for the maximum of $\mathcal{L}$, and in evaluating the curvature matrix of $\mathcal{L}$ at this maximum, we solve

$$\frac{\partial \ln \mathcal{L}}{\partial C} = 0$$  \hspace{1cm} (7)

iteratively by the Newton-Raphson method. Starting from some (sufficiently good) target power spectrum $C$ the correction

$$\delta C = -\left[\frac{\partial^2 \ln \mathcal{L}}{\partial C_2}\right]^{-1} \frac{\partial \ln \mathcal{L}}{\partial C}$$  \hspace{1cm} (8)
gives rapid convergence to the maximum of $\mathcal{L}$.

Taking the log and repeatedly differentiating equation (5)

$$\ln \mathcal{L} = -\frac{1}{2} \left( \Delta^T M^{-1} \Delta + \text{Tr} [\ln M] + N_p \ln 2\pi \right)$$

$$\frac{\partial \ln \mathcal{L}}{\partial C_b} = \frac{1}{2} \left( \Delta^T M^{-1} \frac{\partial S}{\partial C_b} M^{-1} \Delta - \text{Tr} \left[ M^{-1} \frac{\partial S}{\partial C_b} M^{-1} \frac{\partial S}{\partial C'_b} \right] \right)$$

$$\frac{\partial^2 \ln \mathcal{L}}{\partial C_b \partial C'_b} = \frac{1}{2} \left( \Delta^T \left[ M^{-1} \frac{\partial^2 S}{\partial C_b \partial C'_b} M^{-1} - 2 M^{-1} \frac{\partial S}{\partial C_b} M^{-1} \frac{\partial S}{\partial C'_b} M^{-1} \right] \Delta 
- \text{Tr} \left[ M^{-1} \frac{\partial^2 S}{\partial C_b \partial C'_b} M^{-1} - M^{-1} \frac{\partial S}{\partial C_b} M^{-1} \frac{\partial S}{\partial C'_b} M^{-1} \frac{\partial S}{\partial C'_b} \right] \right)$$  \hspace{1cm} (9)

Now if instead of the computationally intensive full curvature matrix we settle for its much simpler ensemble average (ie. the Fisher information matrix) we have

$$F_{bb'} = -\langle \frac{\partial^2 \ln \mathcal{L}}{\partial C_b \partial C'_b} \rangle = \frac{1}{2} \text{Tr} \left[ M^{-1} \frac{\partial S}{\partial C_b} M^{-1} \frac{\partial S}{\partial C'_b} M^{-1} \frac{\partial S}{\partial C'_b} \right]$$  \hspace{1cm} (10)

and equation (8) reduces to

$$\delta C = F^{-1} \frac{\partial \ln \mathcal{L}}{\partial C}$$  \hspace{1cm} (11)

Note that this procedure both locates the maximum and generates the (albeit approximated) covariance matrix $F^{-1}$.

The most computationally expensive calculation here is still the evaluation of the Fisher matrix, for which two methods have been proposed. Noting that, from equation (4), the derivative matrix for each bin

$$\frac{\partial S}{\partial C_b} = \sum_{l \in b} \frac{2l + 1}{4\pi} C_l^b B_l^2 P_l$$  \hspace{1cm} (12)

is independent of iterative step, Bond, Jaffe and Knox \cite{7} calculate them explicitly and solve

$$MX_b = \frac{\partial S}{\partial C_b}$$  \hspace{1cm} (13)

column by column for each bin. The first two rows of table 1 shows the cost of evaluating the Fisher matrix this way.

Alternatively, Tegmark \cite{10} has pointed out that each $(N_p \times N_p)$ Legendre polynomial matrix can be factorised into the product of the corresponding $(N_p \times (2l + 1))$ spherical harmonic matrix and its transpose

$$\frac{2l + 1}{4\pi} P_l = Y_l Y_l^T$$  \hspace{1cm} (14)

where

$$[Y_l]_{im} = Y_{lm}(\theta_i, \psi_i)$$  \hspace{1cm} (15)
for the real spherical harmonic $Y_{lm}$ in the direction of pixel $i$. Now

$$\frac{\partial S}{\partial C_b} = \sum_{l \in b} C_l^b B_l^2 Y_l Y_l^T$$

(16)

and we can use the invariance of the trace of a product of matrices under cyclic permutations to rewrite equation (10) as

$$F_{bb'} = \frac{1}{2} \sum_{l \in b} \sum_{l' \in b'} C_l^b C_{l'}^{b'} B_l^2 B_{l'}^2 \text{Tr} \left[ \left( Y_{l'}^T M^{-1} Y_l \right) \left( Y_{l'}^T M^{-1} Y_l \right)^T \right]$$

(17)

and solve

$$MX_l = Y_l$$

(18)

column by column for each multipole, and

$$Z_{ll'} = Y_l^T X_{l'}$$

(19)

for each pair of multipoles, and hence each pair of bins. The last three rows of table 1 shows the cost of evaluating the Fisher matrix this way.

For CMB observations we have $N_b \ll N_p$, so that the first algorithm (A1) scales as $O(N_b N_p^2)$ in size and $O(N_b N_p^3)$ in time. Similarly $N_l^2 \geq N_p$, with approximate equality for all-sky maps, so that the second algorithm (A2) scales as $O(N_l^4)$ in size and $O(N_l^4 N_p)$ in time. Table 2 shows the implications for a range of future experiments, scaled from implementations of each algorithm applied to an unbinned reduced COBE dataset. Note that no assumption has been made about binning in the MAP and PLANCK datasets.

5 Conclusions

We have implemented two algorithms using the quadratic estimator as a means of determining the maximum likelihood power spectrum and its covariance matrix from a pixelized map of the CMB. Despite previous claims, whilst each is an improvement on direct evaluation of the likelihood function, neither scales better in time than $O(N_p^3)$ in the number of pixels in the map. Ultimately the advantage of each is in a reduction of the scaling prefactor as compared with direct evaluation.

Comparing the two algorithms it is apparent that the choice of which to use for a particular dataset is critical — with timings differing by up to a factor of 1000. Broadly speaking, observations of small patches of the sky, where $N_l \gg \sqrt{N_p}$, should be analysed using A1, whilst all-sky maps, with $N_l \sim \sqrt{N_p}$, should be analysed using A2.

All timings have been scaled from a small dataset analysed on a SUN Ultra II. Two further considerations immediately apply.

- Moving to parallel architectures will give significant reduction in these timings. Implementation of each algorithm on the 512 processor Cray T3E at NERSC indicates that the improvement can be up to a factor of 1000. However, this does assume that we continue to keep all the necessary matrices simultaneously in core; any reduction to vector operations, relocation to disc, or recalculation will dramatically reduce this improvement.
The datasets under consideration will be obtained incrementally over the next 10 years. We should therefore take into consideration Moore’s law — that computer power doubles every 18 months — to allow for corresponding increases in available memory and speed. Current trends do not, however, suggest any significant increase in the total parallel processor time ($O(10^4)$ hours) available to us.

Taken together, we can conclude that these algorithms, judiciously applied, will be sufficient to analyse $10^4$ pixel datasets immediately, the $10^5$ pixel datasets expected in the next 2 years some 6 years from now, and the $10^6$ pixel datasets expected in 5 – 10 years only 16 years from now. However, since we would like to be able to analyse not only the actual datasets as soon as they are obtained, but also simulated datasets in advance of the observations, improved algorithms are still essential.

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References

[1] G. Smoot, astro-ph/9705135
[2] L. Knox, Phys. Rev. D52, 4307 (1995), astro-ph/9504054
[3] W. Hu, N. Sugiyama and J. Silk, Nature 386, 37, (1997), astro-ph/9604166
[4] A. Kosowsky, M. Kamionkowski, C. Jungman and D. Spergel Nucl. Phys. Proc. Suppl. 51B, 49, (1996), astro-ph/9605147
[5] K. M. Górski, Ap. J. 430, L85, (1994), astro-ph/9403066
[6] K. M. Górski, G. Hinshaw, A. J. Banday, C. L. Bennett, E. L. Wright, A. Kogut, G. F. Smoot and P. Lubin Ap. J. 430, L89, (1994), astro-ph/9403067
[7] J. R. Bond, A. H. Jaffe and L. Knox, (submitted to Phys. Rev. D) astro-ph/9708203
[8] A. Kogut, presented at the INPAC/ITP Conference on ‘CMB Data Analysis and Parameter Extraction’, Santa Barbara (November 1997).
[9] S. P. Oh, D. N. Spergel and G. Hinshaw, (in preparation) (1997).
[10] M. Tegmark, Phys. Rev. D55 5895 (1997), astro-ph/9611174.
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X_b = M^{-1} \frac{\partial S}{\partial \xi_b} \quad \forall \ b
\]
\[
\text{Tr} \ [X_b X_{b'}] \quad \forall \ b, b'
\]
\[
X_l = M^{-1} Y_l \quad \forall \ l
\]
\[
Z_{l l'} = Y_l^T X_{l'} \quad \forall \ l, l'
\]
\[
\text{Tr} \ [Z_{l l'} Z_{l l'}^T] \quad \forall \ l, l'
\]

Table 1: Scaling in the calculation of the Fisher matrix \( F \) for the two quadratic estimator algorithms A1 (first two rows), A2 (last three rows).
| DATASET              | $N_p$ | $N_b$ | $N_l$ | SIZE          | TIME          |
|---------------------|-------|-------|-------|---------------|---------------|
|                     |       |       |       | $A1$ $O(N_b N_p^2)$ | $A2$ $O(N_l^4)$ | $A1$ $O(N_b N_p^3)$ | $A2$ $O(N_l^4 N_p)$ |
| COBE                | $10^3$ | 30    | 30    | 240 Mb       | 8 Mb          | 15 min         | 1 min          |
| MAXIMA/BOOMERANG    | $10^4$ to $10^5$ | 20    | 1000  | 16 Gb        | 8 Tb          | 7 days         | 20 years       |
|                     | 20    | 1000  | 1.6 Tb | 8 Tb          | 20 years      | 200 years      |
| MAP/PLANCK          | $10^6$ | 1000  | 1000  | 8 Pb          | 8 Tb          | 1 Myears       | 2 Kyears       |

Table 2: Size and time costs for the calculation of the Fisher matrix $F$ for archetypal datasets on a SUN Ultra II for the two quadratic estimator algorithms $A1$, $A2$. 