MARGINAL DISTRIBUTIONS FOR COSMIC VARIANCE LIMITED COSMIC MICROWAVE BACKGROUND POLARIZATION DATA

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ABSTRACT

We provide computationally convenient expressions for all marginal distributions of the polarization cosmic microwave background (CMB) power spectrum distribution \(P(C_\ell |\sigma)\), where \(C_\ell = \{C_\ell^{TT}, C_\ell^{TE}, C_\ell^{EE}, C_\ell^{BB}\}\) denotes the set of ensemble-averaged polarization CMB power spectra, and \(\sigma = \{\sigma_{TT}, \sigma_{TE}, \sigma_{EE}, \sigma_{BB}\}\) the set of the realization-specific polarization CMB power spectra. This distribution describes the CMB posterior power spectrum for cosmic variance limited data. The expressions derived here are general, and may be useful in a wide range of applications. Two specific applications are described in this paper. First, we employ the derived distributions within the CMB Gibbs sampling framework and demonstrate a new conditional CMB power spectrum sampling algorithm that allows for different binning schemes for each power spectrum. This is useful because most CMB experiments have very different signal-to-noise ratios for temperature and polarization. Second, we provide new Blackwell–Rao estimators for each of the marginal polarization distributions, which are relevant to power spectrum and likelihood estimation. Because these estimators represent marginals, they are not affected by the exponential behavior of the corresponding joint expression, but converge quickly.

Key words: cosmic microwave background – cosmology: observations – methods: numerical

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1. INTRODUCTION

During the last few decades, cosmology has evolved from a data-starved branch of astrophysics into a data-driven high-precision science in which theories may be subjected to stringent observational tests. This revolution has, to a large extent, been driven by steadily improving observations of the cosmic microwave background (CMB), allowing cosmologists to have a close-up look at the very young universe. Two leading experiments were the COBE Differential Microwave Radiometer Experiment (DMR) (Smoot et al. 1992) and WMAP (Bennett et al. 2003) satellite missions, while the third generation experiment, Planck, will be launched later this year.

As observations continue to improve, increasingly demanding requirements are imposed on the data analysis. While rather crude approximations may be acceptable when interpreting low signal-to-noise (S/N) data, the situation is very different in the mid- and high-S/N regime. Here, even “small” effects become clearly visible and may potentially compromise any cosmological conclusion. Using accurate methods in this regime is critical. Some real-world issues relevant to the CMB problem are noncosmological foregrounds, improper noise and/or beam characterization, and suboptimal likelihood approximations.

In 2004, a new approach to CMB analysis was proposed and implemented by Jewell et al. (2004), Wandelt et al. (2004), and Eriksen et al. (2004). Rather than taking the traditional approximate Monte Carlo approach (e.g., Hivon et al. 2002), this new method employs the Gibbs sampling algorithm to facilitate exact (in the maximum likelihood sense), global, and efficient analysis of even high-resolution data sets. Equally important, the Gibbs sampling framework has unique capabilities for error propagation, as it allows for easy marginalization over virtually any auxiliary stochastic field. One important example is that of noncosmological foregrounds.

Since then, the method has been generalized to handle polarized CMB data (Larson et al. 2007), and joint foreground and CMB analysis (Eriksen et al. 2008b), and has been applied most successfully to the WMAP data (O’Dwyer et al. 2004; Eriksen et al. 2007a, 2007b, 2008a). Some useful examples of issues correctly identified by the Gibbs sampler, but missed by other techniques, are (1) the first-year WMAP likelihood bias at \(\ell \lesssim 30\) (Eriksen et al. 2007b; Hinshaw et al. 2007), (2) foreground residuals in the three-year WMAP polarization sky maps (Eriksen et al. 2007b), and (3) residual monopole and dipole components in the three-year temperature sky maps (Eriksen et al. 2008a; Hinshaw et al. 2008). Following up on these methodological advances, the WMAP team adopted the Gibbs sampler as a central component in their analysis of their five-year data, and, in fact, their default low-\(\ell\) temperature likelihood module is precisely the Gibbs-based Blackwell–Rao code written and published by Chu et al. (2005).

While WMAP has done an excellent job of characterizing the large-scale CMB temperature fluctuations, the current frontier in CMB science is polarization. In just a few years, full-sky high-sensitivity data will be available from Planck. And then, very likely, the situation will be quite analogous to that experienced by WMAP in the temperature case—having robust, exact methods that allow for proper characterization and propagation of systematics will be essential in the mid- to high-S/N regime. The Gibbs sampler is among the leading candidates to serve such a purpose.

Unfortunately, the Gibbs sampler, as currently described in the literature, has two major limitations that need to be resolved before this promise can be fulfilled. First, the direct Gibbs sampler is inherently inefficient in the low S/N regime, because the step size between two consecutive samples is determined by cosmic variance alone, whereas the full posterior width is determined by noise. Second, it is nontrivial to establish a full
likelihood approximation from the samples produced by the Gibbs sampler, because of the dimensionality of the underlying space. Both of these issues are currently under development, and reports are expected in the near future (Jewell et al. 2008; Rudjord et al. 2008; H. K. Eriksen et al. 2008, in preparation).

In the present paper, we take a small but important first step toward resolving these issues, by considering the marginal and conditional densities of the probability distribution \( P(C_\ell | \sigma_\ell) \), where \( C_\ell \) is the ensemble-averaged CMB power spectrum and \( \sigma_\ell \) is the observed power spectrum of one given CMB realization. This distribution plays a crucial role within the CMB Gibbs sampling framework. On one hand, it forms one of the two conditionals in the main sampling scheme. On the other hand, it is the kernel of the Blackwell–Rao estimator. Being able to describe this analytically in different forms is therefore very useful. Two specific applications are demonstrated in this paper, describe this analytically in different forms is therefore very useful. Two specific applications are demonstrated in this paper, namely (1) a \( C_\ell \) sampling algorithm that allows for different binning schemes in each of the polarization components, and (2) Blackwell–Rao estimators for each of \( P(C_\ell^T | C_\ell^T, C_\ell^{TE}, d) \), \( P(C_\ell^{TE} | C_\ell^{TE}, d) \), and \( P(C_\ell^{EE} | d) \). Further applications will be demonstrated in the papers mentioned above.

We also note that these expressions are completely general and may prove useful for any other method that considers both \( C_\ell \) and the CMB sky signal as free variables. One such example is the CMB Hamiltonian sampler recently developed by Taylor et al. (2007).

2. NOTATION AND DATA MODEL

We now introduce a statistical model for the CMB observations and define our notation. First, we assume that the data may be modeled by a signal and a noise term,

\[
d(\hat{n}) = s(\hat{n}) + n(\hat{n}).
\]

Here, \( d \) is a three-component \((T, Q, U)\) Stokes’ parameter vector observed in the direction \( \hat{n} \). \( s \) and \( n \) denote similar vectors, describing the CMB field and instrumental noise, respectively. Both the signal and the noise are assumed to be Gaussian distributed with zero mean and covariances \( C \) and \( N \), respectively. (Note that for notational simplicity, we neglect real-world complications such as instrumental beams, frequency-dependent observations, or foreground components in this expression; the topic of this paper is the probability distribution \( P(C_\ell, s) \), and for this, all such issues are irrelevant.)

Next, we additionally assume the CMB field to be statistically isotropic. It is therefore useful to decompose the \((T, Q, U)\) field into spin-weighted spherical harmonics (see, e.g., Zaldarriaga and Seljak 1997 for full details), with coefficients \( \{a^T_{\ell m}, a^E_{\ell m}, a^B_{\ell m}\} \).

Because the spherical harmonics are orthogonal on the full sky, and \( B \) has opposite parity of \( T \) and \( E \), the harmonic space CMB covariance matrix is given by

\[
C_{\ell m, \ell' m'} = \begin{pmatrix}
a^T_{\ell m} a^T_{\ell' m'} & a^T_{\ell m} a^E_{\ell' m'} & a^T_{\ell m} a^B_{\ell' m'} \\
a^E_{\ell m} a^T_{\ell' m'} & a^E_{\ell m} a^E_{\ell' m'} & a^E_{\ell m} a^B_{\ell' m'} \\
a^B_{\ell m} a^T_{\ell' m'} & a^B_{\ell m} a^E_{\ell' m'} & a^B_{\ell m} a^B_{\ell' m'}
\end{pmatrix} \delta_{\ell \ell'} \delta_{mm'}
\]

(2)

\[
= \begin{pmatrix}
C^{TT}_\ell & C^{TE}_\ell & 0 \\
C^{TE}_\ell & C^{EE}_\ell & 0 \\
0 & 0 & C^{BB}_\ell
\end{pmatrix} \delta_{\ell \ell'} \delta_{mm'}.
\]

(3)

In this expression, brackets denote ensemble averages, and the power spectrum \( C_\ell \) therefore corresponds to a theory spectrum, similar to that produced by a Boltzmann code such as CMBFast (Seljak & Zaldarriaga 1996). Note that \( C_{\ell m, \ell' m'} \) is the ensemble-averaged CMB power spectrum of one realization.

Before turning to the main topic of this paper, we recall that, for a probability distribution \( P(x, y) \), the marginal distribution is defined by \( P(x) = \int P(x, y) dy \) and the conditional distribution by \( P(y|x) = P(x, y)/P(x) \). From these, one may also trivially derive Bayes’ theorem, \( P(x|y) = P(y|x)P(x)/P(y) \). Therefore, for uniform priors on both \( C_\ell \) and \( s \), which we assume in this paper, \( P(\sigma_\ell | C_\ell) \propto P(C_\ell | \sigma_\ell) \).

One can also define the realization-specific power spectrum, \( \sigma_\ell \), which is simply the averaged power in each multipole for one given realization,

\[
\sigma_\ell = \frac{1}{2\ell + 1} \sum_{m=-\ell}^{\ell} \left( \begin{array}{ccc}
a^T_{\ell m} a^T_{\ell m} & a^T_{\ell m} a^E_{\ell m} & a^T_{\ell m} a^B_{\ell m} \\
a^E_{\ell m} a^T_{\ell m} & a^E_{\ell m} a^E_{\ell m} & a^E_{\ell m} a^B_{\ell m} \\
a^B_{\ell m} a^T_{\ell m} & a^B_{\ell m} a^E_{\ell m} & a^B_{\ell m} a^B_{\ell m}
\end{array} \right) \delta_{\ell \ell'} \delta_{mm'}.
\]

(4)

Explicitly, \( C_\ell \) is the power spectrum corresponding to some cosmological model and \( \sigma_\ell \) is the power spectrum of one realization drawn from that model. It may therefore be useful to imagine that observations of the CMB sky provide us with \( \sigma_\ell \), and from this we seek to constrain the underlying cosmological theory, parameterized by \( C_\ell \) and summarized by the conditional distribution \( P(C_\ell | \sigma_\ell) \).

With this notation, it is straightforward to write the joint probability distribution for the CMB sky signal, \( s \), the CMB power spectrum, \( C_\ell \), and the data, \( d \),

\[
P(s, C_\ell, d) = P(d | s, C_\ell) P(s, C_\ell)
\]

(6)

\[
\propto e^{-\frac{1}{2} (d-s)^T \Sigma^{-1} (d-s)} P(s, C_\ell)
\]

(7)

and the CMB posterior distribution,

\[
P(s, C_\ell | d) = \frac{P(s, C_\ell, d)}{P(d)} \propto P(s, C_\ell, d).
\]

(8)

These expressions involve two factors, namely the \( \chi^2 = (d - s)^T \Sigma^{-1} (d - s) \) and the CMB probability distribution \( P(s, C_\ell) \). Since we assume that the CMB field is isotropic and Gaussian, as discussed above, the latter may be written as (e.g., Larson et al. 2007)

\[
P(s, C_\ell) = P(s | C_\ell) P(C_\ell)
\]

(9)

\[
\propto \frac{e^{-\frac{1}{2} s^T \Sigma^{-1} s}}{\sqrt{\left| C_\ell \right|}} P(C_\ell)
\]

(10)

\[
= \prod_{\ell m} \frac{e^{-\frac{1}{2} \sum_{aT} (aT_{\ell m})^2}}{\left| C^{TT}_{\ell m} \right|} P(C_{\ell m}^{TT})
\]

(11)

\[
= \prod_{\ell} \frac{e^{-\frac{1}{2} \sum_{aE} (aE_{\ell m})^2}}{\left| C^{EE}_{\ell m} \right|} P(C_{\ell m}^{EE})
\]

(12)

\[
= \prod_{\ell} \frac{e^{-\frac{1}{2} \sum_{aB} (aB_{\ell m})^2}}{\left| C^{BB}_{\ell m} \right|} P(C_{\ell m}^{BB})
\]

(13)

\[
= \prod_{\ell} P(\sigma_\ell | C_\ell) P(C_\ell),
\]

(14)

where \( P(C_\ell) \) is a prior on \( C_\ell \). \( P(\sigma_\ell | C_\ell) \) is recognized as an inverse Wishart distribution when interpreted as a function of \( C_\ell \).
that is, $C_{BB}$ is independent of $(C_{TT}, C_{TE}, C_{EE})$, and follows a one-dimensional inverse Wishart (or inverse Gamma) distribution. We will therefore not consider the BB-component further in this paper. However, we note that if one is interested in exotic models for which $\{TB, EB\} \neq 0$, the expressions derived in this paper will have to be accordingly revised.

3.1. The $(TE, EE)$ Distribution, $P(C_{TE}, C_{EE}|\sigma_t)$

We start by considering the two-dimensional marginal distribution $P(C_{TE}, C_{EE}|\sigma_t)$, which is obtained by integrating $P(C_{TT}, C_{TE}, C_{EE}|\sigma_t)$ over $C_{TT}$. That is, $C_{BB}$ is independent of $(C_{TT}, C_{TE}, C_{EE})$, and follows a one-dimensional inverse Wishart (or inverse Gamma) distribution. We will therefore not consider the BB-component further in this paper. However, we note that if one is interested in exotic models for which $\{TB, EB\} \neq 0$, the expressions derived in this paper will have to be accordingly revised.

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$$P(C_{TE}, C_{EE}|\sigma_t) = \int P(C_{TT}, C_{TE}, C_{EE}|\sigma_t) dC_{TT}$$

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Note that the lower limit in this integral is defined by \( |C_\ell| > 0 \), since the power spectrum covariance matrix in Equation (3) must be positive definite.

If we now define
\[
k \equiv \sigma^2_{\ell} \frac{C^{\text{TE}}_{\ell}}{C^{\text{EE}}_{\ell}} - 2\sigma_{\ell} C^{\text{TE}}_{\ell} + \sigma^2_{\ell} C^{\text{EE}}_{\ell},
\]
and make the change of variable
\[
y = \frac{(2\ell + 1)k}{2(C^{\text{TT}}_{\ell} C^{\text{EE}}_{\ell} - (C^{\text{EE}}_{\ell}))},
\]
this expression is transformed into
\[
P(C^{\text{EE}}_{\ell} \mid C^{\text{TE}}_{\ell} | \sigma_\ell) \propto \left| \sigma_\ell \frac{2\ell + 1}{C^{\text{EE}}_{\ell}} \right| e^{-\frac{\sigma^{2\ell + 1}}{2C^{\text{EE}}_{\ell}}} \int_0^\infty y^{2\ell + 1} e^{-y} dy.
\]
The integral in this expression is simply the Gamma function,
\[
\Gamma \left( \frac{2\ell + 1}{2} \right) = \int_0^\infty y^{2\ell + 1} e^{-y} dy,
\]
and, for our purposes, an irrelevant numerical normalization factor. Thus, the final distribution reads
\[
P(C^{\text{EE}}_{\ell} \mid C^{\text{TE}}_{\ell} | \sigma_\ell) \propto \left| \sigma_\ell \frac{2\ell + 1}{C^{\text{EE}}_{\ell}} \right| \frac{1}{(\sigma^2_{\ell} C^{\text{TT}}_{\ell} + \sigma^2_{\ell} C^{\text{EE}}_{\ell})^{\frac{2\ell + 1}{2}}},
\]
Note that because TT and EE occur symmetrically in Equation (15), the corresponding expression for \( P(C^{\text{TT}}_{\ell} \mid C^{\text{EE}}_{\ell} | \sigma_\ell) \) is obtained by simply interchanging EE and TT in Equation (23).

3.2. The (TT, EE) Distribution, \( P(C^{\text{TT}}_{\ell}, C^{\text{EE}}_{\ell} | \sigma_\ell) \)

Next, we consider \( P(C^{\text{TT}}_{\ell}, C^{\text{EE}}_{\ell} | \sigma_\ell) \), which is obtained by integrating \( P(C^{\text{TT}}_{\ell}, C^{\text{EE}}_{\ell} \mid \sigma_\ell) \) over \( C^{\text{TE}}_{\ell} \). Unfortunately, this distribution does not have a closed expression, but can instead be written in the form
\[
P(C^{\text{TT}}_{\ell}, C^{\text{EE}}_{\ell} | \sigma_\ell) \propto \left| \sigma_\ell \frac{2\ell + 1}{(C^{\text{TT}}_{\ell} C^{\text{EE}}_{\ell})} \right| \cdot I_1(\ell, A, B).
\]
Here \( I_1 \) denotes the integral
\[
I_1 = \int_{-1}^1 e^{-\frac{4(\ell + 1)x}{1 - x^2}} dx,
\]
and we have defined the two dimensionless auxiliary parameters
\[
A = \frac{2\ell + 1}{2} \left( \sigma^2_{\ell} C^{\text{TT}}_{\ell} + \sigma^2_{\ell} C^{\text{EE}}_{\ell} \right)
\]
\[
B = \frac{(2\ell + 1)\sigma^2_{\ell}}{\sqrt{C^{\text{TT}}_{\ell} C^{\text{EE}}_{\ell}}},
\]
However, the fact that \( I_1 \) depends only on two dimensionless parameters and \( \ell \) implies that it can be easily tabulated (and optionally splined for higher accuracy) for each \( \ell \), and thus computationally efficient lookup-tables may be constructed. In most practical applications, which typically require repeated evaluations of \( P(C^{\text{TT}}_{\ell}, C^{\text{EE}}_{\ell} | \sigma_\ell) \), Equation (23) is therefore as useful for \( (C^{\text{TT}}_{\ell}, C^{\text{EE}}_{\ell}) \) as Equation (32) is for \( (C^{\text{TE}}_{\ell}, C^{\text{EE}}_{\ell}) \), although implementationally a little more complicated.

3.3. The Marginal EE Distribution, \( P(C^{\text{EE}}_{\ell} | \sigma_\ell) \)

We now compute the corresponding one-dimensional marginals, and begin with \( P(C^{\text{EE}}_{\ell} | \sigma_\ell) \) by integrating Equation (23) over \( C^{\text{TE}}_{\ell} \). This is simplified by introducing the new variable
\[
y = \frac{\sigma^2_{\ell} C^{\text{TE}}_{\ell} - \sigma^2_{\ell} C^{\text{EE}}_{\ell}}{\sqrt{|\sigma^2_{\ell} C^{\text{EE}}_{\ell}|}}.
\]
The distribution then reads
\[
P(C^{\text{EE}}_{\ell} | \sigma_\ell) = \int P(C^{\text{EE}}_{\ell} \mid C^{\text{TE}}_{\ell} | \sigma_\ell) dC^{\text{TE}}_{\ell}
\]
\[
\propto \frac{\sigma^{2\ell + 1}_{\ell}}{(C^{\text{EE}}_{\ell})^{\frac{2\ell + 1}{2}}} e^{-\frac{\sigma^{2\ell + 1}}{2C^{\text{EE}}_{\ell}}} \int_{-\infty}^{\infty} \left( \frac{1}{y^2 + 1} \right)^{\frac{2\ell + 1}{2}} dy.
\]
The integral in this expression is, for \( \ell > 1 \),
\[
\int_{-\infty}^{\infty} \left( \frac{1}{y^2 + 1} \right)^{\frac{2\ell + 1}{2}} dy = \frac{\Gamma(\frac{3}{2} - \frac{1}{2\ell})}{\Gamma(\frac{3}{2})},
\]
which is a simple numerical constant. The desired marginal distribution therefore reads
\[
P(C^{\text{EE}}_{\ell} | \sigma_\ell) \propto \frac{\sigma^{2\ell + 1}_{\ell}}{(C^{\text{EE}}_{\ell})^{\frac{2\ell + 1}{2}}} e^{-\frac{\sigma^{2\ell + 1}}{2C^{\text{EE}}_{\ell}}},
\]
Again, we note that the corresponding expression for \( P(C^{\text{TT}}_{\ell} | \sigma_\ell) \) is obtained simply by replacing EE with TT.

3.4. The Marginal TE Distribution, \( P(C^{\text{TE}}_{\ell} | \sigma_\ell) \)

Finally, we consider \( P(C^{\text{TE}}_{\ell} | \sigma_\ell) = \int P(C^{\text{TE}}_{\ell} | C^{\text{EE}}_{\ell} | \sigma_\ell) dC^{\text{EE}}_{\ell} \).
As was the case for \( P(C^{\text{TT}}_{\ell}, C^{\text{EE}}_{\ell} | \sigma_\ell) \), this distribution does not have a closed form, but may instead be written in a computationally convenient form
\[
P(C^{\text{TE}}_{\ell} | \sigma_\ell) \propto \frac{\sigma^{2\ell + 1}_{\ell}}{(\sigma^2_{\ell} C^{\text{TE}}_{\ell} + \sigma^2_{\ell} C^{\text{EE}}_{\ell})^{\frac{2\ell + 1}{2}}} \cdot I_2(\ell, C, D),
\]
where \( I_2 \) denotes the integral
\[
I_2 = \int_0^\infty \frac{x^{2\ell + 1} e^{-\frac{x}{2}}}{((x - C)^2 + D^2)^{\frac{2\ell + 1}{2}}} dx.
\]
The two dimensionless auxiliary parameters in this integral are
\[
C = \frac{\sigma^2_{\ell} C^{\text{TE}}_{\ell}}{\sigma^2_{\ell} C^{\text{EE}}_{\ell}},
\]
\[
D = \frac{\sqrt{|\sigma^2_{\ell} C^{\text{EE}}_{\ell}|}}{\frac{2\ell + 1}{2} \sigma^2_{\ell} C^{\text{TE}}_{\ell}}.
\]
Thus, as was the case for \( I_1, I_2 \) also may be tabulated over a two-dimensional grid for each multipole. It is therefore computationally straightforward to evaluate \( P(C^{\text{TE}}_{\ell} | \sigma_\ell) \) at a given value of \( C^{\text{TE}}_{\ell} \), even if it does not have a closed analytical expression.
3.5. The Conditional TE Distribution, $P(C_{\ell}^{TE}|C_{\ell}^{EE}, \sigma_{\ell})$

From the above expressions, we may also derive all possible conditional distributions, since $P(x|y) = P(x, y)/P(y)$. Here we will only explicitly consider the conditional TE distribution,

$$P(C_{\ell}^{TE}|C_{\ell}^{EE}, \sigma_{\ell}) = \frac{P(C_{\ell}^{TE}, C_{\ell}^{EE}|\sigma_{\ell})}{P(C_{\ell}^{TE}|\sigma_{\ell})}$$

(37)

$$\propto \frac{(C_{\ell}^{EE})^{\frac{1}{2}\nu}}{(2\pi \nu)^{\nu/2}} |\sigma_{\ell}|^{\frac{\nu+2}{2}}$$

(38)

which is relevant to several important applications (see, e.g., Section 4).

If we make the same linear transformation of $C_{\ell}^{EE}$ as in Section 3.3, but including an additional $2\ell - 2$ factor,

$$x = \sqrt{\frac{2\ell - 2}{\nu}} \left( C_{\ell}^{EE} \sigma_{\ell} - \sigma_{\ell} C_{\ell}^{EE} \right),$$

(39)

we see that this may be rewritten in a familiar form,

$$P(C_{\ell}^{TE}|C_{\ell}^{EE}, \sigma_{\ell}) \propto \frac{1}{\Gamma\left(\frac{\nu+1}{2}\right)} \left( \frac{\nu+1}{2} \right)^{\frac{\nu}{2}}$$

(40)

$$\cdot \left( x^2 + \frac{1}{2} \right)^{-\nu/2}.$$

We recognize this as the Student’s $t$ distribution with $\nu = 2\ell - 2$ degrees of freedom.

Since one of our goals is to sample from this distribution, it is useful to have its cumulative distribution, $F$, in a closed form

$$F(C_{\ell}^{EE}|C_{\ell}^{EE}, \sigma_{\ell}) = \frac{1}{2} + \frac{1}{\nu} \Gamma\left( \frac{\nu+1}{2} \right) - \frac{1}{2} \Gamma\left( \frac{\nu+1}{2}, \frac{x^2}{\nu+1} \right).$$

(41)

Here $\Gamma$ denotes the hypergeometric function (e.g., Abramowitz & Stegun 1972).

4. CMB GIBBS SAMPLING APPLICATIONS

The analytical expressions derived in Section 3 are the main results of this paper. Being completely general, these may, in principle, be applied to a wide range of practical CMB applications. However, they are particularly useful for methods that consider both the sky signal and the power spectrum $C_{\ell}$ as free variables, such as the CMB Gibbs sampler. In this section, we demonstrate two specific Gibbs-based applications, namely (1) a new $C_{\ell}$ sampling algorithm that supports general binning schemes and (2) new Blackwell–Rao estimators for marginal and conditional distributions.

4.1. A New $C_{\ell}$ Sampling Algorithm

The CMB Gibbs sampler draws samples from the joint posterior, $P(s, C_{\ell}|d)$, by alternately sampling from the two corresponding conditionals (e.g., Jewell et al. 2004; Wandelt et al. 2004; Eriksen et al. 2004),

$$s^{i+1} \sim P(s|C_{\ell}^{i}, d),$$

(42)

$$C_{\ell}^{i+1} \sim P(C_{\ell}|s^{i+1}).$$

(43)

(In these expressions, the arrow indicates sampling from the distribution on the right-hand side.) The former of these distributions is a high-dimensional Gaussian distribution, while the latter, which is the topic of the present paper, is a product of independent inverse Wishart distributions.

There is already a well-known and simple algorithm available in the literature to sample from the inverse Wishart distribution (e.g., Larson et al. 2007, Gupta & Nagar 2000). Let $p$ be the dimension of the target matrix (e.g., $p = 2$ for $(T, E)$) and $\Sigma = (2\ell + 1)\sigma_{\ell}$, then the algorithm goes as follows: (1) draw $2\ell - p$ vectors from a Gaussian distribution with covariance matrix $\Sigma_{i}$; (2) compute the sum of outer products of these vectors; (3) invert this matrix.

This algorithm produces samples for a given multipole $\ell$. However, in low S/N applications it is often desirable to bin many multipoles together, in order to increase the effective S/N of each variable. Because the CMB power spectrum essentially scales as $\mathcal{O}(\ell^{-2})$, it is customary to bin in units of $C_{\ell}(\ell+1)/2\pi$. With this convention, the above algorithm may be generalized to include binning by redefining the covariance matrix as follows:

$$\Sigma_{\ell} = \sum_{i=b}^{\ell} \frac{(\ell+1)}{2\pi} (2\ell + 1) \sigma_{\ell}.$$

(44)

Here $b = [\ell_{\text{min}}, \ell_{\text{max}}]$ indicates the multipole range of the bin under consideration. Note that the total number of modes is now $M = (\ell_{\text{max}} + 1)^2 - \ell_{\text{min}}^2$, and therefore $M$ Gaussian vectors must be drawn from $\Sigma_{\ell}$.

Unfortunately, this method has the serious drawback that the binning scheme must be identical for $C_{\ell}^{TT}$, $C_{\ell}^{EE}$, and $C_{\ell}^{EE}$. This is a problem because the S/N of most experiments is very different for TT than for EE, and one would lose much spectral resolution if one were to bin $C_{\ell}^{TT}$ with a bin size such that the S/N for the corresponding $C_{\ell}^{EE}$ bin is unity.

The new analytical expressions derived in Section 3 allow us to resolve this problem. First, we use the definition of a conditional distribution, and write

$$P(C_{\ell}^{TT}, C_{\ell}^{TE}, C_{\ell}^{EE}|\sigma_{\ell}) = P(C_{\ell}^{TT}|C_{\ell}^{TE}, C_{\ell}^{EE}, \sigma_{\ell}) \cdot P(C_{\ell}^{TE}|C_{\ell}^{EE}, \sigma_{\ell}) \cdot P(C_{\ell}^{EE}|\sigma_{\ell}).$$

(45)

The algorithm may now be written symbolically as follows:

$$C_{\ell}^{EE} \sim P(C_{\ell}^{EE}|\sigma_{\ell})$$

(46)

$$C_{\ell}^{TE} \sim P(C_{\ell}^{TE}|C_{\ell}^{EE}, \sigma_{\ell})$$

(47)

$$C_{\ell}^{TT} \sim P(C_{\ell}^{TT}|C_{\ell}^{TE}, C_{\ell}^{EE}, \sigma_{\ell}).$$

(48)

Then $\{C_{\ell}^{EE}, C_{\ell}^{TE}, C_{\ell}^{TT}\}$ will be a sample drawn from the joint distribution $P(C_{\ell}^{TT}, C_{\ell}^{TE}, C_{\ell}^{EE}|\sigma_{\ell})$. Note that each of these conditional distributions is a one-dimensional distribution, and the correlation with other polarization components comes into play only conditionally, not jointly. One is therefore completely free to specify the binning schemes for each component independently of the others.

We still need to write a sampling algorithm for each of these conditionals. However, since these are all one dimensional, this is a trivial task. The simplest approach, and the one currently implemented in our codes, is to take advantage of the cumulative distribution: suppose we want to draw a sample from a univariate distribution, $P(x)$, and have access to the corresponding cumulative distribution, $F(x)$, then we can draw a uniform variate $\eta \sim U[0, 1]$ and solve for $F(x) = \eta$. The sample $x$ will then be drawn from $P(x)$.

However, a computational issue with this approach is the evaluation of the cumulative distribution. With the notable
exception of $P(C_{\ell}^{\text{TE}}|C_{\ell}^{\text{EE}}, \sigma_{\ell})$ for a single multipole, we do not have explicit analytical expressions for the cumulative distributions. Therefore, in these cases we instead have to map out the analytical probability densities over a grid, and do the integration numerically. Fortunately, this requires only $\sim \mathcal{O}(10^2)$ function evaluations, and is therefore computationally quite fast. The cost of the full Gibbs sampler is anyway hugely dominated by sampling from the sky signal distribution $P(s|C_{\ell}, d)$.

Nevertheless, one might want to consider alternative approaches for applications in which this sampling step may be dominating. In such cases, the rejection sampler (e.g., Liu 2001) appears as a promising candidate. In this approach, one samples from an auxiliary distribution that preferably should approximate the target distribution quite well. Since our distributions are all one dimensional and strongly single-peaked, it should not be difficult to establish such auxiliary functions. Indeed, the Student’s $t$ distribution itself is a typical candidate for such purposes, since it has a quite heavy tail.

In Figure 1 we compare the marginal distributions obtained by the direct inverse Wishart distribution and by the new sampler presented here, only for $\ell = 10$. As expected, they agree perfectly. Next, in Figure 2 we show a single sample from the joint all-$\ell$ distribution $P(C_{\ell}|\sigma_{\ell})$, with appropriate binning schemes for each of $C_{\ell}^{\text{TT}}$, $C_{\ell}^{\text{TE}}$, and $C_{\ell}^{\text{EE}}$. Again, producing a similar sample with the direct inverse Wishart sampler is not possible, as discussed above.

Next, we consider Blackwell–Rao estimators for marginal and conditional distributions, and focus from now on the factorization of $P(C_{\ell}|d)$ given in Equation (46). However, we note that each one of the distributions in Table 1 gives rise to a separate estimator.

First recall the derivation of the Blackwell–Rao estimator (Chu et al. 2005),

\[
P(C_{\ell}|d) = \int P(C_{\ell}, s|d) \, ds
\]

\[
= \int P(C_{\ell}|s, d)P(s|d) \, ds
\]

\[
= \int P(C_{\ell}|\sigma_{\ell})P(\sigma_{\ell}|d) \, D\sigma_{\ell}
\]

\[
\approx \frac{1}{N_{G}} \sum_{i=1}^{N_{G}} P(C_{\ell}|\sigma_{i}).
\]

Thus, the full Blackwell–Rao estimator for $P(C_{\ell}|d)$ is nothing but the sum (or average) of $P(C_{\ell}|\sigma_{i})$ over Gibbs samples, $\sigma_{i}$.

This estimator, as written here, has notoriously poor convergence properties as the dimension of the parameter volume increases (Chu et al. 2005)—it requires an exponential number of samples in order to converge. The reason simply is that the volume of a single Gibbs sample is given by cosmic variance alone, whereas the volume of the full distribution is also determined by noise and sky cut. Therefore, even if the width of $P(C_{\ell}|\sigma_{i})$ for a single multipole is as much as, say, 90% of the
width of $P(C_\ell | d)$, the relative volume fraction in $\ell_{\text{max}}$ dimensions is $f = 0.9^{\ell_{\text{max}}}$. For $\ell_{\text{max}} = 30$, this number is $f = 0.04$, and for $\ell_{\text{max}} = 100$ it is $f = 2.65 \times 10^{-5}$. Clearly, a brute-force Blackwell–Rao approach will not work for high-dimensional spaces unless the volume ratio per multipole is unrealistically large. However, the same problem does not affect the marginal distributions described above, because the number of dimensions is low, and typically just one, by construction.

Let us consider the Blackwell–Rao estimator for $P(C_\ell^{\text{EE}} | d)$ for a single multipole, $\ell$. First, marginalization over other multipoles consists, as usual for Markov Chain Monte Carlo algorithms, of simply disregarding the sample values of all other $\ell$s. Second, marginalization over $C_{\ell \ell}$ and $C_{\ell \ell}^{\text{TE}}$ is done using the expressions derived in Section 3.

$$P(C_\ell^{\text{EE}} | d) = \int \int P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | d) \, dC_\ell^{\text{TT}} \, dC_\ell^{\text{TE}}$$

$$\approx \int \int \sum_i P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | \sigma_i) \, dC_\ell^{\text{TT}} \, dC_\ell^{\text{TE}}$$

$$= \sum_i \int \int P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | \sigma_i) \, dC_\ell^{\text{TT}} \, dC_\ell^{\text{TE}}$$

$$= \sum_i P(C_\ell^{\text{EE}} | \sigma_i)$$

$$= \sum_i \left( \frac{\sigma_i^{\text{EE}}}{C_\ell^{\text{EE}}} \right)^{-\frac{\nu_i}{2}} e^{-\frac{\nu_i}{2} \frac{\sigma_i^{\text{EE}}}{C_\ell^{\text{EE}}}}. \quad (57)$$

Similarly, the Blackwell–Rao estimator for $P(C_\ell^{\text{TE}} | C_\ell^{\text{EE}}, d)$ reads

$$P(C_\ell^{\text{TE}} | C_\ell^{\text{EE}}, d) = \frac{P(C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | d)}{P(C_\ell^{\text{EE}} | d)} \propto P(C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | d)$$

$$\approx \sum_i P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | \sigma_i)$$

$$\propto \sum_i \left( \frac{C_\ell^{\text{EE}}}{\sigma_i^{\text{EE}}} \right)^{-\frac{\nu_i}{2}} e^{-\frac{\nu_i}{2} \frac{\sigma_i^{\text{EE}}}{C_\ell^{\text{EE}}}} \left( \frac{\sigma_i^{\text{TE}}}{C_\ell^{\text{TE}}} - 2\sigma_i^{\text{TT}} C_\ell^{\text{TE}} / \sigma_i^{\text{EE}} \right)^{-\frac{\nu_i}{2}}. \quad (61)$$

First, note that because $C_\ell^{\text{EE}}$ is a constant in this expression, $P(C_\ell^{\text{EE}} | d)$ is also a constant, and can be disregarded after Equation (58). Second, we emphasize that it is crucial to use the full joint expression for $P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | d)$ in this estimator, and not the naive “alternative” $P(C_\ell^{\text{TE}} | C_\ell^{\text{EE}}, d) \approx \sum_i P(C_\ell^{\text{TE}} | C_\ell^{\text{EE}}, \sigma_i)$.

The latter approach would require the underlying Gibbs samples, $\sigma_i$, to be drawn conditionally on $C_\ell^{\text{EE}}$ in original Gibbs analysis, and this is usually not the case.

Finally, we consider the expression for $P(C_\ell^{\text{TT}} | C_\ell^{\text{TE}}, C_\ell^{\text{EE}}, d)$ for a single multipole. However, there is little simplification involved in this expression, as it simply reads

$$P(C_\ell^{\text{TT}} | C_\ell^{\text{TE}}, C_\ell^{\text{EE}}, d) \approx \sum_i P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | \sigma_i)$$

$$\approx \sum_i |\sigma_i|^{2\ell - 2} C_\ell^{\text{EE}}^{\frac{\nu_i}{2}} e^{-\frac{\nu_i}{2} \max(\sigma_i | C_\ell^{\text{EE}})} \, |C_\ell|^{-\frac{\nu_i}{2}} e^{-\frac{\nu_i}{2} \max(\sigma_i | C_\ell^{\text{EE}})}. \quad (64)$$

First, note that because $C_\ell^{\text{EE}}$ is a constant in this expression, $P(C_\ell^{\text{EE}} | d)$ is also a constant, and can be disregarded after Equation (58). Second, we emphasize that it is crucial to use the full joint expression for $P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | d)$ in this estimator, and not the naive “alternative” $P(C_\ell^{\text{TE}} | C_\ell^{\text{EE}}, d) \approx \sum_i P(C_\ell^{\text{TE}} | C_\ell^{\text{EE}}, \sigma_i)$.

As a simple illustration, we plot the three Blackwell–Rao estimators given above for $\ell = 10$ in Figure 3, as computed from a low-resolution simulation ($N_{\text{side}} = 16$, $\ell_{\text{max}} = 47$, Gaussian beam of $10^\circ$ FWHM, and white noise of $\sigma_T = 1 \mu K$ and $\sigma^{O,U} = 0.5 \mu K$ for temperature and polarization, respectively) drawn from a standard $\Lambda$CDM spectrum. As expected, the agreement with direct histograms is excellent, but the smoothness and faster convergence of the Blackwell–Rao estimator make it the preferred choice for most applications.

While these expressions are useful in their own right, for example, for plotting marginal or joint power spectra and the corresponding confidence regions from a set of Gibbs samples (say, by maximizing and/or integrating the Blackwell–Rao estimator for each $\ell$ individually), their main application lies in providing robust estimates of $P(C_\ell^{\text{TT}}, C_\ell^{\text{TE}}, C_\ell^{\text{EE}} | d)$ in terms of univariates. This may open up some very interesting possibilities for stabilizing the exponential behavior of the full multivariate estimator. This topic will be explored further in a future publication.

5. CONCLUSIONS

We have derived computationally convenient expressions for all marginals of $P(C_\ell | \sigma_i)$. These expressions may be useful to any CMB analysis method that considers both the CMB sky signal $s$ and the power spectrum $C_\ell$ as

**Figure 3.** Comparison of three Blackwell–Rao estimators and simple histograms computed from a low-resolution CMB simulation.
unknown parameters. One prominent example is the CMB Gibbs sampler.

We have also presented two specific applications of these expressions. First, we demonstrated a new sampling algorithm for \( P(C_\ell | \sigma_\ell) \) that supports different binning schemes for each polarization component. This is useful because most experiments have very different S/N to temperature and polarization.

Second, we have provided explicit expressions for the Blackwell–Rao estimators for \( P(C_{TT}^\ell | C_{TE}^\ell , C_{EE}^\ell , d) \), \( P(C_{TE}^\ell | C_{EE}^\ell , d) \), and \( P(C_{EE}^\ell | d) \). Together, these three can be used to map out the joint distribution \( P(C_\ell | d) \) for a single multipole in terms of univariate distributions alone. Further, we note that any of the distributions listed in Table 1 gives rise to a separate, and potentially useful, Blackwell–Rao estimator.

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