A Modified $\chi^2$-Test for CMB Analyses

J.A. Rubiño-Martín$^{1*\dagger}$ and J. Betancort-Rijo$^{1,2}$

$^{1}$Instituto de Astrofísica de Canarias, C/ Via Lactea, s/n, 38200 La Laguna, Tenerife, Spain
$^{2}$Departamento de Astrofísica, Universidad de La Laguna, 38200 La Laguna, Tenerife, Spain

ABSTRACT

We present a new general procedure for determining a given set of quantities. To this end, we define certain statistic, that we call ‘modified $\chi^2$ ($\chi^2_M$), because of its similarity with the standard $\chi^2$. The terms of this $\chi^2_M$ are made up of the fluctuations of an unbiased estimator of some statistical quantities, and certain weights. Only the diagonal terms of the covariance matrix explicitly appear in our statistic, while the full covariance matrix (and not its inverse) is implicitly included in the calculation of the weights. Choosing these weights we may obtain, through minimising the $\chi^2_M$, the estimator that provides the minimum RMS, either for those quantities or for the parameters on which these quantities depend. In this paper, we describe our method in the context of Cosmic Microwave Background experiments, in order to obtain either the statistical properties of the maps, or the cosmological parameters. The test here is constructed out of some estimator of the two-point correlation function at different angles. For the problem of one parameter estimation, we show that our method has the same power as the maximum likelihood method. We have also applied this method to Monte Carlo simulations of the COBE-DMR data, as well as to the actual 4-year data, obtaining consistent results with previous analyses. We also provide a very good analytical approximation to the distribution function of our statistic, which could also be useful in other contexts.

Key words: methods: statistical – cosmology: cosmic microwave background – cosmology: cosmological parameters

1 INTRODUCTION

The study of the Cosmic Microwave Background (CMB) anisotropies is providing strong constraints on theories of structure formation. These theories are statistical in essence, so the extraction of the information must be done in a statistical way. In particular, the standard method for analysing a CMB experiment is the maximum likelihood estimator (ML). The procedure is straightforward: maximise the probability of the parameters of the model given the data, $P(\text{parameters}|\text{data})$, over the allowed parameter space. Usually, we take the prior probability for the parameters to be constant, so this is equivalent to maximising the likelihood, $P(\text{data}|\text{parameters})$, via the Bayes’ theorem.

The ML method has been widely applied in CMB analyses, for power spectrum or parameters estimation, (Davies et al. 1987; Górski 1994; Hinshaw et al. 1996a). When computing the likelihood in these problems, we have to deal with the inversion of the covariance matrix of the data, which usually involves $O(N^3)$ operations, being $N$ the number of pixels of the map. The increasing size of the datasets makes this method computationally costful for new experiments, so other methods have been investigated in the last few years to confront the problem. There have been several proposals on this matter. Pioneering work on the problem of power spectrum estimation (Hauser & Peebles 1973; Peebles 1973), based on an evaluation of the $a_{\ell m}$’s coefficients of the multipole expansion of the observed map in the spherical harmonics basis, have been applied to COBE data (Wright et al. 1996). Quadratic estimators have been proposed by several authors (Tegmark 1997; Bond, Jaffe, & Knox 1998) as statistics that give the same parameters that maximise the likelihood, but requiring less computational work.

Nevertheless, alternative statistical methods are required in the field to extract the cosmological information from future CMB experiments (as PLANCK) where the number of data points will be very large (see, e.g. Borrill (1999) for an estimation of the scaling of the computing time with the dataset size).

Here, we propose a new statistical method to analyse a CMB map. In order to illustrate it, we will use the two-point correlation function (CF). We first replace the likeli-
hood of the full map by the likelihood of the fluctuations of an estimator of the CF. Then, we derive the cosmological parameters from it in an efficient manner. If we assume gaussianity for the primordial CMB fluctuations, the CF completely characterises the statistical properties of the field. In this line, it has been suggested [Bashinsky & Bertschinger 2001] that it can be used to obtain the power spectrum or for parameter estimation, because it encodes all the relevant information for that purpose. This approach of considering the CF in CMB analyses has been recently used by other authors [Szapudi et al. 2001a; Kashlinsky et al. 2001; Szapudi et al. 2001b] to estimate the power spectrum. They obtain the CF using different estimators, and integrate it, projecting over the Legendre polynomials, to obtain the CF. Nevertheless, all the procedure described below can be applied to any other estimator.

In this section we will introduce the test, using for this purpose the two-point CF. Hereafter, we will write the estimate of a certain parameter by writing $C_{\ell} = C_{\ell}(n, \Omega, \Omega_k, \Omega_{\Lambda}, H_0, ...).$ In general, we will write $C(\theta | \hat{M})$, being $\hat{M}$ the parameters of the model.

As an example of the general procedure that we propose in this paper, we consider in detail the estimator derived from the following statistic:

$$\chi^2_{\ell}(\hat{M}) = \sum_{k=1}^{n} P_k \left( \frac{E[C(\theta_k)] - C(\theta_k | \hat{M}) - C_N(\theta_k))}{\sigma^2(C(\theta_k))} \right)^2$$  \hspace{1cm} (3)

where $P_k$’s are certain weights to be defined below, and $\sigma^2(C(\theta_k))$ stands for the variance of the estimator $E[C(\theta_k)]$. $C_N(\theta_k)$ represents the discrete CF of the noise. If we have an experiment with uncorrelated noise, this function takes the form

$$C_N(\theta_k) = \begin{cases} \sum_{N} \sigma^2, & \theta_k = 0 \\ 0, & \theta_k \neq 0 \end{cases}$$ \hspace{1cm} (4)

This method is a modification of the standard form of a $\chi^2$-test, for the case when the error of each of the estimators entering $\chi^2$ are independent and gaussianly distributed (hereafter, we mean by standard $\chi^2$-test the case when $P_k = 1$, $\forall k$, and all the terms of the sum in (3) are independent). In the present case, the $E[C(\theta_k)]$ quantities follow very closely a gaussian, but are correlated. For this reason, we have introduced some weights ($P_k$), that will be determined by minimising the dispersion of the estimator derived from equation (3), as we will see in the next section. These quantities will account for the different degree of correlation between terms, and in a general problem, they will be a function $P_k = P_k(C')$, where $C_{ij}$ stands for the correlation matrix between the errors of the estimates of $C(\theta_k | \hat{M})$ and $C(\theta_j | \hat{M})$, i.e.

$$C_{ij} = C_{ij}(\hat{M}) = \langle \left( E[C(\theta_i)] - C(\theta_i | \hat{M}) - C_N(\theta_i) \right) \times \left( E[C(\theta_j)] - C(\theta_j | \hat{M}) - C_N(\theta_j) \right) \rangle$$ \hspace{1cm} (5)

so the variance $\sigma^2(C(\theta_k))$ is related to the $C'$-matrix by

$$\sigma^2(C(\theta_k)) = C'_{ii}$$ \hspace{1cm} (6)

The brackets $< ... >$ represent an average over an ensemble of Universes, i.e., an average over realizations for one fixed CMB model.

In principle, our construction seems to miss information about the correlations when compared to the usual $\chi^2$ procedure to analyse correlated datasets, because in equation (3) only the diagonal terms of the covariance matrix ($C'$) are explicitly shown. Nevertheless, as we will see in the next section, the $P_k$ weights depend on the full covariance matrix and not on its inverse, so all the correlations implicitly enter in that expression.

We will not make a detailed comparison between the usual $\chi^2$ method with the usual full covariance matrix $C'$ (we will refer to this method as the “usual $\chi^2$”) and our $\chi^2_{\ell}$. However, we will illustrate this with an example (see section 6.1). In addition, in Appendix A we present a brief comparison of some characteristics of both methods ($\chi^2_{\ell}$ and the usual $\chi^2$) for the case of linear problems. It is an interesting result that, for gaussian linear problems, if we are estimating only one parameter, the estimates from both
methods are exactly equal, while being different statistics (i.e. they will give different probability contours). Hereafter, we will concentrate in our method, and its application to CMB problems.

It is worth to notice that our \( \chi^2 \) statistic is a different approach to the ML, in the sense that it provides different estimates and probability contours. However, in the case of CMB analyses, we will see below that it has a similar power to the ML, but avoiding the problem of the inversion of the covariance matrix. There is however a minor sense in which our test may formally be considered as an approximation to the ML. It is well-known that the ML is an asymptotically efficient estimator for our problem. Thus, in the limit of infinite size of the sample (or for those problems where an efficient estimator exists, as in linear gaussian problems), then the ML is the only one statistic which renders the minimum variance, and thus any other estimator may be regarded as approximate.

### 2.1 Estimate of the method

Once we have constructed the \( \chi^2 \) test, the estimate for this method is given by the set of values for the parameters that minimise eq. \( \chi^2 \), i.e. the solution to the set of equations \( \partial \chi^2(M)/\partial M = 0 \). For a given problem, we proceed as follows. If we want to estimate a set of \( p \) parameters, \( M = \{\xi_1, ..., \xi_p\} \), we first compute the \( C' \) matrix by assuming an initial value for those parameters, \( \tilde{M} \). Using this matrix, we obtain our estimate by solving the following system of equations,

\[
\frac{\partial \chi^2}{\partial \xi_i} = 0, \quad i = 1, ..., p
\]

(7)

When computing these derivatives with respect to \( \tilde{M} \), we neglect the dependence of \( C' \) on the parameters, which is equivalent to assuming that \( \sigma^2(C(\theta_i)) \) and \( P_k \) are constants in the derivation. This process is iterated until convergence. The reason to keep the \( C' \) matrix fixed in the derivation is that we want to have an unbiased estimator of the parameters.

The evaluation of the \( C' \) matrix can be done by Monte Carlo simulations, but we also propose an analytical approach. It is possible to evaluate equation (8) using the quantities \( \theta_i \), for a multivariate-gaussian field, as is the case for the CMB (see Appendix B).

In the particular case of power spectrum estimation, the set of parameters we have to determine are the \( C_i \)'s themselves, or the band powers in a certain number of multipole bands centred at multipoles \( \ell' \), \( \ell \) (i.e., \( M = \{C_\ell\}_{\ell=1}^{\ell_{\text{max}}} \)). As the theoretical CF \( \tilde{C}_\ell \) is linear in the \( C_i \)'s, we have that eq. (7) is a linear system of \( p \) equations, and the solution can easily be found.

As an example, we present here the equations for the determination of the total power measured by a certain experiment. If we define the function \( f(\theta) \equiv C(\theta)/\sigma^2(\theta) \), which is independent of \( \sigma^2(\theta) \). We can now obtain the analytic expression for the estimate of \( \sigma^2(\theta) \) by minimising eq. (9) with respect to \( \sigma^2(\theta) \), which in this case takes the form

\[
\chi^2_M(\sigma^2(\theta)) = \sum_{i=1}^n P_k E[C(\theta_i)] - \sigma^2(\theta) f(\theta_i)^2 \]

(9)

For simplicity, we will not write the term of the noise CF, but it can be easily included inside the true CF. Inserting the previous expression in equation (9), we obtain, for fixed \( P_k \), an equation for \( \sigma^2(\theta) \). It must be noted that due to the dependence of \( \sigma^2(C(\theta_i)) \) on \( \sigma^2(\theta) \), this equation is not exactly linear. We could solve it iteratively, starting with a given fixed value for \( \sigma^2(\theta) \). However, for all the values of these quantities within the current limits, a first iteration is enough, as we will see, so that the equation determining \( \sigma^2(\theta) \) is effectively linear, and therefore its solution is given by

\[
E[\sigma^2(\theta)] = \left( \sum_{i=1}^n \frac{P_i f_i^2}{\sigma^2(C(\theta_i))} \right)^{-1} \sum_{i=1}^n \frac{P_i f_i^2 E[C(\theta_i)]}{\sigma^2(C(\theta_i))}
\]

(10)

The RMS of this estimator is given by

\[
\text{RMS}(E[\sigma^2(\theta)]) = \left( \sum_{i=1}^n \frac{P_i f_i^2}{\sigma^2(C(\theta_i))} \right)^{-1} \times \left[ \sum_{i=1}^n \frac{P_i f_i^2}{\sigma^2(C(\theta_i))} + \sum_{i \neq j} \frac{f_i f_j P_i P_j C_i C_j}{\sigma^2(C(\theta_i)) \sigma^2(C(\theta_j))} \right]^{1/2}
\]

(11)

where we have defined \( f_i = f(\theta_i) \). The expression within large parentheses in this equation is the RMS of the second sum in equation (10). The first sum within the parentheses correspond to the quadratic addition of the contributions of each term in (10), which is present even when the random variables \( E[C(\theta_i)] \) are independently distributed. The second sum is due to the correlations between any pair of these variables. It should be noted that equation (11) has been obtained assuming that the quantities \( E[C(\theta_i)] \) follow a multivariate gaussian distribution. This is a good approximation if there are enough pixel pairs entering in the sum in (10) (see, for example, [1993], for the CF of the COBE data). Similar calculations for the standard \( \chi^2 \) and the likelihood function can be found in [1992] (hereafter, B93). The matrical expression of the estimate and the RMS for a general linear problem are shown in Appendix A.

### 3 THE \( P_k \) QUANTITIES FOR A GIVEN PROBLEM

The \( P_k \)'s weights in equation (8) are introduced in order to take into account the different degree of correlation of the terms of the sum. Their expression can be obtained once we define exactly what we are interested in. For example, one common criteria for one parameter estimation is to use the estimator which has the minimum RMS. We will consider this criteria here.

For the problem of one parameter estimation described in the previous section, once we have the analytic expression for the RMS, and an initial guess for the \( C' \) matrix, we
can obtain the optimum set of $P_k$’s using the “minimum RMS criteria”. We minimise eq. (11) with respect to the $P_k$’s quantities. We obtain that the $P_k$’s quantities are given by the solution to the implicit set of equations

$$P_k f_k \sum_i \frac{P_i f_i^2}{\sigma^2(C(\theta_i))} + \frac{1}{2} \left( \sum_{i \neq k} f_i f_k C_{ik} \right) \left( \sum_i \frac{P_i f_i^2}{\sigma^2(C(\theta_i))} \right) - f_k \sum_i \frac{f_i^2 P_i^2}{\sigma^2(C(\theta_i))} - f_k \sum_{i \neq j} f_i f_j P_i P_j C'_{ij} = 0, \quad k = 1, ..., p$$

which can be solved numerically, using a Newton-Raphson scheme for nonlinear systems of equations. It should be noted that in the case when $C'_{ij} = 0$, $i \neq j$, equation (12) has the trivial solution $P_k = 1$, as we expected for the standard case without correlations. The estimates obtained with these $P_k$ give us a better guess for $C'$, that could be used in equation (12) to obtain more appropriate values of the $P_k$. However, in practice, we have checked that for all the cases that we consider in this paper, this iteration is not necessary, since over the a priori uncertainty region of the parameter, the variation of the $P_k$ is negligible.

The previous expression, derived for the problem of total power estimation, can also be applied to any problem of one parameter estimation, as follows. Let $M$ be the parameter we are interested in. If we expand the CF in a Taylor series around an initial guess, $M = M_0$, we obtain, up to first order,

$$\Delta C(\theta_k|M) = C(\theta_k|M) - C(\theta_k|M_0) = \frac{\partial C(\theta_k|M)}{\partial M} \bigg|_{M_0} \Delta M + O(\Delta M^2), \quad k = 1, ..., n \quad (13)$$

with $\Delta M = M - M_0$, so we can use equation (12), with

$$f_k = \frac{\partial C(\theta_k|M)}{\partial M} \bigg|_{M_0}, \quad k = 1, ..., n \quad (14)$$

If we use an initial guess close to the real value, this linear approximation will give good results. The $f_k$’s can be obtained numerically for each problem.

When we deal with a problem of several parameters estimation, it is not well defined what has to be minimised. A reasonable criteria for these problems, if we want to estimate the set $M = \{M_1, ..., M_p\}$, is to minimise $\prod_i RMS(E[M_i])$, where we define $RMS(E[M_i])$ as the RMS for each individual parameter. Linearising around our initial guess, $M_0$, we can derive a simple expression for the RMS of each parameter. In this case, we have that

$$\Delta C(\theta_k|M) = \sum_{i=1}^p f_{k,i} \Delta M_i + O(\Delta M^2), \quad k = 1, ..., n \quad (15)$$

where we define

$$f_{k,i} = \frac{\partial C(\theta_k|M)}{\partial M_i} \bigg|_{M_0}, \quad i = 1, ..., p \quad (16)$$

The estimate of the parameters is given by the solution to the linear system of equations $\partial \chi^2_M / \partial M = 0$, where we have again neglected the dependence of $\sigma^2(C(\theta_k))$ on the parameters. The general expression of the covariance matrix of the parameters is shown, for a general linear problem, in Appendix A. If we expand those matrices, we obtain that the general form of this estimate, for our problem, is given by

$$E[\Delta M_i] = \frac{1}{R} \sum_k J_{k,i} P_k \frac{E[C(\theta_k)] - C(\theta_k, M_0)}{\sigma^2(C(\theta_k))}, \quad i = 1, ..., p \quad (17)$$

where $E[\Delta M_i] = E[M_i] - (M_0)_i$, and $R$ and $J$ are numbers obtained from the $f_{k,i}$’s. From (17) we can infer the general expression for the RMS in the case of several parameters, obtaining

$$RMS(E[M_i]) = \frac{1}{R} \left[ \sum_{k,j} J_{k,i} J_{j,i} P_k P_j C'_{kj} \frac{C'_{ij}}{\sigma^2(C(\theta_k))\sigma^2(C(\theta_j))} \right]^{1/2} \quad (18)$$

where $i = 1, ..., p$. Using the previous equation, we can obtain the $P_k$ quantities for any problem, just minimising the product $\prod_i RMS(E[M_i])$ numerically. Summarising, we will have a different expression for the $P_k$’s for each particular problem. An application of these equations for the problem of two parameters estimation can be found in Section 6.1.

4 DISTRIBUTION FUNCTION FOR THE MODIFIED $\chi^2$

The $\chi^2_M$ proposed in eq. (13) corresponds to a sum of quantities which are not independent. If we had set $P_i = 1$, we would have the standard $\chi^2$ statistic, but still with correlations among the terms. Therefore, its distribution function will not be the standard one.

The formal expression for the distribution of a $\chi^2$ constructed from variables which are distributed following a multivariate gaussian distribution is given in Appendix C. This distribution, when applied to CMB analyses, was studied in B03. There, they proposed that the distribution function for the statistic (3) is given by an standard (rescaled) $\chi^2$ function, but with an effective number of degrees of freedom. This proposal is not exact (see also Appendix C), but it turns out to be a very good approximation for the true distribution function, as we shall see in the following section. In a general case, the error in the distribution function using our approximation will be a few percent.

The basis of the approximation is to assume that correlations only reduce the degrees of freedom, but do not change the shape of the distribution. Quantifying this argument, there exist a certain constant, $A$, which makes the statistic

$$U = A \chi^2_M$$

(19)

to be distributed as an ordinary $\chi^2$, with an effective number of degrees of freedom, $n_{eff}$. This number, and the constant $A$, are obtained just by imposing the new distribution to have the mean and the variance of a standard $\chi^2$, i.e.,

$$< U >= n_{eff}, \quad (20)$$

$$MS(U) = < U^2 > - < U >^2 = 2n_{eff} \quad (21)$$

This idea has been used recently by other authors: Wandelt et al. 2000; Hivon et al. 2003.
where $MS$ means mean square. Summarising, our proposal is that once the first and second moments are fixed, the whole distribution will follow a $\chi^2$ very closely. For our problem, we obtain

$$A \equiv \frac{2 < \chi^2 >}{MS(X^2_M)} = \frac{\sum_{i=1}^n P_i}{\sum_{i=1}^n P_i^2 + \sum_{i\neq j} P_i P_j \frac{C_{ij}^2}{\sigma^2(C_{ij}) \sigma^2(C_{ji})}}$$

$$n_{eff} = \frac{2 < \chi^2 >}{MS(X^2_M)} = A \sum_{i=1}^n P_i$$

In this calculation, we needed to compute the $MS$ of eq. 4. This result is obtained using the fact that the data points follow a multivariate gaussian distribution, and it can be found in B93 (see also Appendix B for similar calculations).

In general, $n_{eff}$ is a real number, so we have to consider the analytic extension of a standard $\chi^2$ distribution (which is known as the Gamma distribution function, see for example Stuart & Ord (1994)),

$$dF(\chi^2_{n_{eff}}, n_{eff}) = g(\chi^2_{n_{eff}}, n_{eff}) d\chi^2_{n_{eff}} = \frac{1}{2^{n_{eff}} \Gamma(n_{eff}/2)} \exp(-\chi^2_{n_{eff}}/2) \left(\chi^2_{n_{eff}}/2\right)^{n_{eff}-1} d\chi^2_{n_{eff}}$$

just by replacing the factorial with the gamma function ($\Gamma$). In (21), $dF$ is the probability of finding a value for $U$ between $\chi^2_{n_{eff}}$ and $\chi^2_{n_{eff}} + d\chi^2_{n_{eff}}$, and $g$ stands for the probability density function. Once we know the distribution function, the confidence limits are given by integrating below this curve. We assign a weight to each hypothesis as in a standard $\chi^2$ analysis, integrating the distribution from the obtained value up to infinite,

$$W_{\chi^2} = F(\chi^2_{n_{eff}} > U(X, \hat{M})) = \int_{U(X,\hat{M})}^{+\infty} g(\chi^2_{n_{eff}}, n_{eff}(X, \hat{M})) d\chi^2_{n_{eff}}$$

i.e., the probability of finding a value of $\chi^2_{n_{eff}}$ bigger than or equal to $U(X, \hat{M})$. Here, we explicitly write where the dependence in the data ($X$) and in the parameters ($\hat{M}$) is.

5 CHECKING THE METHOD

In this section, we will test the whole method in the problem of one parameter estimation, but first, we will study the quality of our approximation to the distribution function of a $\chi^2$ with correlations. These two points will be done by means of Monte Carlo simulations. In order to do that, we have chosen the JB-IAC 33 GHz Interferometer (Melnikov et al. 1990) as the reference experiment.

This experiment is a two element interferometer, which operates at 33 GHz, at the Teide Observatory. It has two configurations, with angular resolutions $2^\circ 3 (\ell = 106 \pm 19)$, and $1^\circ 7 (\ell = 208 \pm 18)$, respectively. The window function in both configurations is very narrow, so the results are quoted in terms of total power inside the band (band power). The experiment has given measurements on the power spectrum on both scales (Dicker et al. 1999, Harrison et al. 2000), which are consistent with the Boomerang data (de Bernardis 2000). We have the likelihood analysis implemented for this experiment, so the comparison with the new method will be straightforward. In our analyses, we have used the compact configuration, and only one of the two channels (i.e., the real part of the complex visibility).

The CMB realizations have been done assuming the following values for the cosmological parameters: $n = 1$, $\Omega = 1$, $\Omega_c = 0.03$, $\Omega_k = 0.7$ and $H_0 = 75 km s^{-1} Mpc^{-1}$. For this model, the total power inside the window function (or band power) is $BP = 51.45 \mu K$ for the short configuration ($\ell = 109 \pm 18$). This number is related with $\sigma_{sky}$ by a conversion factor, which is obtained using the flat band power approximation (i.e. $BP = \ell (\ell + 1) C_\ell / 2 \pi$ constant inside the window function) in equation (3). For our instrument, this conversion factor is $BP = 5.44 \sigma_{sky}$, which gives $\sigma_{sky} = 9.46 \mu K$ for the previous model. For this experiment, the sensitivity in a 30s integration is given by $\sigma_{noise} \approx 250 \mu K/\sqrt{N_{days}}$, where $N_{days}$ is the number of observing days. Therefore, the signal-to-noise ratio is given by

$$\omega = \sigma_{sky}/\sigma_{noise}.$$

5.1 Our approximation to the distribution function

The first point is to check the validity of our approximation to the distribution function for a $\chi^2$ with correlations. We will study the case when the $x_i$ quantities entering in the $\chi^2$ follow a multivariate gaussian distribution. This is the case for an (ideal) CMB map, where the temperature at each pixel has two contributions, one coming from gaussian noise, and another one from the cosmological fluctuation field, which is supposed to be also gaussian. Using the CMB terminology from Section 2, we will study the distribution of the statistic

Figure 1. Distribution function for a $\chi^2$ with correlations with $N = 10$ terms. We show the histogram with the frequencies for the rescaled $\chi^2$, obtained from 1000 realizations, for four different cases, varying $w$ (signal-to-noise ratio). We use 10 bins of equal size to sample the distribution function. In all the figures, the dots represent the numbers coming from the realizations, and the error bars show their sampling error. The solid line is our approximation to the distribution function, using the value of $n_{eff}$ from the formula (shown within parentheses in the figure). It is also shown, using dot-dashed lines, the distribution function of a (rescaled) $\chi^2$ with $N = 10$. We can see the effect of the correlations as $w$ increases.

A Modified $\chi^2$-Test for CMB Analyses
Table 1. Values of $n_{\text{eff}}$ and $A$, for $N = 10$.  

| $w$  | Theoretical values$^a$ | Numerical values$^b$ |
|------|------------------------|----------------------|
|      | $n_{\text{eff}}$       | $A$                  |
|      | $n_{\text{eff}}$       | $A$                  |
| 0.34 | 8.4 0.84               | 8.4 0.84             |
| 0.69 | 6.7 0.67               | 6.8 0.67             |
| 1.37 | 5.0 0.50               | 4.8 0.47             |
| 2.74 | 3.9 0.39               | 3.8 0.37             |

$^a$ Computed using eqs. (24) and (25).
$^b$ Computed using 100 CMB realizations, from the numerical value of $\langle \chi^2 \rangle >$ and $\text{MS}(\chi^2)$.

\[ \chi^2 = \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2 + \sigma_{sky}^2} \]  

(26)

and we will compare it with the proposed approximation. This is a particular case of (3), when $P_1 = 1$. We will study in detail this case here, but our results are completely general. It should be noted that our proposal is exact, by definition, in the two limit cases of no correlations at all, and totally correlated points. The first one correspond to the definition of the $\chi^2$ distribution function, and the second one is the case of a $\chi^2$ with $N = 1$.

In Appendix C we present the formal aspect of the distribution function for (26) and we study in detail, analytically, the case $N = 2$. The cases with low $N$ turn out to be the critical ones, because the shape of the distribution function differs strongly from a gaussian. In the limit of high $N$, both our approximation and the real distribution function tend to a gaussian distribution (the same one, by definition), as a consequence of the Central Limit Theorem. Therefore, it is interesting to test our proposal for an intermediate range of values of $N$. We have done so, and we will present here, as an example, the case for $N = 10$.

We generate CMB realizations with noise, for a ten pixels map. From each simulation, we compute (23), and from the whole set of values obtained, we study the histogram with the frequencies, and we compare it with the proposed one, for several values of the signal-to-noise ratio. We show these results in Figure 4. In general, the asymptotic shape of the distribution is very well reproduced, and the largest differences always occur for low values of $\chi^2$. This is precisely the kind of approximation we need, because in a statistical analysis we usually are interested in the tail of the distributions.

We can see that the distribution of the $\chi^2$ with correlations among terms is compatible, inside the numerical precision, with an standard (rescaled) $\chi^2$, with an effective number of degrees of freedom, smaller than $N$.

We have also checked that the numerical values for $n_{\text{eff}}$ and $A$ are correctly given by equations (24) and (25). In Table 1 we compare the values obtained from the simulations with the predicted ones given by the theoretical formulae. Their difference is in all cases smaller than the sampling errors, so we conclude that our expressions give the correct values for these parameters.

5.2 Applying the method to one parameter estimation

We will now test our method in the problem of one parameter estimation. The idea is to compare, by means of Monte Carlo simulations, our method with the Maximum Likelihood on the full map, which is widely accepted as the optimal method for CMB analyses. We will consider in detail the problem of determining the total power measured by a given experiment, so our parameter will be $\sigma_{sky}^2$.

Both the $\chi^2_M$ and the ML are, by construction, almost unbiased methods for determining the total power of an experiment. In order to compare them, we have studied the power of each one. The power of an statistical method, when determining a certain parameter, is characterised by the RMS of the estimate of this parameter. The smaller this value, the more powerful is the method. To compute it, we will use Monte Carlo simulations for a fixed CMB sky plus simulated noise. We will consider different values for the signal-to-noise ratio, and for each one, we will obtain the RMS for each method. Finally, we will also compute the degree of coincidence of both methods, which can be parameterised through the quantity $\text{RMS}(\text{ML}, \chi^2_{M})$, defined as the RMS of the difference between their estimates.

For the experiment we are considering, we have generated simulations for an observation of declination $+41^\circ$, and R.A. range $8h-18h$, for a fixed CMB signal ($\sigma_{sky} = 9.46\mu K$). Each realization contains, for a single channel, 300 data points, with a pixel size of 0.5 degrees. Given that this experiment has a narrow window function, the band power is directly a measurement on the power spectrum.

The values of the $P_k$’s turn out to be not critical in this problem. The solution to the equation (12) is $P_k \approx 1$, $\forall k$, so we use here $P_k = 1$. The results of the realizations are summarised in Table 2. We conclude that, in this problem, the maximum likelihood on the full map and the $\chi^2_M$ method have the same power, within the uncertainty.

If we study the degree of coincidence of both methods, by computing the quantity $\text{RMS}(\text{ML}, \chi^2_{M})$, we conclude that both methods are highly coincident when the signal to noise is low. For example, for $w = 0.13$, the RMS of both methods is $\sim 1150\mu K^2$, and the dispersion between estimates is $590\mu K^2$, roughly half the RMS. So, not only the power of the methods is similar for low $w$, but also the estimates are. For high values of $w$ ($w \gtrsim 0.6$), both methods tend to be independent, in the sense that the degree of coincidence $\text{RMS}(\text{ML}, \chi^2_{M})$ approaches to the value of the RMS.

Once we have the (approximated) distribution function, we can determine the confidence region for one particular experiment. Usually, the size of this region is given by the 68% of the probability. Our error bars has to be interpreted in a frequentist way. That is, if we make lots of simulations, the true signal will lie inside the confidence region of each realization the 68% of the times. It is known that this value does not necessarily represent the 'error bars' defined in the usual Bayesian way, by treating the band-power likelihood function as a probability distribution.

As an example of application of our method, we have analysed the data from Dicker et al. (1999). These data correspond to declination $+41^\circ$, observed with the low resolution configuration ($\ell = 106 \pm 19$). The value obtained using
The total number of points where the CF was evaluated was 68% of the area of the likelihood around the peak, corresponding to ∆σ. In order to compute the Cℓ, we use a value for ∆σ = 20 μK. For any case, our result does not depend on this number. We have also checked that both methods give unbiased estimates, i.e., <E[σ^2_{sky}]> = σ^2_{sky}. We do not include the values for <E[σ^2_{sky}]> in the table for clarity.

We report here the degree of coincidence of both methods, i.e., the quadratic dispersion of the estimates from both ones. The values were obtained from 12 CMB plus noise realizations.

We have obtained the same estimate as the likelihood, but our confidence region is smaller. As we have pointed out, this probably is due to the fact that the confidence region has a different definition in both methods. In order to compare those confidence levels, we perform Monte Carlo simulations, using the measured signal and the experimental noise, and we obtain the equivalence between the confidence levels for both methods. We conclude that the region that contains the 68% of the area of the likelihood around the peak, corresponds to ~75% of the probability in a frequentist sense (i.e., that region contains the true signal the ~75% of the times). This explains why the likelihood gives us bigger error bars in this particular problem. In a general case, we will have to repeat this analysis for the likelihood estimate, in order to compare the sizes of the confidence levels.

### 6 ESTIMATING SEVERAL PARAMETERS

In the previous section, we have proved that our method, when constructed from the CF, has the same power as the likelihood when determining a single parameter (an overall normalisation). We now probe if this is true for a larger number of parameters.

For the case of several parameters estimation, the CF has proved to be a very good statistic in determining the power spectrum of the CMB (Szapudi et al. 2001d). In their paper, they obtain the Cℓ’s by a Gauss-Legendre integration of the CF. When applied to simulations of the Boomerang data (de Bernardis et al. 2004), the error bars for that method, coming from Monte Carlo simulations, are of the same order as the sample variance, which is the theoretical limit to the size of the error bars.

Here, we will apply our method to the COBE Differential Microwave Radiometer data in order to obtain the Cℓ’s in two cases. The first one, using the power law parameterisation of the angular power spectrum, in terms of the spectral index of the primordial spectrum, n (with P(k) ∝ k^n), and the normalisation parameter, Q_{r_{rms−PS}}. In this case, using our notation, we have M = {n, Q_{r_{rms−PS}}}. The dependence of the Cℓ’s in these parameters, for a pure Sachs & Wolfe spectrum (which dominates in the considered multipole range), is given by (Bond & Efstathiou 1987)

\[
C_\ell = \frac{4\pi}{5} Q_{r_{rms−PS}} \frac{\Gamma(\ell + \frac{n-1}{2})\Gamma(\frac{3-n}{2})}{\Gamma(\ell + \frac{3-n}{2})\Gamma(\frac{3}{2})} \left(\frac{2P^2}{\Omega_M^2}\right)
\]

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\]

The second case will be to estimate several Cℓ’s directly, i.e., M = \{C_\ell\}_{\ell=\ell_1}^{\ell=\ell_p}.

### 6.1 Estimating (n, Q_{r_{rms−PS}}) for the COBE data

The CF has been applied for COBE analyses of the (n, Q_{r_{rms−PS}}) parameters by other authors. In Hinshaw et al. (1996), the quadrupole normalisation is inferred using Monte Carlo-based gaussian likelihood analysis for a scale-invariant (n = 1) power-law spectrum. In Bunn, Hoffman, & Silk (1994) (hereafter BHS94), they determine n and Q_{r_{rms−PS}} as the best fit values to the computed CF. They show, by means of Monte Carlo simulations, that this method is not optimal for the determination of those parameters, because they obtain a large RMS when trying to recover them simultaneously (see Table 2 in that paper). Nevertheless, other estimators, such as the direct evaluation of the a_{ℓm}, give smaller RMS’s. We will use here...
the CF, but with our method, to probe whether we obtain good results.

In order to test our method with these two parameters, we perform Monte Carlo realizations of COBE like maps, using a scale invariant power spectrum \( n = 1 \) with a normalization \( Q_{\text{rms-PS}} = (18 \mu K)^2 = 324 \mu K^2 \). We will use the standard COBE pixelization of \( N = 6144 \) pixels (index level 6), in galactic coordinates. We include in our realizations the noise level corresponding to the combined 4-year COBE map of the three frequencies, using the weights quoted in Hinshaw et al. (1996a) (this map is referenced there as 31 + 53 + 90). The CF has been sampled using a 2.6° step, as it appears in that paper (that size correspond to the typical pixel size). Anyway, we have checked that our results are consistent when changing that step. In our calculation of the CF, we use a galactic cut \(|b| > 20°\).

We will use the \( P_k \) quantities given by the minimum of the function \( \text{RMS}(E[n]) \times \text{RMS}(E[Q_{\text{rms-PS}}]) \), as we have discussed in Section 3. Those \( \text{RMS}'s \) can be derived, using the linear approximation to the CF, from equation (18). In this problem, the \( R \) and \( J \) quantities are given by

\[
R = \left( \sum_i \frac{P_i^2}{\sigma^2(C(\theta_i))} \right) \left( \sum_i \frac{P_i f^2}{\sigma^2(C(\theta_i))} \right) - \left( \sum_i \frac{P_i f_1 f_2}{\sigma^2(C(\theta_i))} \right)^2
\]

\[
J_{k,1} = f_{k,1} \left( \sum_j \frac{P_j f_{j,2}^2}{\sigma^2(C(\theta_j))} \right) - f_{k,2} \left( \sum_j \frac{P_j f_j f_{j,2}}{\sigma^2(C(\theta_j))} \right)
\]

where \( n \) stands for \( n \) and \( Q \) for \( Q_{\text{rms-PS}} \). The equation for \( J_{k,2} \) can be obtained from \( J_{k,1} \), just interchanging \( 1 \leftrightarrow 2 \).

In order to check the previous expressions for the \( \text{RMS} \), we use 100 of the above mentioned realizations of COBE like maps \((n = 1; Q_{\text{rms-PS}} = 18 \mu K)\), and we analyse them using several sets of \( P_k \)'s. In this way, we can obtain the real value of the \( \text{RMS} \), and compare it with the number coming from the formula. The results are summarised in Table 3. In all cases, the theoretical numbers obtained from equation (18) are in agreement with the numerical results, so we conclude that the linear approximation to the true CF works well in computing the \( \text{RMS} \). The largest differences occur when we obtain a large \( \text{RMS} \), due to the fact that, in that case, fails the linear approximation to the CF.

The average values recovered for \( n \) and \( Q \) from Monte-Carlo simulations show that the estimator is unbiased, as we would expect. It should be noticed that, in Table 3, the effective number of degrees of freedom is quite small. In all cases, we obtain \( n_{\text{eff}} \lesssim 3 \), and we are using \( n = 70 \). The reason is that the CF contains long-range terms, coming from low multipoles \((\ell \sim 2)\). This fact reduces the degree of freedom drastically, so the choice of the \( P_k \) will be critical in this problem. The numbers obtained when we consider the whole CF and \( P_k = 1 \) are compatible with those in BHS94, but slightly better because we consider the noise of the 4-year COBE map. In that paper, they obtained, using the same galactic cut \((|b| > 20°)\), and the noise from the 2-year map, the values \( \text{RMS}(E[n]) = 0.96 \) and \( \text{RMS}(E[Q_{\text{rms-PS}}]) = 253 \mu K^2 \) (in our units). Nevertheless, we see that considering only the first points, and setting to zero the others, strongly reduces the \( \text{RMS} \) of the estimate, even below the values obtained when they do not consider noise and incomplete sky coverage (they have \( \text{RMS}(E[n]) = 0.36 \) and \( \text{RMS}(E[Q_{\text{rms-PS}}]) = 175 \mu K^2 \)).

Finally, we have applied our \( \chi^2 \)-test for the CF to the actual 4-year COBE data. Our estimates, from the analysis of the 31 + 53 + 90 map, using the galactic cut \(|b| > 20°\), a step of 2.6° to sample the CF, and the optimum set of \( P_k \)'s, are \( E[n] = 1.08 \), and \( E[Q_{\text{rms-PS}}] = 15.2 \mu K \), so our estimate of the parameters, using the true \( \text{RMS} \) from 100
realizations, will be \( n = 1.08 \pm 0.28 \), and \( Q_{\ell}^{1/2} = 15.2 \pm 3.5 \mu K \). This result has to be compared with the likelihood analysis using these data (see Hinshaw et al. [1996a], Table 1). They obtain for this map \( n = 1.25^{+0.26}_{-0.29} \), \( Q_{\ell}^{1/2} = 15.4^{+3.9}_{-2.9} \mu K \). The estimates from both methods are nearly the same, and now the error bars coming from the CF are compatible in size with those coming from the maximum likelihood method. For comparison, using no weights \((P_k = 1)\), we would obtain \( E[n] = 1.10 \pm 0.54 \), and \( E[Q_{\ell}^{1/2}] = (16.0 \pm 4.8) \mu K \), so we can see that using the \( P_k \)'s for this problem is essential.

### 6.2 Estimating band power spectra for COBE data

Finally, we will apply our method to obtain band power spectra for the COBE data. We have used the realizations from the previous subsections to compare with the likelihood analysis using these data (see Hinshaw et al. [1996a], see Table 2 in that paper). We have used exactly the same \( \ell \) range: four multipole bands between \( \ell = 2 \) and \( \ell = 40 \). Those bands are: \( 2 \leq \ell \leq 5 \); \( 6 \leq \ell \leq 10 \); \( 11 \leq \ell \leq 20 \); \( 21 \leq \ell \leq 40 \). Using those realizations, we have checked that the method is unbiased when applied to power spectrum estimation.

When applied to the combination of the 4-year COBE map, we obtain the results that are shown in Table 4. We quote the band power amplitudes in units of the quadrupole normalisation expected for a scale-invariant power-law spectrum within the specified range of \( \ell \). The quoted values for our method have been obtained from the optimal set of \( P_k \) for this problem. When compared with the ML data, we can see that the error bars are of the same order in both cases, as in the previous subsection. So we again obtain a method of a similar power to the likelihood on the pixel map.

The estimates from both methods are consistent in all bins, except the apparent inconsistency at the second one, where the two estimates differ in more than 3 times the size of one error bar. Nevertheless, the statistical significance of that deviation has to be computed as follows: given that we do not know the true value for the band power, when comparing two results we have to consider the difference of both estimates, and so we have to compute the variance of the difference. In this case, the difference is \( 16.7 \mu K - 9.8 \mu K \), and the RMS of the difference of those two estimates is \( \text{RMS} \sim \sqrt{2.6^2 + 2.2^2} \sim 3.4 \mu K \). Here we are assuming the fact that both methods are almost independent, following the results for the case of one parameter estimation, with signal-to-noise ratios of the order of 1. Therefore, we find a deviation of 2.3-sigma level, which corresponds to a fluctuation of 1 in 47 for a normal distribution. This can be understood given that the ML and the \( \chi^2_M \) are two different methods: the first is based on the full map, and the second on the correlation function. Therefore, the estimates will be different in general, although as we can see, both methods have similar power, so there is no reason to consider any one of them as “the estimate”.

Summarising, we have seen that it is possible with our method to perform an analysis with a similar power to the ML, even for the case of several parameters.

### 7 DISCUSSION AND CONCLUSIONS

In this paper we have presented a statistical method to analyse CMB maps. It consists in a variation of an standard \( \chi^2 \)-test for the case when we have correlated points. Here, our test has been constructed from the two-point correlation function, following the proposal from other authors.
that the CF contains all the relevant information concerning the cosmological parameter estimation. In this line, we propose a $\chi^2_M$ based on the CF, which is a different approach from the ‘usual $\chi^2$’ method (which uses the full covariance matrix $C$). Our proposal explicitly uses only the diagonal terms of the covariance matrix of the data, but we introduce certain weights, which now implicitly contain all the correlations. This approach has two important ‘computational’ advantages compared with the ‘usual $\chi^2$’, or with a likelihood based on the CF:

- we do not need to invert the covariance matrix, $C$; all the quantities (the $\chi^2_M$, $n_{eff}$, $A$ and the expression for the RMS) depend on $C$ directly.
- even more, if we have a problem with a low value for $n_{eff}$, the effective number of $P_k$ to use (i.e. the number of $P_k$ which are significantly different from zero) will be also small, typically, of order $O(n_{eff})$. So it is not even necessary to use all the terms of the diagonal.

These advantages are more important when comparing our method with the standard ML analysis on the full map. We do not need to invert the covariance matrix of the map ($N \times N$), and we only need to concentrate on a few numbers, so the problem is computationally accessible if we have to deal with large datasets. It it important to stress here that the $\chi^2_M$ is not an approximation to the ML on the full map, but a different approach (i.e. both methods will give different estimates and probability contours for a given problem). So the $\chi^2_M$ can be applied to any problem, but it has to be checked, by means of Monte Carlo simulations, that the method has a similar power to the maximum likelihood. As we have seen, this is the case for several CMB common problems (power spectrum estimation, and cosmological parameter estimation).

The largest computational effort in our method has to be done estimating the CF, which is a $\sim N^2$ operation. Nevertheless, there are estimators for the CF more efficient [Kashlinsky et al. 2001; Szapudi et al. 2001], so our procedure could be applied to current WMAP data, and PLANCK simulated data, but this will be treated in detail in future works.

Our method can be extended for general noise covariance matrices. We only need to compute $C_N(\theta)$ in the same way as the CF, and introduce it in equation (3). If we have the noise matrix, it is straightforward to obtain $C_N(\theta)$. But, if we do not have the noise matrix, we can obtain an estimate of the correlation function of the noise using MC simulations. This idea has been used recently by other authors [Szapudi et al. 2001]. It must be noted that if the noise changes substantially from pixel to pixel, then we would have to use weights in equation (1) to compute the CF in a more efficient way.

We have also presented an approximation which gives very accurately the distribution function for a $\chi^2$ constructed from a set of multivariate gaussian variables. This proposal can be extended to approximate the distribution function of any quantity made of a sum of squares, each of them distributed (exactly or approximately) following a gaussian distribution.

To conclude, we propose that, if we are interested in obtaining a certain set of parameters, $\hat{M}$, we can use an unbiased estimator of certain quantities depending on these parameters, provided that they contain all the relevant information to these parameters (in our case, we have used the CF at certain angles). From it, we may obtain, by varying the $P_k$’s, the best estimator of those parameters. In this paper, we have tested this proposal, using the two-point CF as the reference estimator, in CMB problems. For the case of one parameter estimation (the normalisation of the spectrum), our method, with the CF, turns out to be as powerful as the ML. When applied to COBE data, we have shown the importance of choosing the right set of $P_k$’s. In the optimum case, we obtain a value for the $RMS$ two or three times smaller than the one obtained without weighting at all. In this problem, the $P_k$’s are critical because the effective number the degrees of freedom is very small. The reason is that when we have strong correlations ($n_{eff}$ small compared with $n$), the structure of these correlations, which is encoded in the $P_k$’s, will be relevant, so there will be a considerable difference between the optimal weights and $P_k = 1$. When analysing CMB data which contain large scales (low multipoles), we are considering correlations over long distances. All the points are correlated with the others due to these low multipoles (quadrupole, octupole,...). In the case of Boomerang data (Szapudi et al. 2001), the effective number of degrees of freedom will be larger (if we throw away the large scales), so the $P_k$’s will be closer to 1, and a standard $\chi^2$ test based on the CF should produce good results.

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APPENDIX A: RELATIONSHIP BETWEEN THE USUAL $\chi^2$ AND THE $\chi^2_M$ FOR GAUSSIAN LINEAR PROBLEMS

In this Appendix we will study the relationship between the usual $\chi^2$ analysis (the standard approach for the case of correlated data points, which uses the full covariance matrix), and our approach, for gaussian problems in which the model depends linearly on the parameters, and with a covariance matrix independent of the parameters. This case is not exactly equal to the usual one in CMB analyses, but it is very close and is particularly suitable for illustration.

We will use here the following notation. Let $\hat{y} = (y_1, ..., y_n)$ be a $1 \times n$ matrix containing the $n$ data points, which, by hypothesis, are distributed following a multivariate gaussian distribution. Let $\hat{\alpha} = (\alpha_1, ..., \alpha_k)$ be a $1 \times k$ matrix whose elements are the $k$ parameters of the model. Let $\hat{x}$ be a $k \times n$ matrix, also given by the model. Their elements are defined so that the mean value of $\hat{y}$, $< \hat{y} >$, is given by the matrix multiplication $\hat{\alpha} \hat{x}$. Finally, let $\hat{M}$ be the covariance matrix of the problem, defined as $\hat{M} = < (\hat{y} - \hat{\alpha} \hat{x})^T (\hat{y} - \hat{\alpha} \hat{x}) >$.
where $T$ stands for the transpose. Using the previous definitions, the usual $\chi^2$ and our $\chi^2_M$ are given, respectively, by

\[
\chi^2 = (\hat{y} - \hat{\delta x})M^{-1}(\hat{y} - \hat{\delta x})^T \tag{A1}
\]

\[
\chi^2_M = (\hat{y} - \hat{\delta x})\hat{V}^{-1}(\hat{y} - \hat{\delta x})^T \tag{A2}
\]

where we have defined the matrix $\hat{V}$ using the diagonal of the covariance matrix, and our weights ($P_i$), in the following way: $\hat{V}_{ij} = M_{ij}/P_i$ for $i = 1, \ldots, n$, and $\hat{V}_{ij} = 0$ for $i \neq j$. It should be noted that the $\hat{V}$ matrix depends implicitly on the weights ($P_i$).

For this family of models under consideration, the optimum estimator is the maximum likelihood, which is given by

\[
L \propto \exp\left(-\frac{1}{2} \chi^2 \right) \det(M) \tag{A3}
\]

Until this point, we have not made use of the fact that the covariance matrix is independent of the parameters. If we use it now, from the last equation we have that the maximum likelihood reduces to the usual $\chi^2$ for this problem. The estimate for both methods is obtained by minimising the previous expressions with respect to the parameters, so we have

\[
E_1[\alpha] = (\hat{y}M^{-1}\hat{x})((\hat{x}M^{-1}\hat{x})^{-1}) \tag{A4}
\]

\[
E_2[\alpha] = (\hat{y}\hat{V}^{-1}\hat{x})((\hat{x}\hat{V}^{-1}\hat{x})^{-1}) \tag{A5}
\]

Hereafter in this section, we will use subscript 1 for the standard (usual $\chi^2$) method, and 2 for the $\chi^2_M$ method. We compute now the covariance matrices of the parameters, $\hat{W}$, which are given by

\[
\hat{W}_1 \equiv \text{Var}[(E_1[\alpha] - <E_1[\alpha]>)] = (\hat{x}M^{-1}\hat{x})^{-1} \tag{A6}
\]

\[
\hat{W}_2 \equiv \text{Var}[(E_2[\alpha] - <E_2[\alpha]>)] = (\hat{x}\hat{V}^{-1}\hat{x})^{-1}((\hat{x}\hat{V}^{-1}\hat{x})^{-1})^{-1} \tag{A7}
\]

Using this notation, the $MS$ for each parameter is given by the corresponding element in the diagonal of $\hat{W}$.

The following point is to compare the estimates of both methods. For the case of one parameter estimation, it can be argued that both method give the same estimate, and therefore have the same $RMS$. The argument is as follows: in this case, the estimate for both methods is a linear combination of the $n$ quantities $\hat{y}_i$. So it could be possible, in principle, to fix the $n$ quantities ($P_i$) to equal the coefficients in expressions A4 and A5. Given that for this particular problem the usual $\chi^2$ is the optimal method (i.e. the one with the minimum variance), and that the corresponding estimator is the only linear one for which this variance is obtained, those $P_i$ quantities which set equal the coefficients in A4 and A5 are exactly the same that would be obtained by minimisation of the $RMS$ of that parameter. We have checked this statement for the critical case where we have a $\chi^2$ with only $n = 2$ terms. In Figure A1 we present several particular examples, showing that for the set of $P_i$ quantities that minimise the $RMS$ for the $\chi^2_M$, we always obtain the same $RMS$ as in the case of the usual $\chi^2$. We have also checked that, for those values of the $P_i$, the estimates from both methods are exactly the same.

Let’s consider now the case of several ($k > 1$) parameters. For this problem, it is not possible in general to obtain a set of $P_i$ quantities which render the $RMS$ of the usual $\chi^2$. In any case, we have checked that it is always possible to choose those quantities to make the estimate for just one of the parameters exactly equal, and so its $RMS$. We have studied this problem in detail for the case of $n = 3$ terms in the $\chi^2$, and $k = 2$ parameters. The results are the following:

- if we choose to minimise the $RMS$ of only one parameter to find the optimal $P_i$ quantities, we can always make the estimate for that parameter exactly equal to the usual $\chi^2$. For those $P_i$ values, the estimator for the other parameter is very close to the optimum, in the sense that the $RMS$ for the other parameter at the most 10% bigger that the optimal one.
- if we minimise the product of the two $RMS$’s, we find in all cases that both estimates are close to the optimal ones, and the largest relative differences between $\hat{W}_1$ and $\hat{W}_2$ are smaller than $\sim 1%$.

Therefore, we can conclude that the criteria to obtain the $P_i$ quantities has an small ambiguity, in the sense that if we are interested in one parameter in particular, we should minimise the $RMS$ for that parameter only. In practice, this ambiguity is not relevant because, for this problem, the differences between the estimates and the obtained $RMS$ values are negligible. Therefore, we will maintain the original proposal of minimising the product of $RMS$’s, which in some sense is equivalent to minimise the average size of the confidence region. All these arguments can be applied to cases with $k > 2$ parameters.

![Figure A1](image.png)
APPENDIX B: USEFUL QUANTITIES FOR MULTIVARIATE GAUSSIAN DISTRIBUTIONS UP TO 4TH ORDER

The probability density function for a multivariate gaussian distribution of \( n \) variables (\( n \)-MGD), \( X = \{X_1, ..., X_n\} \), is given by

\[
g(X) = \frac{1}{(2\pi)^{n/2}|C|^{1/2}} \exp \left( -\frac{1}{2} (X - \bar{X})^T C^{-1} (X - \bar{X}) \right) \tag{B1} \]

where \( C \) is called the covariance matrix, \( |C| \) stands for its determinant, and \( \bar{X} \) is the mean of \( X \). The elements of \( C \) are given by

\[
C_{ij} = \langle X_i - \bar{X}_i, X_j - \bar{X}_j \rangle \tag{B2} \]

We define \( \sigma_i^2 = C_{ii} \). When computing the mean square of equation (3), or the \( C' \) matrix given in (11), we need to know the following quantities: \( \langle X_i^2, X_i^2, X_j \rangle \) and \( \langle X_i, X_j, X_k, X_l \rangle \). We will obtain them here. For a 2-MGD, we can obtain the quantity

\[
\langle X_1^2 X_2^2 \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2\pi \sqrt{|C|}} X_1^2 X_2^2 \times
\]

\[
\times \exp \left( -\frac{1}{2C}(X_1^2 \sigma_1^2 + X_2^2 \sigma_2^2 - 2C_{12}X_1X_2) \right) dX_1 dX_2 =
\]

\[
= \sigma_1^2 \sigma_2^2 + 2C_{12}^2 \tag{B3} \]

For a 3-MGD, we obtain

\[
\langle X_1^2 X_2 X_3 \rangle = 3|C|^2 (A_{22}A_{33} - A_{23}^2)(A_{11}A_{23} - A_{12}A_{13}) - 2|C|A_{23} \tag{B4} \]

where \( A_{ij} \) stands for the elements of the inverse of the \( C \) matrix. Using the same notation, for a 4-MGD, we obtain

\[
\langle X_1 X_2 X_3 X_4 \rangle = |C| \left( 2A_{12}A_{13}A_{24} - A_{14}A_{23} - A_{13}A_{24} - A_{12}A_{13}A_{24} \right) - 3|C|^2 \left( A_{12}A_{34}^2 + A_{14}A_{24}A_{33} - A_{14}A_{23}A_{34} - A_{12}A_{33}A_{44} - A_{13}A_{24}A_{34} + A_{13}A_{23}A_{44} + A_{11}A_{23}A_{24} + A_{11}A_{24}A_{34} - A_{11}A_{22}A_{34} + A_{11}A_{14}A_{22} - A_{12}A_{14}A_{23} - A_{12}A_{13}A_{24} \right) \tag{B5} \]

APPENDIX C: PROBABILITY DISTRIBUTION FUNCTION FOR A \( \chi^2 \) CONSTRUCTED FROM MULTIVARIATE GAUSSIAN VARIABLES

The moment generating function of the quadratic form \( \chi^2 = \sum_{i=1}^{n} \delta_i X_i^2 / \sigma_i^2 \), where the \( X = \{X_1, ..., X_n\} \) variables follow a \( n \)-MGD with zero mean (eq. [B1]), is given by (see Mathai 1982; Stuart & Ord 1994)

\[
G(t) = \prod_{j=1}^{n} \left( 1 - 2t\lambda_j \right)^{-1/2} \tag{C1} \]

In this equation, \( \lambda_1, ..., \lambda_n \) are the eigenvalues of the matrix \( \Sigma \), where \( C \) is the covariance matrix (B2), and \( \Sigma \) is defined as \( \Sigma_{ij} = (\delta_i/\sigma_i^2) \delta_{ij} \), being \( \delta_{ij} \) the Kronecker-delta. From this expression, the distribution function can be obtained by the Laplace inverse transform. Formally, we have

\[
\Psi(n)(\chi^2) = L^{-1}[G(-t)] \tag{C2} \]

where \( L^{-1} \) stands for the inverse Laplace transform (Gradshteyn & Ryzhik 1983, p.1142), and we use the notation \( \Psi_n(\chi^2) \) for the exact distribution function of the \( \chi^2 \). As an example, we will study in detail the case \( n = 2 \), comparing the exact distribution function with our approximation.

C1 Distribution function for \( n=2 \)

The analytical expression for the distribution function can be obtained using (Gradshteyn & Ryzhik 1983), eq. (17.13.9), p.1143, and the convolution theorem for Laplace transforms. We obtain

\[
\Psi_2(\chi^2) = \lim_{t \to 0} \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} \exp \left( -\frac{1}{4\beta}(\alpha + \beta) \right) I_0 \left( \frac{\chi^2}{4\beta} (\beta - \alpha) \right) d\chi \tag{C3} \]

where \( \alpha \) and \( \beta \) are the two eigenvalues of the \( \Sigma C \) matrix, and \( I_0 \) is the zero order \( J \) Bessel function.

For this problem, it is also easy to obtain the analytic expression for the \( k \)-order moment of the distribution, using the binomial expansion. We obtain

\[
< (\chi^2)^k > = \pi^{-1} \sum_{l=0}^{k} \left( \begin{array}{l} k \\ l \end{array} \right) P_l^2 P_{2-l}^2 \sigma_1^{2l} \sigma_2^{2-2l} \times
\]

\[
\times \sum_{j=0}^{l} \left( \begin{array}{l} 2l \\ 2j \end{array} \right) (C_{12})^{2l-2j} 2^{2j} |C| |\Gamma(j+1/2)\Gamma(k-j+1/2) | \tag{C4} \]

We compare both the distribution function and the \( k \)-order moments up to \( k = 4 \) with the values obtained using our approximation. The results quoted here correspond to the case \( P_1 = P_2 = 1 \), and \( \sigma_1^2 = \sigma_2^2 = 1 \), so \( C_{12} \) varies in the range \([0, 1]\). Nevertheless, the results are completely general.

For our problem, we can write \( \alpha = 1 + C_{12}, \beta = 1 - C_{12}, \) and \( n_{eff} = 2(1 + C_{12}^2)^{-1} \). In Figure C1 we present the \( \Psi_2 \) function for the value of \( C_{12} \) which gives us the maximum percentage difference between the exact and the approximated functions. This value corresponds to \( C_{12} = 0.825 \).

The largest percentage difference in the distribution function for this case is reached at \( \chi^2 = 0.388 \), and has a value of \( \approx 17\% \). In terms of the weights, we obtain for this point a difference of a 13\% ( \( W_{12}(true) = 0.73 \) , \( W_{12}(approx) = 0.70 \)). Nevertheless, the power of our approximation is that the largest differences always occur at low values of \( \chi^2 \). The asymptotic shape of the exact distribution function is well reproduced, as we need for a \( \chi^2 \) analysis.

To conclude, we show in Figure C1 the third and fourth order moments, both for the real distribution and the approximation, in the whole range of values for \( C_{12} \). By definition, the first and second moments are equal for the true and the approximate distribution. We see again that the approximation follows quite closely the true function, as we have found from the simulations in Section 5.1.
Figure C2. Skewness and kurtosis for a $\chi^2$ with $N = 2$ terms. We see that the approximation and the true distribution coincide in the two limit cases of $C_{12} = 0$ (no correlations) and $C_{12} = 1$ (totally correlated terms). For comparison, we also show these quantities for a gaussian distribution with the same mean and variance as the exact one (see text for details).

Figure C1. Distribution function for a $\chi^2$ with correlations, with $N = 2$ terms. We have used $P_1 = P_2 = 1$, and $\sigma_1 = \sigma_2 = 1$. We show the case $C_{12} = 0.825$, because for that value we have the largest percentage difference between the true function and our approximation, which is given by $n_{\text{eff}} = 1.2$ and $A = 0.60$. We can see that the largest differences occur at low values of $\chi^2$. The asymptotic values are well reproduced.

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