

# Shrinkage estimation of the power spectrum covariance matrix

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## ABSTRACT

We seek to improve estimates of the power spectrum covariance matrix from a limited number of simulations by employing a novel statistical technique known as shrinkage estimation. The shrinkage technique optimally combines an empirical estimate of the covariance with a model (the *target*) to minimize the *total* mean squared error compared to the true underlying covariance. We test this technique on  $N$ -body simulations and evaluate its performance by estimating cosmological parameters. Using a simple diagonal target, we show that the shrinkage estimator significantly outperforms both the empirical covariance and the target individually when using a small number of simulations. We find that reducing noise in the covariance estimate is essential for properly estimating the values of cosmological parameters as well as their confidence intervals. We extend our method to the jackknife covariance estimator and again find significant improvement, though simulations give better results. Even for thousands of simulations we still find evidence that our method improves estimation of the covariance matrix. Because our method is simple, requires negligible additional numerical effort, and produces superior results, we always advocate shrinkage estimation for the covariance of the power spectrum and other large-scale structure measurements when purely theoretical modelling of the covariance is insufficient.

**Key words:** methods: statistical – large-scale structure of the Universe.

## 1 INTRODUCTION

Large-scale structure statistics, especially power spectra, provide precise constraints on cosmological theories. Accurate measurements are now possible with large-volume surveys and advancing computational power. However, the measured power spectrum is not the only required ingredient for estimating cosmological parameters; the covariance matrix also carries a great deal of information that is vital for properly estimating parameter values and their confidence intervals. Observational effects such as the survey geometry, redshift-space distortions and non-linear clustering make theoretical modelling of the covariance matrix difficult, and often simulations are used to study them in detail. Covariance matrices estimated from a finite number of simulations will contain noise. Cosmological parameter estimation requires the inverse of the covariance matrix to properly weight the measurements. Matrix inversion is an inherently non-linear operation that is sensitive to the noise of all the elements. Chen & Szapudi (2006) showed that when the off-diagonal elements of a covariance matrix are excessively noisy it is better for parameter estimation to use a diagonal approximation of the covariance. This reduces the effects of noise, but ignores important information in the covariance.

Covariance matrices for large-scale structure measurements are often estimated using the unbiased empirical covariance matrix,  $\mathbf{S}$  (see equation 8), a close relative of the maximum-likelihood estimator,  $\mathbf{S}^{(ML)} = \frac{n-1}{n} \mathbf{S}$ . These estimators work well in the regime where the number of repeat observations,  $n$ , is much greater than the number of parameters measured for each observation,  $p$ . However, in the regimes where  $n \sim p$  or  $n \ll p$ , the covariance matrix estimates become ill-conditioned and unstable during inversion, which is necessary for optimal weighting of the data. This is an indication that these estimators do not produce good approximations of the true underlying covariance matrix in these regimes. Efron (1982) provides some insight into the difference between maximum-likelihood as a *summarizer* and as an *estimator*. Maximum-likelihood is an excellent summarizer of data in the sense of trying to represent the important statistical information about a dataset in a small set of numbers. Though maximum-likelihood is asymptotically optimal for estimation in the limit of infinite data, the use of this summary of information for the purpose of making estimates with a finite set of data is not always the best option. Stein (1956) proved that one can construct estimators in high-dimensional ( $d \geq 3$ ) inference problems that outperform maximum-likelihood estimators in the sense of minimizing the *total* mean squared error. Maximum-likelihood produces the best estimates of individual parameters, but the alternatives can often reduce the error on many of the parameters while only slightly increasing the error on a few, resulting in an overall improvement. Stein (1956) also showed that the

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maximum-likelihood estimator has the best performance among estimators that transform correctly under translation, implying that any estimator that outperforms maximum-likelihood will necessarily involve an arbitrary choice.

Schäfer & Strimmer (2005) employ a method known as *shrinkage estimation* to construct covariance matrices for functional genomics measurements in the  $n \ll p$  regime. Their technique optimally combines a high-dimensional estimate that has little or no bias with a low-dimensional estimate that may be biased but has much less variance. The result minimizes the total mean squared error, which is the sum of bias (squared) and variance. They argue that their method can also perform some amount of regularization, resulting in a covariance matrix that has a full set of positive-definite eigenvalues and is well-conditioned (i.e. the ratio of the largest to smallest eigenvalue is not so large that inversion becomes unstable). They employ a lemma from Ledoit & Wolf (2003) to analytically calculate the optimal linear combination of the low- and high-dimensional estimates.

In this paper, our goal is to provide a simple recipe for using shrinkage estimation to improve the covariance matrix of the matter power spectrum from a limited number of simulations over the ubiquitous sample covariance estimator. Our method aims to reduce the total noise while retaining as much information about real covariance in the simulations as possible. Shrinkage estimation achieves this by optimally combining a theoretical model with the empirical estimate. We will assess the improvements our method offers by examining the performance of the covariance matrices through inversion and use in cosmological parameter estimation. Although we focus on the matter power spectrum, the shrinkage technique is relevant for many studies in large-scale structure and cosmology.

The outline of this paper is as follows. In Section 2, we introduce shrinkage estimation and describe its application to covariance matrices. Section 3 applies the shrinkage technique to several toy problems before moving to a more complicated example involving galaxy clustering. We describe our technique for measuring matter power spectra from  $N$ -body simulations in Section 4. In Section 5, we construct several estimates of the power spectrum covariance matrix and compare their performance by estimating cosmological parameters. Finally, we review our results, make recommendations and discuss future directions of this project in Section 6.

## 2 SHRINKAGE ESTIMATION

### 2.1 The method

Much of this section summarizes the introduction to shrinkage estimation given in Schäfer & Strimmer (2005). Suppose we are estimating a vector  $\psi$  (of length  $p$ ) from a set of  $n$  measurements using two different models. One of the models has many free parameters and produces an estimate,  $\mathbf{u}$ , with little (or no) bias, but the variance may be significant due to the number of free parameters. The second model (called the *target*) has many fewer (or no) free parameters and produces an estimate,  $\mathbf{t}$ , which will have smaller variance but may be biased. We construct a new estimate,  $\mathbf{u}^*$ , from a linear combination of these two models, given by

$$\mathbf{u}^* = \lambda \mathbf{t} + (1 - \lambda) \mathbf{u}, \quad (1)$$

where  $\lambda \in [0, 1]$  is called the *shrinkage intensity*. The question now becomes how to choose  $\lambda$  in an optimal way. A common way to

optimize an estimator is to minimize the expected mean squared error, given by the risk function

$$R(\lambda) = \left\langle \sum_{i=1}^p (u_i^* - \psi_i)^2 \right\rangle, \quad (2)$$

where the angle brackets indicate the expectation value. Ledoit & Wolf (2003) introduced an analytic solution for the optimal shrinkage intensity,  $\lambda^*$ . Prior to this solution, shrinkage estimation was much less practical because numerically complicated and expensive methods were necessary to find the optimal shrinkage intensity. The analytic solution is

$$\lambda^* = \frac{\sum_{i=1}^p \text{Var}(u_i) - \text{Cov}(t_i, u_i) - \text{Bias}(u_i)(t_i - u_i)}{\sum_{i=1}^p (t_i - u_i)^2}, \quad (3)$$

where  $\text{Var}$ ,  $\text{Cov}$  and  $\text{Bias}$  are the true variance, covariance and bias, respectively. For a practical estimator, Schäfer & Strimmer (2005) suggest estimating  $\hat{\lambda}^*$  as:

$$\hat{\lambda}^* = \frac{\sum_{i=1}^p \widehat{\text{Var}}(u_i) - \widehat{\text{Cov}}(t_i, u_i) - \widehat{\text{Bias}}(u_i)(t_i - u_i)}{\sum_{i=1}^p (t_i - u_i)^2}, \quad (4)$$

where  $\widehat{\text{Var}}$ ,  $\widehat{\text{Cov}}$  and  $\widehat{\text{Bias}}$  are the unbiased sample estimates of  $\text{Var}$ ,  $\text{Cov}$  and  $\text{Bias}$ , respectively. The Bias term can be ignored if  $\mathbf{u}$  is an unbiased estimator.

### 2.2 Application to covariance matrices

We now specialize the shrinkage estimation technique to covariance matrices. Suppose we have  $n$  sets of data and we measure a data vector  $\mathbf{x}$  of length  $p$  for each of them. Let  $x_i^{(k)}$  be the  $k$ th (of  $n$  total) observation of the  $i$ th (of  $p$  total) element of the data vector. The estimated empirical mean is given by  $\bar{x}_i = \frac{1}{n} \sum_{k=1}^n x_i^{(k)}$ . We define

$$W_{ij}^{(k)} = (x_i^{(k)} - \bar{x}_i)(x_j^{(k)} - \bar{x}_j), \quad (5)$$

$$\overline{W}_{ij} = \frac{1}{n} \sum_{k=1}^n W_{ij}^{(k)}, \quad (6)$$

and write the unbiased empirically estimated covariance matrix of the data,  $\mathbf{S}$ , as

$$S_{ij} = \widehat{\text{Cov}}(x_i, x_j) = \frac{n}{n-1} \overline{W}_{ij}. \quad (7)$$

Explicit substitution results in the usual

$$S_{ij} = \frac{1}{n-1} \sum_{k=1}^n (x_i^{(k)} - \bar{x}_i)(x_j^{(k)} - \bar{x}_j). \quad (8)$$

Similarly we can estimate the covariance of the elements of the covariance matrix of the data, given as

$$\widehat{\text{Cov}}(S_{ij}, S_{lm}) = \frac{n}{(n-1)^3} \sum_{k=1}^n (W_{ij}^{(k)} - \overline{W}_{ij})(W_{lm}^{(k)} - \overline{W}_{lm}), \quad (9)$$

with the variance of an individual entry given by  $\widehat{\text{Var}}(S_{ij}) = \widehat{\text{Cov}}(S_{ij}, S_{ij})$ . For shrinkage estimation we let  $\mathbf{S}$  take the role of  $\mathbf{u}$  and supply a target covariance matrix  $\mathbf{T}$  to take the role of  $\mathbf{t}$ . The optimal shrinkage intensity and resulting covariance matrix  $\mathbf{C}$  are given by

$$\hat{\lambda}^* = \frac{\sum_{i,j} \widehat{\text{Var}}(S_{ij}) - \widehat{\text{Cov}}(T_{ij}, S_{ij})}{\sum_{i,j} (T_{ij} - S_{ij})^2}, \quad (10)$$

$$\mathbf{C} = \hat{\lambda}^* \mathbf{T} + (1 - \hat{\lambda}^*) \mathbf{S}. \quad (11)$$

If the  $\hat{\lambda}^*$  estimate is greater than one, then  $\hat{\lambda}^* = 1$  is enforced, implying that only the target matrix is used. If the  $\hat{\lambda}^*$  estimate is less than zero, then  $\hat{\lambda}^* = 0$  is enforced, implying that only the empirical covariance matrix is used. The numerator of equation (10) implies that as the variances of the elements of  $\mathbf{S}$  decrease (e.g. approaching the  $n \gg p$  regime) the shrinkage estimate smoothly approaches the empirical covariance. The denominator in equation (10) also ensures that if the chosen target matrix is very different from the empirical covariance then the estimator will tend to the empirical covariance. Thus an inappropriate choice of target should not make the final results any worse, but there will be little gain in efficiency.

The  $\text{Cov}(T_{ij}, S_{ij})$  term in the numerator of equation (10) accounts for the fact that  $\mathbf{S}$  and  $\mathbf{T}$  are estimated from the same data. If  $\mathbf{T}$  is fixed then the term is zero. If some of the elements of  $\mathbf{T}$  are taken directly from  $\mathbf{S}$  then the  $\text{Cov}$  term exactly cancels the  $\widehat{\text{Var}}$  term and those elements do not affect the estimate of  $\hat{\lambda}^*$ . Table 2 of Schäfer & Strimmer (2005) shows a variety of worked examples for common targets that may or may not depend on the empirically estimated covariance. In their examples, they ignore moments of higher order than  $\widehat{\text{Var}}(S_{ij})$ .

### 3 TOY EXAMPLES

Before tackling large-scale structure measurements, we present the application of shrinkage estimation to toy models. In Section 3.1, we employ shrinkage to estimate the mean of a noisy vector. For that example, we can calculate the expected shrinkage intensity analytically. In Section 3.2, we present a toy example of covariance estimation.

#### 3.1 Estimating the mean of a noisy vector

In our first toy example of the shrinkage technique, we will estimate the mean of a vector from a set of noisy realizations using the formalism from Section 2.1. Given an input mean vector,  $\psi$ , the distribution for an element of the noisy realization is  $X_i = N(\psi_i, \sigma_i^2)$ , a normal distribution with mean  $\psi_i$  and variance  $\sigma_i^2$ . The  $i$ th element (of  $p$  total) of the  $k$ th realization (of  $n$  total) is written as  $x_i^{(k)}$ , and our high-dimensional estimate of the mean is given by

$$\mathbf{u} = \frac{1}{n} \sum_{k=1}^n \mathbf{x}^{(k)}. \quad (12)$$

Given a fixed target,  $t$ , we will calculate the expected value for the optimal shrinkage intensity,  $\langle \lambda^* \rangle$ , as given by equation (3). If we assume the numerator and denominator are uncorrelated we can write

$$\langle \lambda^* \rangle = \left\langle \frac{\sum_{i=1}^p \text{Var}(u_i)}{\sum_{i=1}^p \langle (t_i - u_i)^2 \rangle} \right\rangle \approx \frac{\sum_{i=1}^p \langle \text{Var}(u_i) \rangle}{\sum_{i=1}^p \langle (t_i - u_i)^2 \rangle}. \quad (13)$$

From our definitions we know that

$$\langle x_i^{(k)} \rangle = \psi_i, \quad (14)$$

$$\langle x_i^{(k)} x_j^{(l)} \rangle = \psi_i \psi_j + \delta_{ij} \delta_{kl} \sigma_i^2 \quad (15)$$

which we can use to find the expectation values of our estimators

$$\langle u_i \rangle = \left\langle \frac{1}{n} \sum_{k=1}^n x_i^{(k)} \right\rangle = \psi_i, \quad (16)$$

$$\langle u_i^2 \rangle = \left\langle \frac{1}{n} \sum_{k=1}^n x_i^{(k)} \frac{1}{n} \sum_{l=1}^n x_l^{(l)} \right\rangle = \psi_i^2 + \frac{1}{n} \sigma_i^2. \quad (17)$$

Fixing the values for  $\psi_i$ ,  $\sigma_i$  and  $t_i$  to be  $\psi$ ,  $\sigma$  and  $t$ , respectively, we predict the shrinkage intensity to be

$$\langle \lambda^* \rangle \approx \frac{\sigma^2}{n(t - \psi)^2 + \sigma^2}. \quad (18)$$

This formula displays the behaviour we expect. As  $n$  becomes large,  $\langle \lambda^* \rangle$  approaches zero and we will rely mostly on the empirical estimate of the mean. As  $t$  approaches  $\psi$ ,  $\langle \lambda^* \rangle$  approaches unity as we have chosen the perfect target. We can also calculate the expected mean squared errors for the high-dimensional, low-dimensional and shrinkage estimators and find they are given by

$$\langle \text{MSE}(\mathbf{u}) \rangle = p \frac{\sigma^2}{n}, \quad (19)$$

$$\langle \text{MSE}(\mathbf{t}) \rangle = p(\psi - t)^2, \quad (20)$$

$$\langle \text{MSE}(\mathbf{u}^*) \rangle = p \left[ \langle \lambda^* \rangle^2 (\psi - t)^2 + (1 - \langle \lambda^* \rangle^2) \frac{\sigma^2}{n} \right], \quad (21)$$

respectively.

We generated simulations to check the validity of our analytic predictions. Each simulation starts by generating the  $n$  realizations  $\mathbf{x}^{(k)}$ . The sample mean  $\mathbf{u}$  is calculated for the set of realizations and used with the target  $\mathbf{t}$  to generate the shrinkage estimate  $\mathbf{u}^*$ . The shrinkage intensity,  $\hat{\lambda}^*$ , for the set of realizations is calculated using equation (4) and jackknife resampling of equation (12) is used to estimate the  $\widehat{\text{Var}}(u_i)$  term. We generated 100 simulations for each set of input parameters we tested and the results are shown in Table 1. The results of our simulations match the analytical predictions reasonably well and also show that the shrinkage estimator outperforms both the empirical estimate and the target in a mean squared error sense.

#### 3.2 Estimating the covariance

Our second toy model applies the formalism of Section 2.2 for shrinkage estimation of a covariance matrix. In this case, the analytical predictions would be prohibitively tedious, so we present only the results of simulations. Each simulation starts by generating the realizations,  $\mathbf{x}^{(k)}$ , where the distribution of each element is  $X_i^{(k)} = N(0, \sigma^2)$ . From each set of realizations, we construct two estimates of the covariance matrix. The Monte Carlo (MC) method uses the standard empirical covariance estimate as given by equation (8). We also compute a shrinkage version of the Monte Carlo estimator (MC+S) from equation (11) using the identity matrix as a target. The two estimators are compared by inspecting the eigenvalue spectra and by computing the mean squared error between the estimate and the known true covariance matrix, which is  $\sigma^2 \mathbf{I}$  where  $\mathbf{I}$  is the identity matrix. The mean squared error between two matrices  $\mathbf{A}$  and  $\mathbf{B}$  is given by the Frobenius norm of the difference,

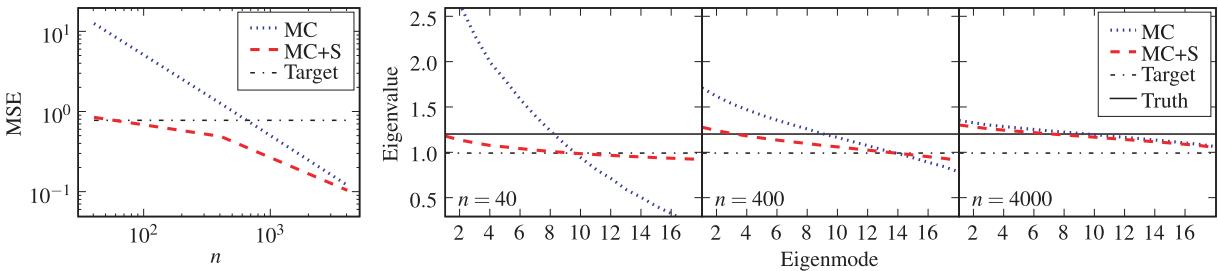
$$\|\mathbf{A} - \mathbf{B}\|_F^2 = \sum_{i,j} |A_{ij} - B_{ij}|^2. \quad (22)$$

For our simulations we fixed  $p = 18$  and  $\sigma = 1.1$  and compared the performance of the covariance estimators as a function of the number of realizations,  $n$ . We ran 100 simulations for each value of  $n$  and averaged the results. For  $n = 40, 400$  and  $4000$ , the shrinkage intensities were  $\hat{\lambda}^* = 0.92 \pm 0.08$ ,  $0.61 \pm 0.06$ ,  $0.136 \pm 0.006$ . Fig. 1 shows the results for the two estimators as well as the results when only using the target. The shrinkage estimator gives a mean squared error that is equal to or less than both the empirical covariance and the target by itself for all  $n$ . The eigenvalue spectrum for

**Table 1.** Shrinkage estimation of the mean of a noisy vector.

| Input  |          |     |     |     | Output                      |                   |                         |  |                                       |  |                                     |                                   |                            |
|--------|----------|-----|-----|-----|-----------------------------|-------------------|-------------------------|--|---------------------------------------|--|-------------------------------------|-----------------------------------|----------------------------|
| $\psi$ | $\sigma$ | $t$ | $n$ | $p$ | $\langle \lambda^* \rangle$ | $\bar{\lambda}^*$ | $\Delta\bar{\lambda}^*$ | $\langle \text{MSE } (\mathbf{u}^*) \rangle$ | $\overline{\text{MSE}}(\mathbf{u}^*)$ | $\langle \text{MSE } (\mathbf{u}) \rangle$ | $\overline{\text{MSE}}(\mathbf{u})$ | $\langle \text{MSE } (t) \rangle$ | $\overline{\text{MSE}}(t)$ |
| 1.1    | 1.0      | 1.0 | 100 | 100 | 0.50                        | 0.509             | 0.003                   | 0.50   | 0.52                                  | 1.00                                       | 1.02                                | 1.00                              | 1.00                       |
| 1.2    |          |     |     |     | 0.20                        | 0.205             | 0.0002                  | 0.80   | 0.80                                  | 1.00                                       | 0.99                                | 4.00                              | 4.00                       |
|        | 0.9      |     |     |     | 0.45                        | 0.459             | 0.003                   | 0.45   | 0.46                                  | 0.81                                       | 0.80                                | 1.00                              | 1.00                       |
|        |          | 0.9 |     |     | 0.20                        | 0.201             | 0.0003                  | 0.80   | 0.80                                  | 1.00                                       | 1.00                                | 4.00                              | 4.00                       |
|        |          |     | 50  |     | 0.67                        | 0.696             | 0.008                   | 0.67   | 0.71                                  | 1.00                                       | 2.00                                | 1.00                              | 1.00                       |
|        |          |     |     | 50  | 0.50                        | 0.529             | 0.01                    | 0.25   | 0.26                                  | 0.50                                       | 0.49                                | 0.50                              | 0.50                       |

Results of simulations to test shrinkage estimation of the mean of a noisy vector. The first-five columns are the input values for the simulations. The first row gives the fiducial values and subsequent rows only indicate parameters that were varied. The remaining columns list analytically predicted (indicated by  $\langle \cdot \rangle$ ) and measured (where  $\bar{a}$  and  $\Delta a$  indicate the sample mean and standard deviation for  $a$ ) quantities from the outputs of the simulations. We used 100 simulations for each set of input parameters. See Section 3.1 for an explanation of the parameters and quantities.



**Figure 1.** Comparison of the Monte Carlo (MC) and shrinkage (MC+S) estimates for the toy-model covariance from Section 3.2. The plot at left-hand side shows the mean squared error (MSE) between the estimate and the known input covariance as a function of the number of realizations,  $n$ . Results using only the target are also shown. The plots at right-hand side show the eigenvalue spectra for the covariance estimators using different numbers of realizations,  $n$ . The known true eigenvalue spectrum and the eigenvalues of the target are also shown. All plots represent the averages of 100 simulations for each number of realizations,  $n$ .

the shrinkage estimator is also closer to the correct spectrum than for the empirical covariance at fixed  $n$ . This indicates that using the shrinkage estimator is in some sense equivalent to using more simulations.

#### 4 SIMULATIONS AND MEASUREMENTS

We divide the Hubble Volume (Evrard et al. 2002)  $\Lambda$  cold dark matter ( $\Lambda$ CDM) simulation into 4096 subvolumes, each with a sidelength of  $187.5 \text{ Mpc } h^{-1}$ . We measure the power spectrum in each subvolume using a simple code that implements the same basic algorithm as presented in Szapudi et al. (2005) and employs a fast Fourier transform (FFT). The FFT was performed on a  $64^3$  grid and the power spectrum was measured in 18 logarithmically spaced bins from  $k = 0.0367$  to  $k = 0.920$ . For plotting and model comparison purposes, we calculate the average  $k$  from the actual modes in each bin for the bin centres. The power spectrum calculated on a pixelized grid is the product of the true power spectrum with (square of) the Fourier transform of the pixel window function. Our measured power spectrum can be written as  $P_{\text{meas}}(\mathbf{k}) = P(\mathbf{k})/|\tilde{W}_p(\mathbf{k})|^2$  where the Fourier transform of the pixel window function,  $\tilde{W}_p$ , is given by

$$\tilde{f}(k) = \frac{\sin[\pi k/(2\pi/L)]}{\pi k/(2\pi/L)}, \quad (23)$$

$$|\tilde{W}_p(\mathbf{k})|^2 = \tilde{f}^2(k_x)\tilde{f}^2(k_y)\tilde{f}^2(k_z), \quad (24)$$

and  $L$  is the length of the side of a pixel. Our pixels are  $2.93 \text{ Mpc } h^{-1}$  on each side.

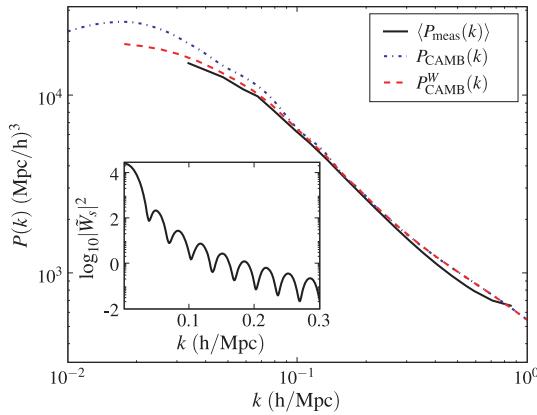
We used CAMB (Lewis, Challinor & Lasenby 2000) to calculate a model transfer function and matter power spectrum using cosmological parameter values to match the Hubble Volume (Evrard et al. 2002)  $\Lambda$ CDM simulation:  $\Omega_m = 0.3$ ,  $\Omega_\Lambda = 0.7$ ,  $h = H_0/100 \text{ km s}^{-1} \text{ Mpc}^{-1} = 0.7$ ,  $\Omega_b h^2 = 0.0196$  and  $n_s = 1$ . We normalized the resulting power spectrum,  $P_{\text{CMB}}(k)$ , to have a (linear)  $\sigma_8 = 0.9$  and then applied the non-linear HALOFIT (Smith et al. 2003) correction. Thus the normalization matches linear theory for large scales (low  $k$ ), but the shape includes non-linear clustering corrections at smaller scales (higher  $k$ ).

The measured power spectrum is the convolution of the true power spectrum with the squared Fourier transform of the survey window function. When testing a model for the power spectrum we must perform this convolution before comparing it to our measurement. The convolved power spectrum,  $P^W$ , is given by

$$P^W(k) = \int d\mathbf{q} P(k - \mathbf{q}) |\tilde{W}_s(\mathbf{q})|^2, \quad (25)$$

where  $P$  is the input (theoretical) power spectrum. Because the survey is the same shape as our pixels we can write the (normalized) survey window function in terms of the pixel window function as  $|\tilde{W}_s|^2 = (L/2\pi)^6 |\tilde{W}_p|^2$ , where  $L$  is now the survey sidelength. To simplify the convolution we used the spherically averaged transform of the window function (calculated via Monte Carlo) and reduced the convolution of the spherically symmetric power spectrum to a two-dimensional integral, given by

$$P^W(k) \approx 2\pi \int_0^\infty dq q^2 |\tilde{W}_s(q)|^2 \int_{-1}^1 dx P\left(\sqrt{k^2 + q^2 - 2kqx}\right). \quad (26)$$



**Figure 2.** Plot of the input theoretical power spectrum ( $P_{\text{CAMB}}$ ), the theoretical power spectrum convolved with the survey window function ( $P_{\text{CAMB}}^W$ ), and the averaged power spectrum measured from all of the subvolumes ( $\langle P_{\text{meas}} \rangle$ ). Inset shows the spherically averaged survey window function.

In practice the integral over  $dx$  was done with Romberg integration and the integration over  $dq$  was performed with the extended trapezoidal rule at the  $k$  values where we had calculated the spherically averaged  $|\tilde{W}_s(\mathbf{k})|^2$ . Power spectrum values inside the integral were evaluated using cubic spline interpolation in  $(\log k, \log P)$  and power law extrapolation at low and high  $k$ . Fig. 2 shows the input theoretical power spectrum ( $P_{\text{CAMB}}$ ), the convolved model power spectrum ( $P_{\text{CAMB}}^W$ ), and the average of the measured power spectra from all of the subvolumes ( $\langle P_{\text{meas}} \rangle$ ). The inset shows the spherically averaged survey window function.

We wish to evaluate our covariance estimates in the context of cosmological parameter fitting. Given the relatively small volume of each of our subvolumes we decided to fit for only the power spectrum normalization in each subvolume, parameterized by  $\sigma_8$  (linear). We write the log-likelihood (for a fixed covariance matrix) as

$$d(\sigma_8) = P_{\text{meas}}(k) - \left( \frac{\sigma_8}{0.9} \right)^2 P_{\text{CAMB}}^W(k, \sigma_8 = 0.9), \quad (27)$$

$$\log \mathcal{L}(\sigma_8) \propto -\frac{1}{2} \mathbf{d}^T \mathbf{C}^{-1} \mathbf{d} = -\frac{1}{2} \chi^2, \quad (28)$$

where  $\mathbf{C}$  is the covariance matrix being tested. We use  $\sigma_8$  to fit for the amplitude of the power spectrum in the linear regime, and we assume that the difference in shape in the non-linear regime is minimal for values of  $\sigma_8$  that are close to our fiducial model of  $\sigma_8 = 0.9$ . We numerically find the maximum-likelihood value,  $\hat{\sigma}_8$ , and define the upper and lower  $1\sigma$  error bars,  $\pm \Delta$ , where

$$\log \mathcal{L}(\hat{\sigma}_8 \pm \Delta) - \log \mathcal{L}(\hat{\sigma}_8) = -1/2.$$

Our likelihood analysis assumes that the bandpower measurements of the power spectrum are normally distributed. For most of our bandpowers this is a good approximation, but there are several for which an offset lognormal distribution (Bond, Jaffe & Knox 2000) would be more accurate. This could cause some bias in our recovered value of  $\hat{\sigma}_8$ , but it should not affect our assessment of the relative performance of different covariance estimators. The covariance matrices for the normal and offset lognormal cases are related by a change of variables.

**Table 2.** Statistics of  $\hat{\sigma}_8$  and error-bar estimates.

| C                       | $\langle \hat{\sigma}_8 \rangle$ | $\sigma_{\hat{\sigma}_8}$ | $\langle \Delta \rangle$ | $\sigma_\Delta$ |
|-------------------------|----------------------------------|---------------------------|--------------------------|-----------------|
| Reference               | 0.870                            | 0.041                     | 0.042                    | 0.002           |
| Monte Carlo             | 0.853                            | 0.088                     | 0.031                    | 0.006           |
| Monte Carlo Target Only | 0.870                            | 0.042                     | 0.014                    | 0.002           |
| Monte Carlo + Shrinkage | 0.872                            | 0.042                     | 0.027                    | 0.008           |
| Jackknife               | 0.790                            | 0.102                     | 0.015                    | 0.005           |
| Jackknife Target Only   | 0.869                            | 0.044                     | 0.013                    | 0.003           |
| Jackknife + Shrinkage   | 0.850                            | 0.047                     | 0.021                    | 0.007           |

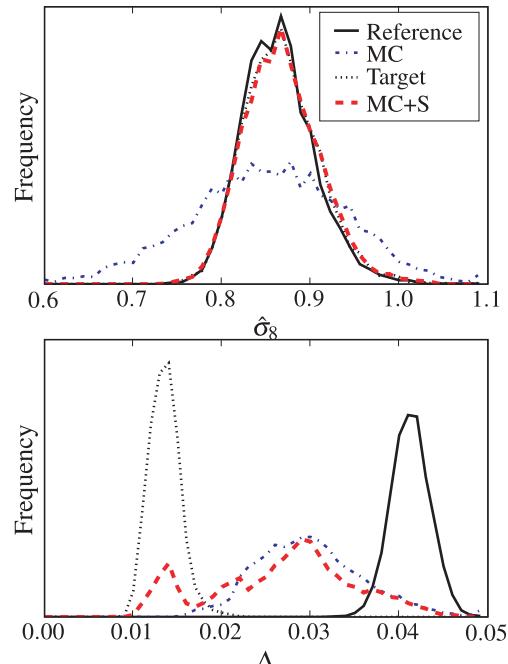
The mean and standard deviation of the estimates of the maximum-likelihood estimate,  $\hat{\sigma}_8$ , and the  $1\sigma$  error bar,  $\Delta$ , using different methods to estimate the covariance matrix.

## 5 COVARIANCE MATRIX ESTIMATES

In this section we compare the performance of several techniques for estimating the covariance matrix of our power spectrum measurements. As a baseline comparison we calculate the covariance matrix from all 4096 subvolumes using equation (8). For each method of covariance matrix estimate we measure  $\hat{\sigma}_8$  and  $\Delta$  using the power spectra measured from the subvolumes and show the distributions of the  $\hat{\sigma}_8$  and  $\Delta$  values. The mean and standard deviations of those quantities are presented in Table 2.

### 5.1 Reference

As a reference, we estimate the covariance matrix of our power spectrum measurement by applying equation (8) to our measurements from all 4096 subvolumes. There are  $18 \times 19/2 = 171$  independent elements in the covariance matrix, thus we are in the regime where we have many more realizations than elements to be estimated and the usual covariance estimator should give reasonable results. The solid-black line in Fig. 3 is a histogram of the results of



**Figure 3.** (Area normalized) distributions of maximum-likelihood value,  $\hat{\sigma}_8$ , and error bar,  $\Delta$ , estimates for the Reference, Monte Carlo (MC), Monte Carlo Target only (Target), and the Monte Carlo + Shrinkage (MC+S) covariance matrix estimates.

estimating  $\hat{\sigma}_8$  using the reference covariance matrix and the power spectra measured from each of the 4096 subvolumes. The upper panel shows the distribution of  $\hat{\sigma}_8$  and the lower panel shows the distribution of the error-bar estimates (absolute value of both upper and lower). The mean and standard deviation of these histograms are presented in Table 2. The agreement between the width of the best-fitting distribution,  $\sigma_{\hat{\sigma}_8}$ , and the mean error-bar estimate,  $\langle \Delta \rangle$ , indicates that the covariance matrix is properly estimating the likelihood distribution. The width of the error-bar distribution,  $\sigma_\Delta$ , is small, indicating that the error-bar estimate is usually very close to the correct value. The mean of the maximum-likelihood estimates,  $\langle \hat{\sigma}_8 \rangle$ , is 0.870 instead of our known input value of 0.9, but we know that our modelling of the power spectrum into the non-linear regime is not perfect so this small offset is not worrisome for our purposes. For the remainder of this section we assume that the results using the reference covariance matrix are a good approximation to those that would be obtained using the true underlying covariance matrix. See Section 6 for further discussions.

## 5.2 Monte carlo

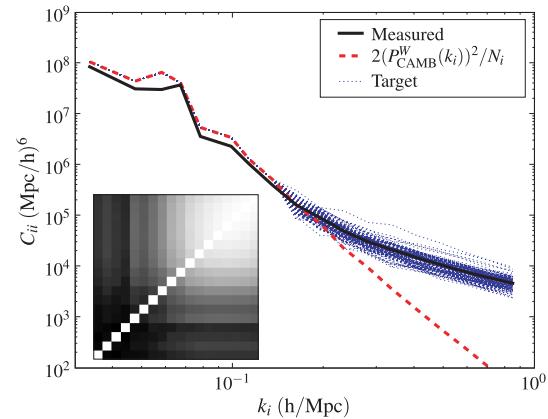
Next we test covariance matrices estimated with equation (8) but using a small number of subvolumes, which we call the Monte Carlo method. We use sets of 40 (randomly chosen, non-overlapping) subvolumes to test the regime where we have more simulations than diagonal elements of the covariance matrix (18), but fewer simulations than independent elements (171). From 4096 subvolumes, we can create 102 separate covariance matrix estimates. To obtain smooth histograms in Fig. 3, we test each covariance matrix estimate against 40 randomly chosen  $P(k)$  measurements from other subvolumes. The statistics in Table 2 are calculated using one randomly chosen  $P(k)$  measurement per covariance matrix. The statistics do not depend on how many randomly chosen  $P(k)$  measurements are used for each covariance matrix estimate. The upper panel of Fig. 3 shows that the distribution of  $\hat{\sigma}_8$  is too wide, indicating that a parameter analysis using a covariance matrix estimated with this method will often return a value far from the mean. The lower panel of Fig. 3 shows that the error bar is typically underestimated by  $\sim 25$  per cent. The width of the estimated error bar distribution is also much wider than for the reference covariance matrix estimate. These effects are the result of using a very noisy estimate of the covariance matrix.

## 5.3 Monte carlo + shrinkage

Our first test of the shrinkage approach is to apply shrinkage estimation to the Monte Carlo method described in the previous section. First we need to choose a target covariance matrix,  $\mathbf{T}$ . In linear theory we expect the covariance matrix of the power spectrum to be diagonal. Off-diagonal terms arise in practice from the survey window function and non-linear clustering effects. We use a diagonal target matrix to simulate a situation where we have some idea about the structure of the covariance matrix but we know our model is not exact. Our target matrix takes the form

$$T_{ij} = \begin{cases} 0 & i \neq j \\ 2 [P_{\text{CMB}}^W(k_i)]^2 / N_i \langle k_i \rangle \leq 0.14 h \text{ Mpc}^{-1} \\ S_{ii} & \langle k_i \rangle > 0.14 h \text{ Mpc}^{-1}, \end{cases} \quad (29)$$

where we use a different method in the linear and non-linear regimes. For bins in the linear regime we use our convolved model for the power spectrum,  $P_{\text{CMB}}^W(k_i)$ , and the number of  $k$  modes in each bin,  $N_i$ , to predict the covariance (e.g. Hamilton, Rimes &



**Figure 4.** Plot of the diagonal elements of the reference covariance matrix estimated from all of the subvolumes, of a linear theory model for the covariance, and of the 102 target matrices for the Monte Carlo + Shrinkage estimates. Inset shows the reference correlation matrix in a linear stretch.

Scoccimarro 2006). In the non-linear regime, we use the diagonal of the empirically estimated covariance from the 40 subvolumes. Fig. 4 shows the diagonal elements of the reference covariance matrix, the linear theory model and the 102 target matrices. Inset is the reference correlation matrix,  $R_{ij} = C_{ij} / \sqrt{C_{ii} C_{jj}}$ , showing that the covariance matrix is strongly diagonal until well into the non-linear regime. Our results are robust to changes in the non-linear cut-off by several bins in either direction.

We calculate the optimal shrinkage intensity,  $\hat{\lambda}^*$ , for each of the 102 Monte Carlo estimates,  $\mathbf{S}$ , according to equation (10). We apply the  $\text{Cov}(T_{ij}, S_{ij})$  term to the diagonal elements of  $\mathbf{T}$  that are taken from  $\mathbf{S}$ . We find values for  $\hat{\lambda}^*$  distributed evenly between 0.1 and 1.0 (see Fig. 7). We produce each of our 102 new estimates of the covariance matrices,  $\mathbf{C}$ , from a linear combination of  $\mathbf{S}$  and  $\mathbf{T}$  according to equation (11). We perform the same tests as described in section 5.2 and compare the results in Fig. 3 and Table 2. The most striking result is that the maximum-likelihood estimates,  $\hat{\sigma}_8$ , follow a very similar distribution to that for the reference matrix, indicating that the parameter values are now correctly estimated. The error bars are still underestimated, but the distribution is very similar to that for the normal Monte Carlo estimator.

Fig. 3 and Table 2 also show results using only the diagonal target. The values of  $\hat{\sigma}_8$  follow the correct distribution, indicating that the estimated parameter values are fine, but the error bars are much more severely underestimated. This is expected because our target matrix is diagonal and we are using information from far enough into the non-linear regime to know that we are missing some important covariance. It is now clear that the estimated error-bar distribution of the shrinkage estimator is a combination of the Monte Carlo and target distributions. The shrinkage intensity can serve as a proxy for whether the estimated error bars are likely to be similar to those for the Monte Carlo or the target. See Section 6 for further discussions.

In summary, the shrinkage of the empirically estimated covariance against our target matrix outperforms either matrix by itself. Using just the empirically estimated covariance brings in too much noise which causes error in the estimation of  $\hat{\sigma}_8$  itself. Using only the diagonal target mitigates the noise problems, but ignores important covariance. The shrinkage estimator uses the best aspects of both, keeping the part of the covariance that is well estimated but drastically reducing the total amount of noise.

#### 5.4 Jackknife

Recently a resampling technique known as the jackknife method has been used to estimate covariance matrices for large-scale structure measurements from the data set itself. The method works by dividing the data volume into  $n$  cells of roughly the same size and recalculating the measurement  $n$  times, each time with a different cell left out. The variance between the measurements can be adjusted to try and calculate the variance corresponding to the entire volume. In practice one replaces equation (5) with

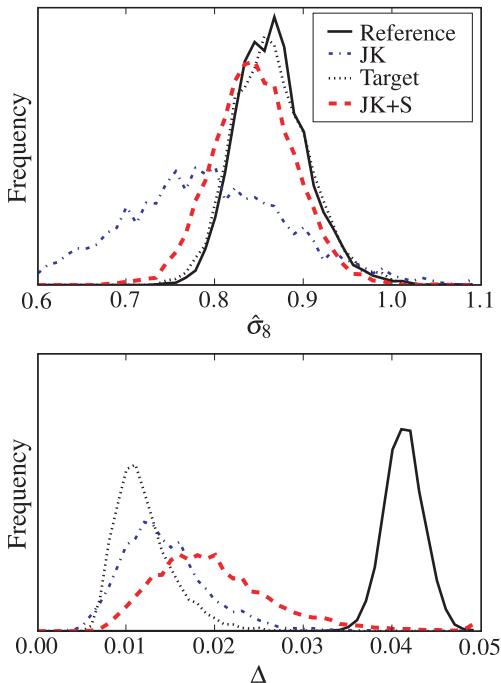
$$W_{ij}^{(k)} = \frac{(n-1)^2}{n} \left( x_i^{(k)} - \bar{x}_i \right) \left( x_j^{(k)} - \bar{x}_j \right), \quad (30)$$

and then calculates the covariance matrix with equation (7), resulting in the usual

$$S_{ij} = \frac{n-1}{n} \sum_{k=1}^n \left( x_i^{(k)} - \bar{x}_i \right) \left( x_j^{(k)} - \bar{x}_j \right). \quad (31)$$

We divided each subvolume into  $3^3 = 27$  cells and modified our code to calculate the power spectrum with one cell removed. Our code incorporates a volume correction, the lowest order edge correction in Fourier space. For each of the 4096 subvolumes, we estimate  $\hat{\sigma}_8$  and  $\Delta$  using the power spectrum and the jackknife covariance matrix from the same subvolume. The results are compared to the reference case in Fig. 5 and listed in Table 2.

The distribution of  $\hat{\sigma}_8$  is much wider than for the reference covariance matrix, indicating that the noise in the covariance estimate causes incorrect parameter estimation. This is similar to the result for the Monte Carlo method. The jackknife estimates of  $\hat{\sigma}_8$  also peak at a noticeably lower value than for the reference covariance, though the two histograms are in roughly  $1\sigma$  agreement given the width of the distribution for the jackknife case. The error bars estimated in the jackknife case are typically underestimated by a factor of almost three compared to the reference covariance matrix and



**Figure 5.** (Area normalized) distributions of maximum-likelihood value,  $\hat{\sigma}_8$ , and error bar,  $\Delta$ , estimates for the Reference, Jackknife (JK), Jackknife Target only (Target) and the Jackknife + Shrinkage (JK+S) covariance matrix estimates.

nearly an order of magnitude compared to the actual width of the jackknife distribution of  $\hat{\sigma}_8$ .

#### 5.5 Jackknife + shrinkage

Our final method of estimating the covariance matrix applies shrinkage to the jackknife estimator to see if we can achieve enhanced robustness. We use the same method to construct a target matrix as described in Section 5.3, using the diagonal of the jackknife estimated covariance matrix in the non-linear regime. We calculate the shrinkage intensity,  $\hat{\lambda}^*$ , and covariance estimate for each of the 4096 covariance matrices as described in Section 2.2, but substituting equation (30) for equation (5) throughout. We find values for  $\hat{\lambda}^*$  distributed evenly between 0.0 and 1.0 (see Fig. 7). We run the same tests as described in Section 5.4 and the results are shown in Fig. 5 and Table 2.

As with the shrinkage version of the Monte Carlo estimator, the shrinkage version of the jackknife estimator shows significant improvement in the actual estimated parameter,  $\hat{\sigma}_8$ . However, the central value and width are not quite as good as for the reference case. There is some improvement in the estimation of the error bar, though the error bars are still systematically underestimated by a factor of roughly two compared to the reference.

Fig. 5 and Table 2 also show the results of estimating  $\hat{\sigma}_8$  and  $\Delta$  using only the diagonal targets used in the shrinkage version of the jackknife estimator. Again, the diagonal target matrix does well for estimating  $\hat{\sigma}_8$  due to the lack of noise, but it gives the worst estimates of the error bars.

In this case, the shrinkage version of the jackknife estimator did the best job of estimating the error bars, and it was only slightly worse than the diagonal approximation at recovering the distribution of  $\hat{\sigma}_8$ . Again, shrinkage estimation is doing an excellent job of keeping information about covariance while reducing the total noise.

## 6 DISCUSSIONS AND CONCLUSIONS

We have introduced shrinkage as a technique for improving estimates of the covariance matrix for power spectrum measurements. We tested our methods on dark matter simulations and showed improvement over the empirically estimated covariance matrix from a limited number of simulations or jackknife resamplings. In order to clearly assess the potential improvement from using shrinkage estimation, we chose an intentionally difficult scenario where traditional methods of estimating the covariance were unlikely to yield satisfactory results. All of these methods would perform better if we allowed ourselves more simulations per Monte Carlo estimate or if we did not push as far into the non-linear clustering regime. The shrinkage technique would still outperform the other methods, but perhaps the differences would be less obvious.

A good estimate of the covariance matrix of a power spectrum measurement is essential for extracting cosmological information via parameter fitting. Including the covariance between different bins is a good step towards properly estimating the confidence intervals on cosmological parameters. However, the increased number of free parameters of a full-covariance estimate (as opposed to a diagonal approximation) can cause the covariance estimate to be noisy if only a relatively small number of simulations are available. This noise can adversely affect the estimate of the parameter itself. A diagonal approximation to the covariance can be more easily constrained with a limited number of simulations, leading to better estimates of the parameter values. However, the confidence

intervals can be severely underestimated if actual covariance is ignored. Neither alternative is appealing. If a similar measurement was performed with the two-point correlation function, the Fourier dual of the power spectrum, a full-covariance matrix is especially important as bins will be strongly correlated, even in the linear clustering regime. Realistic survey geometries will also cause additional covariance on large scales for the power spectrum.

Shrinkage estimation is an optimal way of combining a model with many degrees of freedom and a model with few degrees of freedom to minimize the total error on the covariance estimate. In our example, the shrinkage versions of the Monte Carlo and jackknife estimators clearly outperformed their counterparts without shrinkage, with the shrinkage version of the Monte Carlo estimator producing the best results. The lemma of Ledoit & Wolf (2003) as employed by Schäfer & Strimmer (2005) allows a mathematically and numerically simple way of calculating the optimal shrinkage intensity. This means that there is minimal addition work required to use a shrinkage version of a covariance estimator. Shrinkage estimation can result in a massive improvement in the limit of a small number of simulations and will not adversely affect the covariance estimate in the limit of a large number of simulations. For these reasons, we always recommend the use of the shrinkage versions of covariance estimators in all regimes.

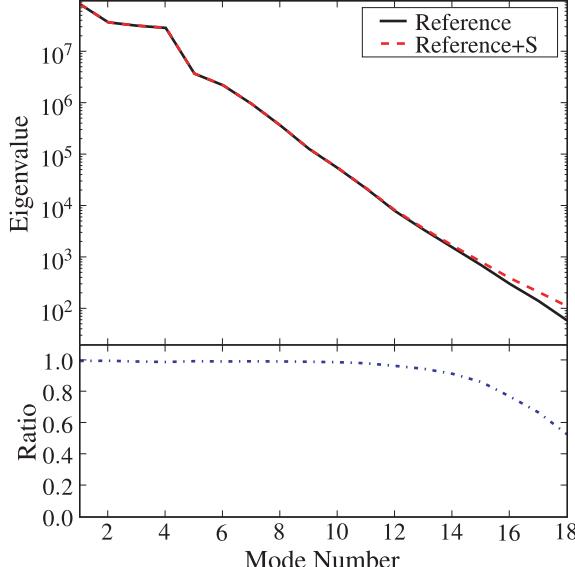
We briefly investigated the effects of shrinkage estimation in the limit of a large (though not infinite) number of simulations. We applied shrinkage estimation to our reference covariance matrix estimated from all 4096 subvolumes using the target from equation (29) and found an optimal shrinkage intensity  $\hat{\lambda}^* = 0.0096$ . This number is the same order as the relative noise we expect in each element of the matrix,  $1/\sqrt{4096} = 0.0156$ . We then calculated the eigensystems of both matrices. The dot products of the corresponding eigenvectors always exceeded 0.996, indicating that they are essentially identical. The (sorted) eigenvalue spectra are shown in Fig. 6. The eigenvalues are the same to within 1 per cent for the first 10 eigenmodes. After the 10th eigenmode the eigenvalues

from the reference matrix become increasingly smaller compared to the shrinkage version. By the final eigenmode the difference is  $\sim 50$  per cent. The shrinkage version of the reference matrix should be a more accurate estimate of the true underlying covariance matrix. The non-linear nature of matrix inversion can cause errors  $\gg 1$  per cent even when individual elements of the covariance matrix are estimated to  $\sim 1$  per cent. We ran our parameter estimation test using the shrinkage version of the reference matrix and found that  $\langle \hat{\sigma}_8 \rangle$  moved by less than 0.5 per cent. This is small compared to the width of the distribution, which is  $\sim 5$  per cent. The average minimum  $\chi^2$  did improve from 52.4 to 41.1 with the shrinkage version of the covariance matrix, though this is still large for  $18 - 1 = 17$  degrees of freedom. The remaining discrepancy is dominated by bias from problems with modelling the power spectrum into the non-linear regime or power loss in the simulation at smaller scales due to low resolution, not a grossly inaccurate estimate of the variances. The amplitude is mainly sensitive to smooth eigenmodes, which have large eigenvalues, so there is little change in the estimated value. Parameters that are more sensitive to the shape of the power spectrum may be more sensitive to the lower eigenvalue modes and show more than a 1 per cent change. The impact of these differences could be estimated with a study of the information content of the power spectrum covariance in terms of cosmological parameter confidences (i.e. Neyrinck & Szapudi 2007), but this is beyond the scope of this paper.

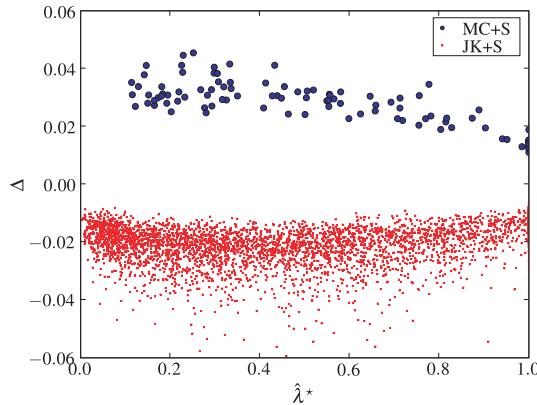
We employed a very simple diagonal target matrix in this paper, but better targets can clearly improve the efficiency of the shrinkage technique. A much more realistic model for covariance on small scales could be constructed using the halo model. For realistic measurements it may also be advantageous to model some of the effects of survey geometries, redshift-space distortions and clustering bias. Targets that depend on a small number of free parameters may be very useful for some of these effects (e.g. clustering bias). Targets can also be developed for a wide range of large-scale structure measurements in addition to the power spectrum. The exploration of more sophisticated targets is beyond the scope of this paper and is left to future studies.

Ultimately, we would like to develop more diagnostics of the performance of our covariance estimates. Fig. 7 shows the estimated error bar,  $\Delta$ , as a function of the shrinkage intensity,  $\hat{\lambda}^*$ , for the shrinkage versions of the Monte Carlo and jackknife estimators. There is clearly some correlation for the shrinkage version of the Monte Carlo estimator, so knowledge of  $\hat{\lambda}^*$  could help one gauge how much the error bars are underestimated. The exploration of such diagnostics should proceed as better targets are developed.

The difficulties in estimating the power spectrum covariance matrix in the context of making precision cosmological measurements are of even greater concern for higher-order clustering measurements. Higher-order clustering measurements have a configuration space with more degrees of freedom than the power spectrum (or two-point correlation function). Even a lower resolution measurement will have more bins and a much larger covariance matrix, and noise will cause larger deviations in the inverse matrix. Theoretical modelling of the covariance matrix for an  $N$ -point correlation function generally involves correlations up to the  $2N$ -point (e.g. Szapudi 2008), making the models more uncertain. The ability to optimally combine simulations and a theoretical model with a small number of free parameters will make dramatic improvements. Shrinkage estimators could also be used for covariance matrices of measurements outside of large-scale structure, including the cosmic microwave background power spectrum. Finally, we note that Section 2.1 makes no specific references to covariance matrices and



**Figure 6.** Plot of the (sorted) eigenvalue spectrum for the Reference covariance matrix, empirically estimated from 4096 subvolumes, and the shrinkage of that reference covariance matrix against our diagonal target (Reference+S). The lower panel shows the ratio of these eigenvalue spectra.



**Figure 7.** Plot of estimated error bar,  $\Delta$ , as a function of the shrinkage intensity,  $\hat{\lambda}^*$ , for the shrinkage versions of the Monte Carlo (MC+S) and jackknife (JK+S) methods. For clarity all of the MC+S error bars are plotted as positive and all of the JK+S as negative.

that shrinkage is a general estimation technique. We are studying additional applications of shrinkage estimation for cosmological measurements.

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