The Effect of Covariance Estimator Error on Cosmological Parameter Constraints

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Extracting parameter constraints from cosmological observations requires accurate determination of the covariance matrix for use in the likelihood function. We show here that uncertainties in the elements of the covariance matrix propagate directly to increased uncertainties in cosmological parameters. When the covariance matrix is determined by simulations, the resulting variance of the each parameter increases by a factor of order $1 + N_b/N_s$ where $N_b$ is the number of bands in the measurement and $N_s$ is the number of simulations.

I. INTRODUCTION

Upcoming galaxy surveys\cite{15} aim to measure cosmological parameters at the percent level. Achieving this lofty goal will require overcoming a number of well-known theoretical systematics: bias in translating the matter distribution to the galaxy distribution\cite{15},\cite{17}, uncertainties in the predictions for the dark matter spectrum\cite{5,9}, baryonic contamination of the power spectrum in weak lensing\cite{10,11}, outliers in photometric redshifts\cite{12}, and theoretical systematics: bias in translating the matter density to the CMB power spectrum\cite{8,9}, mis-estimating the covariance matrix\cite{14}, and uncertainties in parameter errors. We then focus on the case when the sample covariance is estimated from simulations and dub parameter errors. We then focus on the case when the covariance matrix is estimated from simulations and dub the additional uncertainty covariance estimator error.

Covariance estimator error is straightforward to compute when the measurements $x$ are Gaussian distributed, the dependence of the covariance on cosmology is neglected, and the sample covariance estimator is used. Then, the covariance estimator error enhances the variance of every parameter by a factor of order $(1 + N_b/N_s)$ with $N_s$ the number of simulations used for the estimate. We go beyond the Gaussian case with the example of the weak lensing power spectrum, where we use existing simulations to compute the covariance estimator error. The degradation is very similar to the Gaussian case. We conclude by tabulating the covariance estimator error for existing surveys.
**II. SIMPLE EXAMPLE**

Suppose the set of measurements $x_i^d$ each is designed to measure a single parameter $x$, and consider the case when the covariance matrix is diagonal, so $C_{ij} = \delta_{ij}\sigma_i^2$. Then, the inverse of the covariance matrix $\Psi = C^{-1}$ is also diagonal with elements $\Psi_i = \sigma_i^{-2}$. In this simple case, we need to minimize

$$\chi^2(x) = \sum_i (x_i^d - x)^2 \Psi_i;$$

(2)

in so doing, we arrive at an estimate for $x$:

$$\hat{x} = \frac{\sum_i x_i^d \Psi_i}{\sum_i \Psi_i}. \quad (3)$$

The uncertainty on this estimate can be obtained by computing $(\langle \hat{x} - x \rangle^2)$, which leads to

$$\Delta x^2 = \frac{\sum_{ij} \Psi_i \Psi_j (x_i^d x_j^d)}{[\sum_i \Psi_i]^2} - x^2.$$

(4)

The angular brackets around $x_i^d x_j^d$ refer to an average over the distribution from which the $x_i^d$ are drawn. This distribution is assumed to be Gaussian with mean $x$ and variance $C_i^i$, where $^i$ indicates this is the true variance, not necessarily equal to the covariance $C$ (or its inverse $\Psi$) used to estimate $x$. Therefore, the variance of our estimator is

$$\Delta x^2 = \frac{\sum_i C_i^i \Psi_i^2}{[\sum_i \Psi_i]^2}.$$

(5)

If we had access to the true covariance matrix, then $C_i^i \Psi_i$ would be equal to unity and the sum in the numerator would be simply equal to that in the denominator, leaving the variance on our estimator to be $\Delta x^2 = 1/\sum_i \Psi_i$, which, in the limit of equal errors on each of the $N_b$ measurements, reduces to the standard $\sigma^2/N_b$.

Let’s consider though the impact of not knowing exactly what the covariance matrix is. Write

$$\Psi_i = \Psi_i^i + \Delta \Psi_i.$$

(6)

Then the error on $x$ is

$$\Delta x^2 = \frac{1}{\sum_j (\Psi_j^i + \Delta \Psi_j)^2} \sum_i C_i^i [\Psi_i^i + \Delta \Psi_i]^2.$$

(7)

Taylor expanding leads to

$$\Delta x^2 = \frac{1}{\Psi_i^i} + \text{new terms}. \quad (8)$$

The first set of these new terms are linear in $\Delta \Psi$. These lead to fluctuations in the error, meaning that the error we assign to our estimator will be wrong \[15\]. However, $\Delta \Psi$ is just as likely to fluctuate up as it is down, so the linear terms do not lead to a systematic bias on the error, only an uncertainty on the error. The second set of terms is quadratic in $\Delta \Psi$, and this set is more pernicious as it leads to a larger error in the estimator of $x$. That is, the estimated value of $x$ will be drawn from a distribution with a systematically larger variance than if the covariance matrix were known exactly.

Let’s compute this error in our simple model. The second order terms are

$$\Delta x^2 = \left. \frac{\sum_i \Delta \Psi_i^2}{[\sum_i \Psi_i]^2} + \sum_i C_i^i \Delta \Psi_i^2 \right|_{\text{second order}}$$

Suppose the fluctuations in the covariance matrix are such that \[15\]

$$\langle \Delta \Psi_i \Delta \Psi_j \rangle = \alpha \delta_{ij} \Psi_i^2.$$  

(10)

Then, the first term in Eq. (9) will be of order $N_b^{-2}$. The second on the other hand is of order $N_b^{-1}$ so it dominates and we are left with

$$\Delta x^2 = \frac{1 + \alpha}{\sum_i \Psi_i}.$$ 

(11)

If the uncertainty in the covariance matrix is driven by a finite number of simulations $N_s$, then we will see that $\alpha \approx 1/N_s$. We call the new term covariance estimator error, and it simply increases the errors on our estimate of $x$. Although one can drive this error down by running many simulations, the number of (expensive) simulations required in the era of percent level measurements is apparently greater than a hundred, difficult but manageable. Unfortunately, this very simple case of diagonal errors does not capture the full danger of the situation. In the more realistic case that the covariance matrix is not diagonal, $\alpha$ scales as $N_b/N_s$, so if there are measurements in a large number of bands, it will become harder and harder to reduce the covariance error.

**III. COVARIANCE ERROR IN THE GENERAL CASE**

We now generalize this treatment in three ways: First, we allow the covariance matrix to have off-diagonal elements, so $\Psi_{ij} = C_{ij}^{-1}$ is no longer just a diagonal matrix. Second, we allow for more than one parameter; instead of $x$, we envision fitting for a full set of parameters, $p_\alpha$. Finally, the measurements are likely not direct estimates of the parameters. If we call the data in $N_b$ bands $x_i^b$, then we want to extract values of the cosmological parameters $p_\alpha$ from these measurements. The theoretical predictions for these measurements, call them $x_i$, depend on the parameters: $x_i = x_i(p_\alpha)$, usually in some complicated way. For simplicity, we shift all parameters so the true values are equal to 0. Then the predictions $x_i(p = 0)$ are equal to the true values $x_i^t$. The measured values will not be
exactly equal to \( x^t \), but we expect the mean over many realizations to equal to the true set:

\[
\langle x^d_i \rangle = x^t_i \tag{12}
\]

and the spread is given by the covariance matrix

\[
C^{-1}_{ij} \equiv \langle (x^d_i - x^t_i)(x^d_j - x^t_j) \rangle. \tag{13}
\]

where again superscript \(^t\) denotes the true value. We will extract the best fit values of the parameters by minimizing Eq. \( \mathbf{11} \). Note again that the covariance matrix here is not equal to the true one; this is the effect we want to explore: what happens to our parameter extraction when the covariance matrix is wrong?

Let’s decompose the \( \chi^2 \) into two pieces:

\[
\chi^2(p) = \chi_0^2(p) + \Delta \chi^2(p) \tag{14}
\]

where

\[
\chi_0^2 \equiv \sum_{ij} (x^d_i - x_i(p))(C^{-1})^{-1}_{ij}(x^d_j - x_j(p)) \tag{15}
\]

and the term due to the uncertainty in the covariance matrix is

\[
\Delta \chi^2 \equiv \sum_{ij} (x^d_i - x_i(p))\Delta \Psi_{ij}(x^d_j - x_j(p)) \tag{16}
\]

where

\[
\Delta \Psi_{ij} = C^{-1}_{ij} - (C^t)^{-1}_{ij}. \tag{17}
\]

Both \( \chi_0^2 \) and \( \Delta \chi^2 \) are functions of \( p \), and we can Taylor expand both around \( p = 0 \). Apart from an irrelevant constant, the standard piece is

\[
\chi_0^2(p) \simeq -2 \sum_{ij} \frac{\partial x_i}{\partial p_\alpha} (C^{-1})^{-1}_{ij}(x^d_j - x^t_j)p_\alpha + F_{\alpha \beta} p_\alpha p_\beta \tag{18}
\]

where

\[
F_{\alpha \beta} = \frac{1}{2} \frac{\partial \chi_0^2}{\partial p_\alpha \partial p_\beta} \simeq \sum_{ij} \frac{\partial x_i}{\partial p_\alpha} (C^t)^{-1}_{ij} \frac{\partial x_j}{\partial p_\beta}. \tag{19}
\]

The approximate equality on the second line follows since operating with the derivative twice on \( x^d \) leaves a factor of \( x^d_i - x_i \), which averages to zero. Before turning to the effects of the new piece, it is worth recalling the derivation for the mean and variance of the estimator for \( \hat{p}_\alpha \) using the standard terms. Minimizing the Taylor expanded \( \chi_0^2 \) with respect to \( p_\alpha \) leads to the estimator

\[
\hat{p}_\alpha = F^{-1}_{\alpha \beta} \sum_{ij} \frac{\partial x_i}{\partial p_\beta} (C^t)^{-1}_{ij}(x^d_j - x^t_j). \tag{20}
\]

Since \( \langle (x^d_i - x_i) \rangle = 0 \), the mean of this estimator is zero, equal to the true value, so the estimator is unbiased. The expected variance is obtained by squaring Eq. \( \mathbf{20} \) and using the fact that \( \langle (x^d_i - x_j)(x^d_j - x_j) \rangle = C_{ij} \)

\[
\langle \hat{p}_\alpha \hat{p}_\alpha' \rangle = F^{-1}_{\alpha \beta} F^{-1}_{\alpha' \beta'} \sum_{ij} \frac{\partial x_i}{\partial p_\beta} (C^t)^{-1}_{ij} \frac{\partial x_j}{\partial p_\beta'} = F^{-1}_{\alpha \alpha'}. \tag{21}
\]

where the second equality follows from recognizing the sum over \( i, j \) as the definition of \( F \) and then setting \( F^{-1}F = I \). So \( F^{-1} \) is the projected covariance matrix on the parameters if \( C \) is known exactly.

To account for the effect of the uncertainty in the covariance matrix, we now Taylor expand \( \Delta \chi^2 \) in Eq. \( \mathbf{14} \):

\[
\Delta \chi^2 \simeq -2 \sum_{ij} \frac{\partial x_i}{\partial p_\alpha} \Delta \Psi_{ij}(x^d_j - x^t_j)p_\alpha + \Delta F_{\alpha \beta} p_\alpha p_\beta \tag{22}
\]

with

\[
\Delta F_{\alpha \beta} \equiv \sum_{ij} \frac{\partial x_i}{\partial p_\alpha} \Delta \Psi_{ij} \frac{\partial x_j}{\partial p_\beta}. \tag{23}
\]

The changes to \( \chi^2 \) translate into a new estimator for the parameters:

\[
\hat{p}_\alpha = [F + \Delta F_{\alpha \alpha'}^{-1}] \frac{\partial x_i}{\partial p_\alpha} \left[ \Psi^t + \Delta \Psi_{ij}(x^d_j - x^t_j) \right]. \tag{24}
\]

Just as in the toy model of \( \mathbf{11} \), we can expand this estimator in powers of \( \Delta \Psi \), and – subject to the caveats mentioned below – the estimator will remain unbiased but its variance will increase.

Although we are interested in the terms second order in \( \Delta \Psi \) as these lead to larger errors on the parameters, it is worth pausing to comment here on two situations where the linear terms could lead to a bias: (i) when the covariance matrix depends on the parameters and this dependence is ignored by fixing \( C \) and (ii) when the fluctuations in \( \Delta \Psi \) are correlated with fluctuations in the data. To illustrate consider the simple situation where the elements of the inverse covariance matrix are monotonically decreasing functions of \( p \) (e.g., in the diagonal case, when \( p \) is the amplitude, the cosmic variance will be larger when \( p \) increases and therefore elements of the inverse covariance matrix will be smaller when \( p \) is greater than zero). Then, the assumed fixed value of \( \Psi \) will be less than the true value when \( p < 0 \) and greater than the true value when \( p > 0 \); equivalently \( \Delta \Psi \) will start negative and turn positive as \( p \) passes through zero. If the fluctuations in \( \Delta \Psi \) are correlated with fluctuations in the data, then the first term in Eq. \( \mathbf{22} \) has mean zero. The second will be negative when \( p < 0 \) and positive when \( p > 0 \). This will then mistakenly favor regions of parameter space with \( p < 0 \). A full understanding of the bias induced by neglecting the parameter dependence of the covariance matrix is beyond the scope of this paper (in particular, the determinant in the prefactor of the likelihood also needs to be considered) \([17]\), but this simple example makes some of the dangers explicit. The
where $N_s$ is the number of parameters in the fit and has the restriction, $N_p < N_b$. Eq. (27) is our main result, demonstrating that uncertainty in the covariance matrix propagates directly to a new source of uncertainty in the estimate of parameters. This uncertainty is proportional to $F_{s\beta}^{-1}$, which is equal to the parameter covariance in the absence of this additional error. So covariance error does not alter the shape of the constraints, but does inevitably lead to looser constraints.

A simple way to think of this degradation is to recall that the parameter covariance matrix is inversely proportional to $f_{\text{sky}}$, the fraction of sky covered by a survey. Covariance error enters in an identical way, so if the new variance captured in Eq. (27) has coefficient $B(N_b - N_p)$ equal to 0.1, for example, the result is equivalent to throwing away 10% of the data set.

**A. Gaussian limit**

Taylor et al. [15] computed the values of $A$ and $B$ in the Gaussian case (after correcting for the bias in the inverse covariance estimator [14]):

$$A = \frac{2}{(N_s - N_b - 1)(N_s - N_b - 4)}$$

$$B = \frac{N_s - N_b - 2}{(N_s - N_b - 1)(N_s - N_b - 4)}$$

As in the toy model of §4 in the (common) limit that $N_s \gg N_b \gg N_p$, the variance is enhanced over the standard variance by a factor of $(1 + N_b/N_s)$. This is our main conclusion.

**B. Weak Lensing Spectra**

We can compute covariance estimator error for non-gaussian fields by using a subset of available simulations. As an example, we use the suite of weak lensing simulations from [18, 19], assuming that the true covariance matrix is obtained from the scatter in all the simulations (1000 total). Then using only some of the simulations, we estimate $\Delta \Psi$ and therefore $B$ by taking the difference in $\Psi$ from the smaller and full set of simulations. The resulting estimate of $B$ is shown in Figure 1 compared with the Gaussian prediction. It is seen that, even for this highly non-gaussian field, Eq. (28) gives a good fit to the simulation samples. There are two reasons one might expect $B$ to exhibit a different dependence on $N_s$, 1) the two-point function of a Gaussian random field is not itself Gaussian distributed, 2) nonlinear gravitational evolution skews the statistics of the cosmological mass density field away from Gaussian. However, because the two-point function estimator is a sum of squares of the density perturbations, the distribution of the estimator may tend to a Gaussian as the number of modes in a (wavenumber or angular) bin becomes large. Figure 1 is consistent with this explanation.

**C. Current surveys**

Table 1 demonstrates the effect of simulation covariance error for some recently published cosmological surveys (which estimated covariance matrices from simulation realizations rather than from the data). We find that the degradation ranges from 5-15%.

**IV. CONCLUSIONS**

We derived a new contribution to parameter uncertainties from the uncertainty in sample data covariance matrices estimated from simulations. This error adds in quadrature with other sources of parameter uncertainty.
and scales with the ratio of the number of data bins to the number of simulation realizations.

Current surveys use hundreds of simulations, but even this large number leads to an underestimate of parameter uncertainties by \(\sim 5\text{-}15\%\). Future surveys, which will be sensitive enough to measure in hundreds of bins will require of order \(10^4\) simulation realizations (per cosmological model) to prevent 5-10\% degradation in the parameter uncertainties. Mitigation schemes such as shrinkage estimators [23], emulators [17, 24], and large-scale mode-resampling [25] will be important to reduce these computational requirements to tractable levels.

When the covariance matrix varies with cosmology (as is generally the case), there will be additional contributions to the covariance estimator error. We will derive these contributions in future work, but expect them to be sub-dominant to the primary result we present in this paper as long as the model for the cosmology-dependent covariance is accurate enough to ensure that the fluctuations, \(\Delta \Psi\), in the covariance estimator are approximately independent of cosmology.

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