Sample size effects in multivariate fitting of correlated data

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Abstract

A common problem in analysis of experiments or in lattice QCD simulations is fitting a parameterized model to the average over a number of samples of correlated data values. If the number of samples is not infinite, estimates of the variance of the parameters ("error bars") and of the goodness of fit are affected. We illustrate these problems with numerical simulations, and calculate approximate corrections to the variance of the parameters for estimates made in the standard way from derivatives of the parameters' probability distribution as well as from jackknife and bootstrap estimates.

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I. INTRODUCTION

A common problem in analysis of experiments or of Monte Carlo simulations is fitting a parameterized model to the average over a number of samples of correlated data values. In particular, lattice QCD calculations typically require fitting operator correlators, which are a function of distance between the operators, to sums of exponentials with unknown amplitudes and masses. If the number of samples is not infinite, estimates of the variance of the parameters (“error bars”) and of the goodness of fit are affected. This can be viewed as a generalization of the well known rule “replace $N$ by $N - 1$ in the denominator” in calculating the error on an average to the case where the error is on a parameter estimated by a fit to correlated data points. We calculate approximate corrections to the variance of the parameters (see Fig. 1 for a graphical example) for estimates made in the standard way from derivatives of the parameters’ probability distribution as well as from jackknife and bootstrap estimates. (The distribution of parameter estimates is not exactly Gaussian, so the variance of the parameters is not quite the whole story.) Without compensating for sample size effects, none of these methods give unbiased estimates of the parameters’ variance.

Many numerical simulation programs or experiments involve two or more stages of fitting, where the parameters resulting from the first stage are the data input to the second stage. For example, in computations of meson decay constants in lattice QCD the first stage involves fitting a correlator of meson operators to exponentials and extracting the mass and amplitude, and the second stage involves fitting these masses and amplitudes to functions of the quark masses and lattice spacings to allow extrapolation to the chiral and continuum limits. (See for example Refs. [1] and [2].) For example, in Ref. [1] about 600 hadron masses and amplitudes are computed in the first stage of fitting, and these 600 numbers and their (co)variances are in turn the data for the fitting in the second stage. While an unbiased estimate of the variance of the parameters is always welcome, it is particularly important in this case since many parameters in the first stage of fitting are used as inputs (data) in the second stage of fitting, and if their errors are systematically too large or too small the apparent goodness of fit in the second stage of fitting will be very good or very bad respectively.
II. THE PROBLEM

We consider a problem where we need to fit a function of $P$ parameters to an average of $N$ samples, where each sample consists of $D$ data points. We use subscript indices to label the component of the data vectors and superscript indices to label the samples. Thus $x_i^a$ is the $i$’th component of the $a$’th sample, with $0 \leq i < D$ and $0 \leq a < N$. Each sample is assumed to be normally distributed, but the different components of the $D$ dimensional sample are generally correlated. Averages over samples will be denoted by overbars. We will need to imagine averaging over many trials of the experiment, and we will use angle brackets to denote such an average: $\langle x_i \rangle$.

So, for example

\[
\begin{align*}
\bar{x}_i &= \frac{1}{N} \sum_a x_i^a \\
\bar{x}_i x_j &= \frac{1}{N} \sum_a x_i^a x_j^a \\
\bar{x}_i \bar{x}_j &= \frac{1}{N} \sum_a x_i^a \frac{1}{N} \sum_b x_j^b
\end{align*}
\]

(1)

The covariance matrix ("of the mean") for one trial is

\[
C_{ij} = \frac{1}{N} (\bar{x}_i \bar{x}_j - \bar{x}_i \bar{x}_j) = \frac{1}{N^2} \sum_a x_i^a x_j^a - \frac{1}{N^3} \left( \sum_a x_i^a \right) \left( \sum_b x_j^b \right)
\]

(2)

This covariance matrix will fluctuate around the true covariance matrix, obtainable only in the limit $N \rightarrow \infty$. Note we use $\frac{1}{N}$ instead of $\frac{1}{N-1}$ in normalizing $C_{ij}$. For our purposes, the difference between these normalizations is best included with the other order $\frac{1}{N}$ effects to be discussed.

Fit parameters $p_\alpha$, with $0 \leq \alpha < P$, are obtained by minimizing

\[
\chi^2 = \left( \bar{x}_i - x_i^f(p_\alpha) \right) (C^{-1})_{ij} \left( \bar{x}_j - x_j^f(p_\alpha) \right)
\]

(3)

where $x_i^f(p_\alpha)$ is the value of $\bar{x}_i$ predicted by the model. As pointed out in Ref. 3, since we are stuck with estimates of the covariance matrix and the $\bar{x}_i$ obtained from the same samples, they are correlated.
First change to a convenient coordinate system (alas, available only in theory, not in practice). For the moment we assume that our fit model is good, so that the \( x_i^f(p_\alpha) \) can be adjusted to equal the true averages of the \( x_i \). Shift the coordinates so that \( \langle x_i \rangle \) is zero. Then rotate the coordinates so that the true covariance matrix is diagonal, and rescale them so that \( \langle (x_i^a)^2 \rangle = 1 \). (So far, we have followed Ref. [3].) We now have \( \langle x_i^a x_j^b \rangle = \delta_{ij} \delta^{ab} \), and the true covariance matrix is the unit matrix.

Make a further rotation so that the changes in the \( x_i^f(p_\alpha) \) as the \( p_\alpha \) vary around their true values are in the first \( P \) components, and so that the changes in the \( x_i^f(p_\alpha) \) as the first parameter \( p_0 \) varies are in the first component. Now we can rescale \( p_0 \) so that \( \frac{\partial p_0}{\partial x_0} = 1 \), which simply means that \( p_0 \) is the average \( \bar{x}_0 \). In doing this we have assumed that \( p_0 \) is linear enough in the \( \bar{x}_i \) or that the fluctuations in the \( \bar{x}_i \) are small enough.

In this basis, write the covariance matrix (from the data in this experiment) and its inverse in blocks,

\[
C \equiv \begin{pmatrix} U & V \\ V^T & W \end{pmatrix} \quad \text{and} \quad C^{-1} \equiv \begin{pmatrix} A & B \\ B^T & E \end{pmatrix} \tag{4}
\]

where the matrices \( U \) and \( A \) are \( P \) by \( P \), \( V \) and \( B \) are \( P \) by \( D - P \) and \( W \) and \( E \) are \( D - P \) by \( D - P \).

Now \( \chi^2 \) is given by

\[
\chi^2 = \left( \bar{x}_i - x_i^f \right) \left( C^{-1} \right)_{ij} \left( \bar{x}_j - x_j^f \right), \tag{5}
\]

where only the first \( P \) components of \( x_i^f \) are nonzero. For example, with two parameters

\[
\chi^2 = \begin{pmatrix} \bar{x}_1 - x_1^f, \bar{x}_2 - x_2^f, \bar{x}_3, \ldots \end{pmatrix} \begin{pmatrix} A & B \\ B^T & E \end{pmatrix} \begin{pmatrix} \bar{x}_1 - x_1^f \\ \bar{x}_2 - x_2^f \\ \bar{x}_3 \\ \vdots \end{pmatrix} \tag{6}
\]

The \( x_i^f \) are found from minimizing \( \chi^2 \):

\[
0 = \frac{\partial \chi^2}{\partial x_i^f} = 2A_{i+j} \left( \bar{x}_{j^*} - x_{j^*}^f \right) + 2B_{i+j} \bar{x}_{j^*} \tag{7}
\]
where here and in many subsequent equations starred indices run from 0 to \( P - 1 \) and primed indices from \( P \) to \( D - 1 \), and the factor of two comes from differentiating with respect to the \( x_i^f \) on both sides of \( \text{Eq. 5} \) and using the fact that \( C^{-1} \) is symmetric.

This is solved by
\[
x_i^f = \bar{x}_{i^}\; + \; A^{-1}_i^j B_{j^k^l} \bar{x}_k^l
\]

From \( CC^{-1} = 1 \) and \( \text{Eq. 4} \)
\[
UA + VB^T = 1
\]
\[
UB + VE = 0
\]
\[
V^T A + WB^T = 0
\]
\[
V^T B + WE = 1
\]

Using the third of Eqs. \( \text{9} \) remembering that \( A \) and \( W \) are symmetric, we get an alternate to \( \text{Eq. 8} \)
\[
B = -AVW^{-1}
\]
\[
A^{-1} B = -VW^{-1}
\]
\[
x_i^f = \bar{x}_{i^}\; - \; V_{i^j^} W^{-1}_{j^k^l} \bar{x}_k^l
\]

From this equation we see that, in this basis, parameter number zero, \( x_0^f \), does not depend on the other of the first \( P \) components, \( \bar{x}_{i^}\) with \( 1 \leq i^ < P \). Thus the distribution of parameters depends only on the combination \( D - P \equiv d \).

Similarly for \( \chi^2 \):
\[
\chi^2 = (-\bar{x} B^T A^{-1} \bar{x}) \left( \begin{array}{cc} A & B \\ B^T & E \end{array} \right) \left( \begin{array}{c} -A^{-1} B \bar{x} \\ \bar{x} \end{array} \right)
\]
\[
= \bar{x} (-B^T A^{-1} B + E) \bar{x}
\]

5
Now insert $W^{-1}W = 1$ and use the third and fourth equations in 9

$$
\chi^2 = \overline{x} W^{-1} (-WB^T A^{-1} B + WE) \overline{x}
= \overline{x} W^{-1} (V^TA A^{-1} B + WE) \overline{x}
= \overline{x} W^{-1} (V^TB + WE) \overline{x}
= \overline{x} W^{-1}_{ij} \overline{x}_j
$$

But $W$ is just the covariance matrix for the last $D - P$ components of $\overline{x}$ in this basis, so the statistical properties of $\chi^2$ are exactly the same as a $D - P$ dimensional problem with no fit parameters, and the distribution of $\chi^2$, as expected, depends only on the number of degrees of freedom, $d \equiv D - P$. We note that the distribution of $\chi^2$ (more properly, $T^2$) is known. Since it is important here and closely related to the estimates of parameter errors, we quote the result in Appendix I.

### III. NUMERICAL EXAMPLE

To illustrate the effects of sample size, we begin with a numerical example, using the basis described above. In this example, $N$ Gaussian distributed random data vectors with $D = 25$ were generated. The data was fit with $P = 5$ parameters, which are just the first $P$ components of the average data vector. This was repeated for many trials. The black octagons in Fig. 1 show $N$ times the variance (over trials) of one of the parameters, where the asymptotic value is one. These black octagons are the correct answer for the variance of the parameter, and this is the variance that we wish to estimate from our experiment, where we only have one trial to work with. We see that for finite $N$ the parameters fluctuate by an amount larger than the asymptotic value.

We also show the average over trials of the variance estimated from derivatives of the parameter probability, the average over trials of the variance estimated from a single elimination jackknife analysis, and the average from a bootstrap analysis. For the jackknife and bootstrap, the plot contains average variances both for the case where the full sample covariance matrix was used in each resampling and where a new covariance matrix was made using the data in each jackknife or bootstrap sample. Red squares are average variances from the
FIG. 1: Number of samples times the variance (square of the error) of a parameter in fitting correlated data, and averages over trials of several methods for estimating this variance. The horizontal line indicates the asymptotic value, $\text{variance}(x_0) = 1/N$. $N$ is the number of samples; the meaning of the plot symbols is described in the text.
usual “derivative” method. Blue diamonds are from a single elimination jackknife analysis where a new covariance matrix was made for each jackknife sample. The two blue bursts (on top of the red squares) use the full sample covariance matrix in each jackknife resample. Similarly, the green fancy plusses are from a bootstrap analysis, using the covariance matrix from the original sample. The green crosses are estimates from a bootstrap analysis where a new covariance matrix was made for each bootstrap sample.

We see that correct answer deviates from the asymptotic value for finite $N$, and that the various methods for estimating this variance produce biased estimates of the variance of the parameter.

**IV. LARGE $N$ EXPANSION**

Most of the effects shown in Fig. 1 can be understood analytically. We can expand the covariance matrix in each trial around its true value,

$$C_{ij} = \frac{1}{N} \{ \delta_{ij} + (\bar{x}_i \bar{x}_j - \delta_{ij} - \bar{x}_i \bar{x}_j) \}$$ \hspace{1cm} (13)

Here the term in parentheses has fluctuations of order $1/\sqrt{N}$ and an average of order $1/N$. Thus its square will also have expectation value $\approx 1/N$.

Then

$$C_{ij}^{-1} = N \delta_{ij} - N (\bar{x}_i \bar{x}_j - \delta_{ij} - \bar{x}_i \bar{x}_j) + N (\bar{x}_i \bar{x}_k - \delta_{ik} - \bar{x}_i \bar{x}_k)(\bar{x}_k \bar{x}_j - \delta_{kj} - \bar{x}_k \bar{x}_j) + \ldots$$ \hspace{1cm} (14)

Using the fact that integrals of polynomials weighted by Gaussians are found by pairing the $x_i^a$ in all possible ways, or making all possible contractions, we can develop rules for calculating these expectation values. We will use parentheses to list the pairings. For
example, with (12) indicating that the first and second $x$ are paired,

$$
\langle x_i x_i x_j x_j \rangle
= x_i x_i x_j x_j \ (12)(34)
+ x_i x_i x_j x_j \ (13)(24)
+ x_i x_i x_j x_j \ (14)(23)
$$

(15)

Using

$$
\langle x^a_i x^b_j \rangle = \delta_{ij} \delta^{ab}
$$

and

$$
\overline{x_i} = \frac{1}{N} \sum_a x^a_i
$$

we get the Feynman rules for contractions of barred quantities.

1. Each contraction gives a $\delta_{ij}$ for the lower indices it connects.

2. Each bar gives a $1/\sqrt{N}$, whether it covers a single $x$ or two, $\overline{x_i}$ or $\overline{x_i x_j}$ — see Eq.11

3. Each continuous line made of overbars and contraction symbols gives a factor of $N$. This is from the $\sum_{abc...} \delta^{ab} \delta^{bc} ...$, which has $N$ nonzero terms. For example, $\overline{x_i} \overline{x_j x_k} \overline{x_l} \ (12)(34)$ is one continuous line, while $\overline{x_i} \overline{x_j x_k} \overline{x_l} \ (14)(23)$ is two lines (one is a loop). This results in every loop giving an extra factor of $N$ relative to other contractions with the same number of fields.

Since an open line (not a loop) with $C$ contractions has $2C$ $x$’s and $C + 1$ bars, but a loop with $N$ contractions has $2C$ $x$’s and $C$ bars, these rules can be rephrased as:

1. Each contraction gives a $\delta_{ij}$ for the lower indices it connects.

2. Each $x$ gives a factor of $1/\sqrt{N}$.

3. Each loop gives a factor of $N$.

In the expansion of $C^{-1}$ we find the combination $\overline{x_i x_j} - \delta_{ij} x_i x_j$, which we will denote by $\overline{x_i x_j}$. This occurs frequently enough that we should state special rules for it.
In evaluating an expression containing \( \overline{x_i x_j} \) there will be contractions where the \( x_i \) and \( x_j \) in \( x_i x_j \) are contracted with each other. These contractions just cancel the \( \delta_{ij} \). The terms with \( x_i \) and \( x_j \) contracted give a \( -\delta_{ij}/N \). Thus a “tadpole” where \( \overline{x_i x_j} \) (12) contracts with itself just gives a \( -\delta_{ij}/N \). (This includes the \( N^{-1/2} \) from each of the \( \overline{x} \)'s.)

Now consider terms where \( \overline{x_i x_j} \) is part of an open line, like

\[
\overline{x_i x_j x_j} \quad (12)(34)
\]

In this case the \( \overline{x_i x_j} \) and the \( -\overline{x_i x_j} \) cancel, so \( \overline{x_i x_j} \) can never be part of an open line. But if this object is part of a loop, like in

\[
\overline{x_i x_j x_k x_l} \quad (13)(24)
\]

the \( \overline{x_i x_j} \) part is part of the loop, but the \( -\overline{x_i x_j} \) part breaks the loop. Thus the four paths hidden in these double bars give

\[
N - 2 + 1 = (N - 1)\delta_{ik}\delta_{jl}
\]

Similarly, a loop of three double bars gives \( 2^3 = 8 \) terms, \( N - 3 + 3 - 1 = (N - 1) \), and any loop made up entirely of \( \overline{x_i x_j} \)'s gives a factor of \( N - 1 \) times the appropriate Kronecker \( \delta \)'s.

As trivial examples,

\[
\begin{align*}
\langle \overline{x_i x_j} \rangle &= \overline{x_i x_j} \quad (12) = \frac{1}{N} \delta_{ij} \\
\langle \overline{x_i x_j} \rangle &= \overline{x_i x_j} \quad (12) = \delta_{ij} \\
\langle N C_{ij} \rangle &= 1 + \overline{x_i x_j} \quad (12) = \left(1 - \frac{1}{N}\right) \delta_{ij}
\end{align*}
\]

We are also interested in the variances of averaged quantities. For the variance of something, \( \text{var}(X) = \langle X^2 \rangle - \langle X \rangle^2 \), we need the “connected part” of \( \langle X^2 \rangle \). We use a vertical bar to denote this, and we only need contractions where some of the lines cross the bar.
As an example, for the variance of an arbitrary element of $C$ to lowest order,

$$\langle \text{var} (C_{ij}) \rangle = \langle C_{ij}^2 \rangle - \langle C_{ij} \rangle^2_{\text{no sum } ij}$$

$$= \frac{1}{N^2} \left( 1 + \frac{\bar{X}_i \bar{X}_j}{N} \right)_{NS}$$

$$= \frac{1}{N^2} \left( \bar{X}_i \bar{X}_j \right)$$ (13)(24) + (14)(23)

$$= \frac{N - 1}{N^4} (\delta_{ii} \delta_{jj} + \delta_{ij} \delta_{ij})_{NS}$$

$$= \frac{1}{N^2} \frac{2}{N}; \ i = j$$

$$= \frac{1}{N^2} \frac{1}{N}; \ i \neq j$$ (24)

The last line is written to display that the fractional variance on the diagonal element is $\frac{2}{N}$.

In equations where the components are separated into starred indices, $0 \leq i^* < P$ and primed indices, $P \leq i' < D$, contractions of primed with starred indices are zero, contractions of starred with starred indices give delta functions with $\delta_{i^* i^*} = P$, and primed with primed use $\delta_{i' i'} = D - P$.

V. VARIANCE (AND HIGHER MOMENTS) OF THE PARAMETERS

In this section we examine the variances of the parameters – that is, the error bars on our answers. First we calculate how much the parameters actually vary over many trials of the experiment. Then we calculate the average of common ways of estimating this variance — from derivatives of the probability, from an “eliminate J” jackknife analysis or from a bootstrap resampling (using either the covariance matrix from the full sample, or a new covariance matrix made from each jackknife or bootstrap resample). The differences allow us to find and correct for bias in our error estimates resulting from the finite sample size.

For the actual variance of our parameters, use Eq. 10. Since we are in a coordinate system where the average of this quantity is zero, we don’t need to worry about taking the connected part.
\[ \left< x_0^f x_0^f \right> = \left< \overline{x_0} \overline{x_0} \right> + 2 \left< \overline{x_0} V_0^j W^{-1}_{j'k'} x_{k'} \right> + \left< \overline{x_0} W^{-1}_{j'k'} V_{k'0}^T V_{0m'} W^{-1}_{m'n'} x_{n'} \right> \tag{25} \]

Since \( V \) and \( W \) are made entirely of double bars and can therefore only be part of a loop, and primed indices can’t contract with index zero, the middle term (cross term) is zero.

We compute this to order \( \frac{1}{N^3} \).

\[ \left< x_0^f x_0^f \right> = \left< \overline{x_0} \overline{x_0} \right> + \left< \overline{x_0} \left( \delta_{j'm'} - \overline{x_0} x_{m'} + \overline{x_0} x_{p'} \overline{x_0} x_{m'} + \ldots \right) \left( \overline{x_m} x_0 \right) \right> \left< \overline{x_0} x_{n'} \right> \left( \delta_{n'k'} - \overline{x_0} x_{k'} + \overline{x_0} x_{r'} \overline{x_0} x_{k'} + \ldots \right) \overline{x_{k'}} \right> \tag{26} \]

The leading term, \( \left< \overline{x_0} \overline{x_0} \right> \), is just \( \frac{1}{N} \).

The term with six \( x \)’s has only one contraction:

\[ x_j^f \overline{x_j^f} x_0^f \overline{x_0^f} x_{k'} \overline{x_{k'}} \overline{x_0^f} \tag{16}(25)(34) \]

\[ = \frac{N - 1}{N^3} d \tag{27} \]

where \( d \equiv D - P \).

There are two equal terms with eight \( x \)’s. There are three nonzero contractions of this term. Ignoring the \( N^{-4} \) parts, these are

\[ -2 x_j^f \overline{x_j^f} x_{m'} \overline{x_{m'}} x_0^f \overline{x_0^f} x_{k'} \overline{x_{k'}} \tag{18}(27)(34)(56) = \frac{-2}{N^3} \delta_{j'k'} \delta_{j'm'} \delta_{m'k'} \delta_{00} \]

\[ -2 x_j^f \overline{x_j^f} x_{m'} \overline{x_{m'}} x_0^f \overline{x_0^f} x_{k'} \overline{x_{k'}} \tag{18}(23)(47)(56) = \frac{+2}{N^3} \delta_{j'k'} \delta_{j'm'} \delta_{m'k'} \delta_{00} \]

\[ -2 x_j^f \overline{x_j^f} x_{m'} \overline{x_{m'}} x_0^f \overline{x_0^f} x_{k'} \overline{x_{k'}} \tag{18}(24)(37)(56) = \frac{-2}{N^3} \delta_{j'k'} \delta_{j'm'} \delta_{m'k'} \delta_{00} \tag{28} \]

Here the plus sign on the second contraction comes from the tadpole. The second and third contractions cancel, so we just have

\[ \frac{-2}{N^3} d^2 \tag{29} \]
To order $\frac{1}{N^3}$ we only need two loop contractions from the terms with ten $x$’s. There are three such terms, but two of them are equal.

$$\left\langle x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{k'} x'_{k'} \right\rangle + 2 \left\langle x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{m'} x'_{m'} x_0 x_{k'} x_k' \right\rangle$$

(30)

Each term has two contractions:

$$\frac{x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{m'} x'_{m'} x_0 x_{k'} x_k'}{x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{m'} x'_{m'} x_0 x_{k'} x_k'} \quad (1, 10)(28)(39)(47)(56)$$

$$= \frac{1}{N^3} \left( d + d^2 \right)$$

(31)

$$\frac{2 x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{m'} x'_{m'} x_0 x_{k'} x_k'}{x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{m'} x'_{m'} x_0 x_{k'} x_k'} \quad (1, 10)(24)(35)(69)(78)$$

$$+ \frac{2 x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{m'} x'_{m'} x_0 x_{k'} x_k'}{x_j^0 x_j^0 x_{m'} x_0 x_{n'} x_{m'} x'_{m'} x_0 x_{k'} x_k'} \quad (1, 10)(25)(34)(69)(78)$$

$$= \frac{2}{N^3} \left( d + d^2 \right)$$

(32)

Putting it all together,

$$\left\langle x_0^f x_0^f \right\rangle = \frac{1}{N} + \frac{N - 1}{N^3} \left( d \right) + \frac{-2}{N^3} \left( d \right) + \frac{3}{N^3} \left( d + d^2 \right)$$

$$= \frac{1}{N} + \frac{d}{N^2} + \frac{d(d + 2)}{N^3} + \ldots$$

(33)

Thus the fluctuations in the parameters are larger than the asymptotic value $\frac{1}{N}$. from the covariance matrix.

As noted above, the probability distribution of the parameters is not exactly Gaussian. Higher moments of this distribution can be obtained in the same way. At leading order in $\frac{1}{N}$ there is only one independent diagram for the connected part of each moment, and we find, for $M$ even,

$$\left\langle \left( x_0^f \right)^M \right\rangle_{\text{connected}} = \frac{(D - P) (M - 1)!}{N^M}$$

(34)
VI. ESTIMATES OF THE PARAMETERS’ VARIANCE

In practice, the most common method for estimating the variance of the parameters is to use the covariance matrix for the parameters. (See, for example, Ref. \[5\].) In our coordinate system, this matrix is just $A^{-1}$, and our estimate for the variance of parameter zero is $(A^{-1})_{00}$. Using the third and first of Eqs. \[9\],

\[
B^T = -W^{-1}V^T A \\
1 = UA - VW^{-1}V^T A \\
A^{-1} = U - VW^{-1}V^T
\]

(35)

Then, our estimate for the variance of parameter zero is

\[
var(x_0)_{derivative} = A^{-1} \\
= U_{00} - V_{0k'}W_{k'l'}^{-1}V_{l'0}^T \\
= \frac{1}{N}(\delta_{00} + \overline{x_0x_0}) \\
- \frac{1}{N}(\overline{x_0x_{k'}})(\delta_{k'l'} - \overline{x_{k'}x_{l'}} + \overline{x_{k'}x_{m'}}\overline{x_{m'}x_{l'}} \ldots)x_{l'}x_0)
\]

(36)

For the order $\frac{1}{N}$ correction we only need the $\delta_{k'l'}$ from $W^{-1}$, and find

\[
N\,var(x_0)_{derivative} = \delta_{00} + \overline{x_0x_0} (12) - \overline{x_0x_{k'}}\overline{x_{k'}x_0} (14)(23) \\
= 1 - \frac{1}{N} - \frac{N-1}{N^2}(D-P) \\
= 1 - \frac{1}{N}(1 + D - P)
\]

(37)

The order $1/N^2$ contribution to this estimate vanishes, as sketched in Appendix II. If $D = P = 1$ this is just $\frac{1}{N}\langle 1 + \overline{x_0x_0} \rangle = 1 - \frac{1}{N}$, the standard correction for a simple average, reflecting our normalization of the covariance matrix. Comparing to the desired result in Eq. \[33\], we see that this is an underestimate of the variance of the parameters. The difference between this error estimate and the correct one above is that this estimate assumes that the
covariance matrix remains fixed while the data points vary, while the correct answer takes into account the correlations between the data points and the covariance matrix (constructed from these same data points).

VII. VARIANCE OF JACKKNIFE AND BOOTSTRAP PARAMETERS

The variance of the parameters is also often estimated by a jackknife or bootstrap analysis. In these methods the fit is repeated many times using subsets of the data sample, and the variance of the parameters is estimated from the variance over the jackknife or bootstrap samples. Both the jackknife and bootstrap can be done either using the covariance matrix from the full sample in fitting each jackknife or bootstrap sample, or by remaking a covariance matrix for each resample. Using the full sample covariance matrix amounts to seeing how the parameters vary with fixed covariance matrix, that is, by varying $x_i^\ast$ and $x_k'$ in Eq. 8 with $A_{rj}^{-1}, B_{j'k'}$ held fixed. This is the same question as is answered by $\text{var}(x_0^d)_{\text{derivative}}$ in Eq. 37. Since the change in the parameters is linear in $x_i^\ast$ and $x_k'$, it doesn’t matter if the $x_i$ are varied infinitesimally (by taking derivatives) or slightly (jackknife) or fully (bootstrap). In this case, the variance of the parameters will have the same bias as does Eq. 37 — no new calculation is necessary, although there is a slight difference due to the normalization of the covariance matrix used here.

Remaking the covariance matrix for each resample includes correlations of the covariance matrix and data, but not in quite the desired way. The calculations above can be extended to calculate the expectation value of the parameter variance for the jackknife analysis in which the covariance matrix is recomputed for each jackknife sample. An “eliminate $J$” jackknife consists of making $N/J$ resamples, each omitting $J$ data vectors (numbers $nJ$ through $(n + 1)J - 1$), and hence having $N_J \equiv N - J$ elements. We will denote averages in the $n$'th jackknife sample with a superscript $(n)$. The average of $x^a$ in the $n$'th jackknife sample is

$$\bar{x^a(n)} = \frac{1}{N_J} \left( \sum_{n \in (n)} x^a \right)$$  \hspace{1cm} (38)

where $J$ data vectors (starting with number $nJ$) were deleted from the full sample. The
variance of this quantity (over the jackknife samples) is

\[ \frac{J}{N(N - J)} \tag{39} \]

so we generally multiply the variance over the jackknife samples by \( \frac{N-J}{J} \) to get the expected variance of the mean \( \frac{1}{N} \).

We now compute the variance of the parameters in the jackknife fits. In doing this we will need averages of products of quantities from different jackknife ensembles. Without losing generality, we can think of these as ensembles number zero and one, which differ only in their first \( J \) data elements. Thus, expectation values of sums over values in different ensembles may produce factors of \( N_J - J \) instead of \( N_J \), where \( N_J \) is the number of samples in the jackknife, and is really \( N - J \). (\( N_J - J = N - 2J \) is the number of samples in common between two different jackknife resamples.)

For example, using \( (n) \) to denote quantities in the \( n \)'th jackknife sample (\( x_{aj}^{(n)} \) is the \( j \)'th component of the \( a \)'th data vector in jackknife sample \( (n) \)), for \( n \neq m \),

\[
\langle x_j^{(n)} x_k^{(m)} \rangle = \langle \frac{1}{N_J} \sum_a x_{aj}^{(n)} \frac{1}{N_J} \sum_b x_{bk}^{(m)} \rangle \\
= \frac{1}{N_J^2} \sum_{ab} \delta_{jk} \bar{\delta}^{ab} \\
= \frac{N_J - J}{N_J^2} \delta_{jk} \tag{40}
\]

where we define \( \bar{\delta}^{ab} = 1 \) if \( a = b \) and \( a, b \in (J, N - 1) \), 0 otherwise. Thus the sum over \( a \) and \( b \) gives a factor of \( N_J - J \) instead of \( N_J \).

From Eq. 39 parameter 0 in jackknife fit \( (n) \) is

\[ x_0^{(n)f} = x_0^{(n)} + V_{0j}^{(n)} W_{j'k''}^{-1} x_{k''}^{(n)} \tag{41} \]

and the variance of this parameter over the jackknife samples is

\[
\text{var}_J(x_0^{f}) = \left\langle \left( \frac{x_0^{(n)} - x_0^{(n)}}{x_j^{(n)} - x_j^{(n)}} W_{j'k''}^{-1}(n) V_{i'0}^{T(n)} - \frac{J}{N} \sum_m \left( x_0^{(m)} - x_{k''}^{(m)} W_{k''i''}^{-1} V_{i''0}^{T(m)} \right) \right) \rightangle \\
\times \left\langle \left( x_0^{(n)} - V_{0j'}^{(n)} W_{j'k''}^{-1}(n) x_{k''}^{(n)} - \frac{J}{N} \sum_p \left( x_0^{(p)} - V_{0j'}^{(p)} W_{j'k''}^{-1} x_{k''}^{(p)} \right) \right) \right\rangle \tag{42}
\]
This is more complicated than Eq. 25 because the mean over jackknife samples is not exactly zero. Also, the sums over sample vectors now sometimes give \( N_J \), sometimes \( N_J - 1 \), and sometimes \( N_J - J \), so some of the shortcuts developed above won’t work any more. Note the \( J/N \) is correct – there are \( N/J \) jackknife resamples, each containing \( N_J = N - J \) elements.

In Eq. 42 the sums contain terms where \( n = m \) and terms where \( n \neq m \). Separate the diagonal and off-diagonal terms in the sums, and use the fact that all non-diagonal terms are equal, \( \sum_m \) contains \( N/J - 1 \) terms with \( m \neq n \), and \( \sum_{mp} \) has \( N/J \) diagonal terms and \( (N/J)(N/J - 1) \) off diagonal:

\[
\text{var}_J(x_0) = \left\langle \left(1 - \frac{J}{N}\right) \frac{x_0^{(n)}}{x_0} - \left(1 - \frac{J}{N}\right) \frac{x_0^{(m)}}{x_0} - 2 \left(1 - \frac{J}{N}\right) \frac{x_0^{(n)}}{x_0} V_{0i'} W_{i'k'}^{-1(n)} \frac{x_0^{(n)}}{x_0} - \frac{x_0^{(n)}}{x_0} W_{j'k'}^{-1(n)} V_{j'i'} T_{n} V_{0i'}^{-1(0)} W_{i'k'}^{-1(n)} \frac{x_0^{(n)}}{x_0} - \frac{x_0^{(n)}}{x_0} W_{j'k'}^{-1(n)} V_{j'i'} T_{n} V_{0i'}^{-1(0)} W_{i'k'}^{-1(n)} \frac{x_0^{(n)}}{x_0} \right\rangle_{n \neq m} \tag{43}
\]

where \( n \neq m \). To evaluate this expression we need:

\(a\) \( \langle \frac{x_0^{(n)}}{x_0} \frac{x_0^{(n)}}{x_0} \rangle \)

\(b\) \( \langle \frac{x_0^{(n)}}{x_0} \frac{x_0^{(m)}}{x_0} \rangle_{n \neq m} \)

\(c\) \( \langle \frac{x_0^{(n)}}{x_0} V_{0i'} W_{i'k'}^{-1(n)} \frac{x_0^{(n)}}{x_0} \rangle \)

\(d\) \( \langle \frac{x_0^{(n)}}{x_0} V_{0i'} W_{i'k'}^{-1(m)} \frac{x_0^{(m)}}{x_0} \rangle_{n \neq m} \)

\(e\) \( \langle \frac{x_0^{(n)}}{x_0} W_{j'k'}^{-1(n)} V_{j'i'} T_{n} V_{0i'}^{-1(0)} W_{i'k'}^{-1(n)} \frac{x_0^{(n)}}{x_0} \rangle \)

\(f\) \( \langle \frac{x_0^{(n)}}{x_0} W_{j'k'}^{-1(n)} V_{j'i'} T_{n} V_{0i'}^{-1(0)} W_{i'k'}^{-1(m)} \frac{x_0^{(m)}}{x_0} \rangle_{n \neq m} \) \tag{44}

Here \(a\), \(c\) and \(e\), which involve only jackknife sample \( (n) \), are the same as in the previous section with the replacement of \( N \) by \( N_J \). Because \( W^{-1(n)} \) and \( V^{(n)} \) consist only of double
barred quantities which can’t be part of an open line, and primed and unprimed indices can’t contract, (c) vanishes. For (d) we can imagine expanding all the \( \bar{x}_i x_j^{(m)} \)’s into pieces, \( \bar{x}_i x_j^{(m)} - \delta_{ij} - \bar{x}_i (m) x_j^{(m)} \). and making all contractions. There is only one factor of \( x \) from jackknife sample \( (n) \), which must contract with something from \( (m) \). Thus, all of these terms differ from (c) by replacement of exactly one factor of \( N_J \) by \( N_J - J \), and therefore also sum to zero.

Similarly (e) and (f) differ by the replacement of one or more factors of \( N_J \) by \( N_J - J \). Thus, their difference will be one order in \( \frac{J}{N} \) less than their value. This means that to get the first correction to the asymptotic form, we need only keep the lowest order term in part (e), and the analogous contraction for part (f).

\[
\begin{align*}
(a) \quad \langle x_0^{(n)} x_0^{(n)} \rangle &= \frac{1}{N_J^2} \sum_{ab} x_0^{a(n)} x_0^{b(n)} = \frac{1}{N_J} \\
(b) \quad \langle x_0^{(n)} x_0^{(m)} \rangle &= \frac{1}{N_J^2} \sum_{ab} x_0^{a(n)} x_0^{b(m)} = \frac{N_J - J}{N_J^2} \\
(c) \quad \langle x_j^{(n)} x_j^{(n)} x_0^{(n)} x_0^{(n)} x_k^{(n)} x_k^{(n)} \rangle &= \frac{N_J}{N_J^3} (D - P) \\
&= \frac{N_J - 1}{N_J^3} (D - P) \\
(f) \quad \langle x_j^{(n)} x_j^{(n)} x_0^{(m)} x_0^{(m)} x_k^{(m)} x_k^{(m)} \rangle &= \frac{N_J - 2J - 1 + \ldots}{N_J^3} (D - P)
\end{align*}
\]

Here (a), (c) and (e) are the same as in the previous section. To evaluate (f) we need to separate the two terms in the double overbar (the delta function isn’t there since the indices can never be equal), since they may give different numbers of factors of \( N_J - J \). This evaluation proceeds as:
Now the (16)(25)(34) contraction gives

\[
(f) \approx \left\langle \frac{\left(\sum_{j'j} x_{j'}^{(n)} x_{j'}^{(m)} \right)^2}{\sum_{k'k} x_k^{(m)}} \right\rangle_{n \neq m}
= \left\langle \frac{\left(\sum_{j'j} x_{j'}^{(n)} x_{j'}^{(m)} \right)^2}{\sum_{k'k} x_k^{(m)}} \right\rangle_{n \neq m}
- \left\langle \frac{\left(\sum_{j'j} x_{j'}^{(n)} x_0 \right)^2}{\sum_{k'k} x_k^{(m)}} \right\rangle_{n \neq m}
- \left\langle \frac{\left(\sum_{j'j} x_0 x_{j'} \right)^2}{\sum_{k'k} x_k^{(m)}} \right\rangle_{n \neq m}
+ \left\langle \frac{\left(\sum_{j'j} x_0 x_0 \right)^2}{\sum_{k'k} x_k^{(m)}} \right\rangle_{n \neq m}
\]

= \frac{1}{N^6} \sum_{abcdef} \left\langle \frac{\left(\sum_{j'j} x_{j'}^{(n)} x_{j'}^{(m)} \right)^2}{\sum_{k'k} x_k^{(m)}} \right\rangle_{n \neq m}
\]

Now the (16)(25)(34) contraction gives

\[
= \frac{1}{N^6} \sum_{abcdef} \left( \delta_{j'k'} \delta_{af} \delta_{j'k'} \delta_{bd} \delta_{00} \delta_{bd}
- \delta_{j'k'} \delta_{af} \delta_{j'k'} \delta_{be} \delta_{00} \delta_{bd}
- \delta_{j'k'} \delta_{af} \delta_{j'k'} \delta_{bd} \delta_{00} \delta_{cd}
+ \delta_{j'k'} \delta_{af} \delta_{j'k'} \delta_{be} \delta_{00} \delta_{cd} \right)
\]

\[
= \frac{1}{N^6} \left( N^2_J (N_J - J)^2 - 2N_J (N_J - J)^2 + (N_J - J)^3 \right) (D - P)
\]

\[
= \frac{1}{N^6} \left( N^4_J - 2N^3_J J - N^3_J + \ldots \right) (D - P)
\]

\[
= \frac{1}{N^3_J} \left( N_J - 2J - 1 + \ldots \right) (D - P)
\]

Putting the pieces together, the variance of the parameter over the jackknife samples is

\[
(1 - J/n) \left( \frac{J}{N^2_J} + \frac{2J(D - P)}{N^3_J} \right)
= \left( \frac{N - J}{N} \right) \left( \frac{J}{(N - J)^2} \right) \left( 1 + \frac{2(D - P)}{N} + \ldots \right)
\]
Comparing with Eq. 39 which is for \( D = P \), we see that there is an extra factor of 
\[ 1 + \frac{2(D - P)}{N} \] 
(independent of \( J \)). However, by comparison with Eq. 33 we see that this effect is too large by a factor of two, so the jackknife variance for the parameters is also biased.

The leading corrections to the bootstrap estimate of the parameters’ variance can be done in a similar way. To be specific, our bootstrap procedure is to make \( B \) resamplings, each made by choosing \( N \) data vectors with replacement from the original set of \( N \) vectors, and calculate the variance of the parameters over the bootstrap resamples. Similarly to Eq. 42, the average over trials of the bootstrap estimate of the variance is

\[
\text{var}_B(x_0^f) = \left\langle \left( \frac{x_0^{(n)}}{x_0^{(m)}} - x_0^{(n)} W_{j'j''}^{-1}(n) V_{j''0}^{(n)} - \frac{1}{B} \sum_m \left( \frac{x_0^{(m)}}{x_0^{(m)}} - x_0^{(m)} W_{j'j''}^{-1}(m) V_{j''0}^{(m)} \right) \right) \left( \frac{x_0^{(n)}}{x_0^{(n)}} - x_0^{(n)} W_{j'j''}^{-1}(n) x_0^{(m)} \right) - \frac{1}{B} \sum_p \left( \frac{x_0^{(p)}}{x_0^{(p)}} - V_{j'j''}^{(p)} W_{j'j''}^{-1}(p) x_0^{(p)} \right) \right) \right\rangle
\]

(50)

which, after separating diagonal and off-diagonal terms in the sums, becomes

\[
\left( 1 - \frac{1}{B} \right) \left\langle \begin{array}{c}
\frac{x_0^{(n)}}{x_0^{(n)}} x_0^{(n)} \\
\frac{x_0^{(n)}}{x_0^{(m)}} x_0^{(m)} \\
- \frac{x_0^{(n)}}{x_0^{(n)}} x_0^{(m)} x_0^{(m)} \\
- 2 x_0^{(n)} V_{0j'}^{(n)} W_{j'j''}^{-1}(n) x_0^{(n)} x_0^{(n)} \\
+ 2 x_0^{(n)} V_{0j'}^{(m)} W_{j'j''}^{-1}(m) x_0^{(m)} x_0^{(m)} \\
+ x_0^{(n)} W_{j'j''}^{-1}(n) V_{j''0}^{(n)} V_{0j'}^{(n)} W_{j'j''}^{-1}(n) x_0^{(n)} x_0^{(n)} \\
- x_0^{(n)} W_{j'j''}^{-1}(n) V_{j''0}^{(m)} W_{j'j''}^{-1}(m) x_0^{(m)} x_0^{(m)} \\
\end{array} \right\rangle \right\}_{n \neq m}
\]

(51)

The overall \( 1 - \frac{1}{B} \) is the expected factor for difference between the average over the original sample and average over bootstraps. Label the parts as in Eq. 44 where now \( (n) \) means the \( n \)'th bootstrap resample.

For part (a),

\[
\left\langle \frac{x_0^{(n)}}{x_0^{(n)}} \frac{x_0^{(n)}}{x_0^{(n)}} \right\rangle = \frac{1}{N^2} \sum_{ab} \left\langle x_0^{a(n)} x_0^{b(n)} \right\rangle
\]

(52)

where, in this section, the superscript \( a(n) \) means the number of the data vector in the original set that was chosen to be the \( a \)'th member of bootstrap resample \( (n) \). For example,
if for $N = 3$ our bootstrap ensemble members were members 0, 1 and 0 of the original ensemble, then $0(n) = 0, 1(n) = 1$ and $2(n) = 0$. We will get contributions with nonvanishing expectation value when $a(n) = b(n)$. If a member of the original ensemble is chosen $m$ times in the bootstrap sample, then there will be $m^2$ contributions. Thus the total is the sum over all members of the original ensemble of the square of the number of times that member was chosen for this bootstrap sample. The probability distribution for the number of times a member appears in the bootstrap sample is a binomial distribution with probability $p = 1/N$. The average square of the number of times a member appears in a bootstrap resample is just the second moment of this distribution, etc.

$$\langle (n_i) \rangle = 1$$
$$\langle (n_i)^2 \rangle = 2 - \frac{1}{N}$$
$$\langle (n_i)^3 \rangle = 5 - \frac{6}{N} + \frac{2}{N^2} \quad (N > 2) \quad (53)$$

Thus the expectation value of $(a)$ is $\frac{1}{N^2} N \left( 2 - \frac{1}{N} \right) = \frac{2}{N} - \frac{1}{N^2}$.

Part (b) is the expectation value of the number of times a member was chosen in bootstrap resample $(n)$ times the number of times it was chosen in resample $(m)$. These two are independent, so we get just the product of the averages, or $\frac{1}{N^2}$.

For part (c), break the double bar into its two components.

$$(c) = -2 \left\langle x_0^{(n)} x_0^{(n)} x_0^{(n)} x_{i'}^{(n)} x_{i'}^{(n)} \right\rangle + 2 \left\langle x_0^{(n)} x_0^{(n)} x_0^{(n)} x_{i'}^{(n)} x_{i'}^{(n)} \right\rangle$$
$$= -\frac{2}{N^3} \sum_{abc} \left\langle x_0^{a(n)} x_0^{b(n)} x_{i'}^{c(n)} x_{i'}^{d(n)} \right\rangle + \frac{2}{N^4} \sum_{abcd} \left\langle x_0^{a(n)} x_0^{b(n)} x_{i'}^{c(n)} x_{i'}^{d(n)} \right\rangle \quad (54)$$

In the first term we get a contribution when $a(n) = b(n) = c(n)$. For each of the $N$ members of the original ensemble we therefore get $n^3_0$ terms, where $n_0$ is the number of times that member appeared in the bootstrap resample, so we get $N \left( 5 - \ldots \right) (D - P)$, where the $D - P$ is from the implicit sum over $i'$. In the second term we get contributions when $a(n) = b(n)$ and $c(n) = d(n)$. The probabilities of these two conditions are not quite independent, since if one member of the original ensemble is chosen multiple times in the bootstrap resample the other members will be chosen fewer times. This effect will be suppressed by a power of
\[ \frac{1}{N}, \text{ so to leading order we just have } \langle n^2 \rangle^2 = 4N^2 (D - P). \] Putting in the two and overall factors of \( N \) from the left, \((c) = \frac{-2(D-P)}{N^2} + \ldots \).

Parts \((d), (e)\) and \(f\) are done similarly, where to this order in \( \frac{1}{N} \) we only need the loop contraction in parts \((e)\) and \((f)\).

Putting it together

\[
\text{var}_B(x^f_0) = \left(1 - \frac{1}{B}\right) \frac{1}{N} \left(1 + \frac{D - P - 1}{N}\right) \tag{55}
\]

**VIII. CORRECTING SMALL BIASES**

Once the biases in the various estimates of the error on the parameter have been calculated, it is a simple matter to correct for them. In particular, we should multiply variance estimates from the derivative method by \( F_{\text{deriv}} \) in Eq. \ref{eq:56}. Note this assumes the covariance matrix was normalized as in Eq. \ref{eq:2}. For the jackknife or bootstrap done with the full sample covariance matrix, multiply the variance by \( F_{\text{reuse}} \). This differs from \( F_{\text{deriv}} \) only in the 1 in the denominator, the well known correction for the difference between the sample average and the true average, which was not included in our normalization of \( C \). For the jackknife or bootstrap analysis where a new covariance matrix is made for each jackknife or bootstrap sample, multiply the variance by \( F_{\text{jackknife, remake}} \) or \( F_{\text{bootstrap, remake}} \). Of course, if you are rescaling error bars instead of the variance, you should use the square root of the factor below. (In \( F_{\text{bootstrap, remake}} \) we assumed that the \( \frac{B-1}{B} \) in Eq. \ref{eq:51} has already been accounted for.)

\[
F_{\text{deriv}} = \frac{1 + \frac{1}{N} (D - P) + \frac{1}{N^2} (D - P) (D - P + 2) \ldots}{1 - \frac{1}{N} (1 + D - P) + \frac{0}{N^2}}
\]

\[
F_{\text{reuse}} = \frac{1 + \frac{1}{N} (D - P) + \frac{1}{N^2} (D - P) (D - P + 2) \ldots}{1 - \frac{1}{N} (D - P) + \frac{0}{N^2}}
\]

\[
F_{\text{jackknife, remake}} = 1 - \frac{1}{N} (D - P) \ldots
\]

\[
F_{\text{bootstrap, remake}} = 1 + \frac{1}{N} \ldots \tag{56}
\]
In Fig. 2 we plot the order $\frac{1}{N}$ forms for the variance of the parameter and the various methods of estimating it together with the numerical data. The horizontal axis has been inverted to $\frac{1}{N}$. Figure 3 shows the same data, with the estimates for the variance corrected for

**IX. COMPARISON TO NUMERICAL RESULTS**

In Fig. 2 we plot the order $\frac{1}{N}$ forms for the variance of the parameter and the various methods of estimating it together with the numerical data. The horizontal axis has been inverted to $\frac{1}{N}$. Figure 3 shows the same data, with the estimates for the variance corrected for
FIG. 3: Numerical results from Fig. 1 corrected for bias up to corrections of order $\frac{1}{N^2}$ for the jackknife with remade covariance matrices and order $\frac{1}{N^3}$ for the methods with fixed covariance matrix.

bias (up to errors of order $\frac{1}{N^2}$ or $\frac{1}{N^3}$). Here the lines for the actual variance of the parameter (black) and for the derivative or resampling with the full sample covariance matrix (red) are second order in $\frac{1}{N}$, while the line for the jackknife with remade covariance matrices (blue) is only first order in $\frac{1}{N}$. As an aside, we note that although the lowest order corrections for
the bootstrap with remade covariance matrices are smaller than for the other methods, the
next order corrections appear to be larger.

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Appendix I

Since estimating the goodness of fit is as important as estimating the errors on the pa-
rameters, we quote some results here. Note that what we call $\chi^2$ (with the covariance matrix
estimated from our data) is more properly called $T^2$, but we stick with the common usage
in the lattice gauge community.

The probability distribution for $\chi^2$ is known[6]. In terms of $N$ and $d$,

$$
Prob(\chi^2) = \frac{N^{-d/2} \Gamma(N/2)}{\Gamma(d/2) \Gamma((N - d)/2)} (\chi^2)^{(d-2)/2} \left(1 + \frac{1}{N \chi^2}\right)^{-N/2}
$$

We can compare to the $\chi^2$ distribution:

$$
Prob(\chi^2) = C (\chi^2)^{(d-2)/2} e^{-\chi^2/2}
$$

and see that in the limit of large $N$ they are the same.

From moments of Eq. 57 we see that the mean and variance of $\chi^2$ depend on the sample
size. Using
\[ I(D, N) \equiv \int_0^\infty d(\chi^2)(\chi^{D-2}/2) \left( 1 + \frac{1}{N} \chi^2 \right)^{-N/2} = \frac{N^{D/2} \Gamma(D/2) \Gamma((N-D)/2)}{\Gamma(N/2)} \] (58)

\[ \langle \chi^2 \rangle = \frac{I(D+2, N)}{I(D, N)} = \frac{N^D/2}{N-D^2/2} = \frac{D}{1 - D+2} \] (59)

\[ \langle (\chi^2)^2 \rangle = \frac{I(D+4, N)}{I(D, N)} = \frac{N^2D/2}{(N-D^2/2)(N-D^4/2)} = \frac{D(D+2)}{(1 - D^2/2)(1 - D+4/2)} \] (60)

(Note this is using our normalization of the covariance matrix).

Taking the connected part, or variance, and expanding in $\frac{1}{N}$, this is
\[ \text{var}(\chi^2) = 2d \left( 1 + \frac{3d + 6}{N} \right) \] (61)

Estimates of confidence levels, or probability (over trials) that $\chi^2$ would exceed the value in your experiment, can be found by integrating Eq. 57.

**Appendix II**

The customary estimate for the variance of the parameters, or from jackknife or bootstrap resamplings with the covariance matrix held fixed, has zero coefficient at the next order.

\[ N \text{var}(x_0^f)_{\text{derivative}} = A_{00}^{-1} = U_{00} - V_{0k'} W_{k'\ell}^{-1} V_{\ell0}^T \]
\[ = \frac{1}{N} \left( \delta_{00} + \bar{x}_0 \bar{x}_0 \right) \]
\[ - \frac{1}{N} \left( \bar{x}_0 \bar{x}_{k'} \right) \left( \delta_{k'\ell} - \bar{x}_k \bar{x}_{k'} + \bar{x}_{k'} \bar{x}_{m'} \bar{x}_{m'} \bar{x}_{\ell} \ldots \right) \bar{x}_{\ell} \bar{x}_0 \] (62)
Again, we only need two loop contractions from the terms with eight $x$'s.

\[
N\text{varest}(p_0) = \delta_{00} \tag{63}
\]

\[
+ \overline{x_0x_0} \tag{12}
\]

\[
- \overline{x_0x_k'} \overline{x_k'x_0} \tag{14}(23)
\]

\[
+ \overline{x_0x_k'} \overline{x_k'x_l'} \overline{x_l'x_0} \tag{16}(23)(45)
\]

\[
+ \overline{x_0x_k'} \overline{x_k'x_l'} \overline{x_l'x_0} \tag{16}(24)(35)
\]

\[
+ \overline{x_0x_k'} \overline{x_k'x_l'} \overline{x_l'x_0} \tag{16}(25)(34)
\]

\[
- \overline{x_0x_k'} \overline{x_k'x_l'} \overline{x_l'm'} \overline{x_m'x_0} \tag{18}(27)(35)(46)
\]

\[
- \overline{x_0x_k'} \overline{x_k'x_l'} \overline{x_l'm'} \overline{x_m'x_0} \tag{18}(27)(36)(45)
\]

\[
= 1 - \frac{1}{N} - \frac{N - 1}{N^2} (D - P)
\]

\[
+ \frac{N - 1}{N^3} (D - P)^2 + \frac{N - 1}{N^3} (D - P)
\]

\[
+ \frac{N - 1}{N^3} (-1)(D - P) - \frac{(N - 1)^2}{N^4} (D - P)
\]

\[
- \frac{(N - 1)^2}{N^4} (D - P)^2
\]

\[
= 1 - \frac{1}{N} (1 + D - P) + \frac{0}{N^2} \tag{64}
\]

If $D = P = 1$ this is just $\frac{1}{N} \langle 1 + \overline{x_1x_1} \rangle = 1 - \frac{1}{N}$ as it must be.