Undesirable effects of covariance matrix techniques for error analysis

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Abstract

Regression with $\chi^2$ constructed from the covariance matrix should not be used for some combinations of covariance matrices and fitting functions. Using the technique for unsuitable combinations can amplify systematic errors. This amplification is uncontrolled, and can produce arbitrarily inaccurate results that might not be ruled out by a $\chi^2$ test. In addition, this technique can give incorrect (artificially small) errors for fit parameters. I give a test for this instability and a more robust (but computationally more intensive) method for fitting correlated data.

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Recently there has been some interest in the analysis of correlated data, and people seeking more sophisticated analysis techniques have often performed regression, using the covariance matrix to construct $\chi^2$ [1]. DeGrand [2], DeTar and Kogut [3] and Gottlieb et al. [4] use the technique to analyze lattice gauge theory results, while Abreu et al. [5] and Wosiek [6] use it to analyze scaled factorial moment data. I show here that this analysis technique can amplify systematic errors, unlike simpler, more robust techniques.

This technique is simple in principle – transform the data to an uncorrelated basis, use regression to fit the data in this basis, then transform back to the laboratory frame. However, some of the results obtained by this procedure are very odd. In particular, Gottlieb et al. [4], Toussaint [7] and Wosiek [6] find that this procedure can produce best-fit lines that fall below all data points, and even below all error bars!

In this paper, I first discuss the proposed treatment of correlated data, and show that in a gedanken experiment without systematic errors this treatment produces exactly the desired results. In a very similar gedanken experiment with arbitrarily small systematic errors, this procedure amplifies the errors in the data; therefore, this treatment of data is not robust. I use these simple gedanken experiments instead of the scaled factorial moment data or the lattice gauge theory results for purposes of presentation, as the effect observed in the different data sets is qualitatively the same. I then give a more robust alternative procedure for fitting correlated data, and in the course of this discussion a test for the stability of the regression is shown.

The experimental procedure is very simple. Consider $N$ trial measurements of $I$ data points, $y_i$. Calculate the covariance matrix from these data,

$$C_{ij} = \frac{1}{N-1} \left[ \sum_{n=1}^{N} (y_{i,n} - y_i)(y_{j,n} - y_j) \right], \quad (1)$$

where

$$y_i = \frac{1}{N} \sum_{n=1}^{N} y_{i,n}. \quad (2)$$

Fit the data with the curve $f_i(\alpha)$, where $\{\alpha\}$ is the set of free parameters, by minimizing

$$\chi^2 = \sum_{i=1}^{I} \sum_{j=1}^{I} (y_i - f_i)(C^{-1})_{ij}(y_j - f_j). \quad (3)$$

I illustrate this procedure with a gedanken experiment to measure the mean voltage of a generator that produces random voltages $v$ with probability distribution $p(v)$. The generator charges a capacitor, and I then measure the voltage on the capacitor twice, calling the two measurements $y_1$ and $y_2$. Each measurement has some (uncorrelated) “measurement noise” in addition to the fluctuations due to the random voltage generator; I assume that this noise may be different for the two measurements.

After $N$ trials, the experimentally determined covariance matrix is

$$C = \frac{1}{N-1} \begin{pmatrix} \sigma^2 + \epsilon_1^2 & \sigma^2 \\ \sigma^2 & \sigma^2 + \epsilon_2^2 \end{pmatrix}, \quad (4)$$
where

\[ \sigma^2 = \int dv p(v) v^2 - \left[ \int dv p(v) v \right]^2 \]  \tag{5}

is the contribution to the covariance matrix from the distribution of random voltages, and \( e_{1(2)}^2 \) is the contribution of noise from the set of first (second) measurements.

Fitting to the function \( f_1 = f_2 = V \), \( \chi^2 \) is minimized when

\[ V = \frac{e_1^{-2}(y_1) + e_2^{-2}(y_2)}{e_1^{-2} + e_2^{-2}} \]  \tag{6}

where \( \langle y_{1(2)} \rangle \) is the average value for the first (second) measurement. It is clear from Eq. (6) that \( V \) is the average of \( \langle y_1 \rangle \) and \( \langle y_2 \rangle \), properly weighted for measurement error, and so the analysis procedure is very successful at fitting the curve for this gedanken experiment.

The experimental error is given by

\[ \sigma_V^2 = \frac{2}{\left. \frac{d^2}{dV^2} \chi^2 \right|^{-1}}. \]  \tag{7}

Taking \( \chi^2 \) from eq. (3) and \( C \) from eq. (4) gives

\[ \sigma_V^2 = \frac{\sigma^2 + 1/(e_1^{-2} + e_2^{-2})}{N - 1}. \]  \tag{8}

Again, this technique works well, clearly giving the correct error in the cases \( \sigma = 0 \) and \( \sigma \to \infty \).

Now, I modify the gedanken experiment slightly, by assuming that the capacitor discharges somewhat between the two measurements. I therefore assume that the first measurement is unchanged, but that the voltage is reduced by a factor \( \gamma \) at the time of the second measurement. I could alternatively assume that the scales of the voltmeters are slightly different, but I wish to have all systematic effects occur before measurement rather than during it.

In this case, the experimentally determined covariance matrix is

\[ C = \frac{1}{N - 1} \begin{pmatrix} \sigma^2 + e_1^2 & \gamma \sigma^2 \\ \gamma \sigma^2 & \gamma^2 \sigma^2 + e_2^2 \end{pmatrix}. \]  \tag{9}

After an infinite number of measurements \( \langle y_1 \rangle = \overline{v} \) and \( \langle y_2 \rangle = \gamma \overline{v} \), where \( \overline{v} \) is the mean value of the random voltage. Fitting again to the function \( f_1 = f_2 = V \), \( \chi^2 \) is minimized when

\[ V = \frac{\gamma e_1^2 + e_2^2}{(\gamma - 1)^2 \sigma^2 + e_1^2 + e_2^2} \overline{v}. \]  \tag{10}

The procedure gives systematic errors for this second experiment, as \( V \) is always less than \( \overline{v} \). This is not totally unexpected, because the discharge of the capacitor between the measurements gives a systematically lower value of \( y_2 \). If \( \gamma = 1 \), as in the first experiment, all systematic errors vanish. For any other value of \( \gamma \), however, \( V \) can have
any value between zero and $\bar{V}$. By contrast, a naive least-squares fit always yields a value for $V$ between $\gamma \bar{V}$ and $\bar{V}$. Thus, the covariance matrix technique can produce large systematic errors from arbitrarily small intrinsic systematic errors.

One might think that $\chi^2$ should be large whenever the fit is very bad ($V \ll \bar{V}$). However, this is not the case if the sample size is too small. In the limit $\sigma \to \infty$, where the fit is the worst,

$$\chi^2 \to (N-1) \left( \frac{\bar{V}}{\sigma} \right)^2.$$  \hspace{1cm} (11)

Thus, $\chi^2$ will be acceptably small whenever $N < (\sigma/\bar{V})^2$, so that an infinite number of events may be required to rule out the worst fits.

One might then expect that, if $\chi^2$ is acceptably small, the error in $V$ will be large enough that $V$ is within a few standard deviations of $\bar{V}$. However, in the limit $(\gamma - 1)\sigma \gg e_1, e_2$,

$$\sigma^2_V = \frac{(\gamma^2 e_1^2 + e_2^2)\sigma^2 + e_1^2 e_2^2}{(N-1)(\gamma - 1)^2} \to \frac{\gamma^2 e_1^2 + e_2^2}{(N-1)(\gamma - 1)^2} \ll \frac{\sigma^2}{N-1}. \hspace{1cm} (12)$$

Thus, it is quite possible to have simultaneously $V \ll \bar{V}$, $\chi^2$ small, and $(V - \bar{V})^2 \gg \sigma^2_V$.

Now I try a more robust technique, constructing the best estimator by minimizing the variance in

$$V = ay_1 + (1 - a)y_2.$$  \hspace{1cm} (13)

The variance is

$$\sigma^2_V = \langle V^2 \rangle - \langle V \rangle^2,$$

$$= a^2 \left( \langle y_1^2 \rangle - \langle y_1 \rangle^2 \right) + 2a(1-a) \left( \langle y_1 y_2 \rangle - \langle y_1 \rangle \langle y_2 \rangle \right) + (1-a)^2 \left( \langle y_2^2 \rangle - \langle y_2 \rangle^2 \right) \hspace{1cm} (14)

$$= \frac{1}{N-1} \left\{ a^2 \left( (\gamma - 1)^2\sigma^2 + e_1^2 + e_2^2 \right) - 2a \left[ \gamma(\gamma - 1)\sigma^2 + e_2^2 \right] + \left[ \gamma^2\sigma^2 + e_2^2 \right] \right\}. \hspace{1cm} (15)$$

The condition $d\sigma^2_V/da = 0$ then gives

$$a = \frac{\gamma(\gamma - 1)\sigma^2 + e_2^2}{(\gamma - 1)^2\sigma^2 + e_1^2 + e_2^2}, \hspace{1cm} (16)$$

$$V = \frac{\gamma e_1^2 + e_2^2}{(\gamma - 1)^2\sigma^2 + e_1^2 + e_2^2},$$

$$\sigma^2_V = \frac{(\gamma e_1^2 + e_2^2)^2 \sigma^2 + (\gamma(\gamma - 1)\sigma^2 + e_2^2)^2 e_1^2 + ((\gamma - 1)\sigma^2 - e_1^2)^2 e_2^2}{(N-1)(\gamma - 1)^2\sigma^2 + e_1^2 + e_2^2}. \hspace{1cm} (17)$$

The value of $V$ is the same for the two techniques, and $\sigma^2_V$ is the same when $\gamma = 1$. In the limit $e_1, e_2 \to 0$ I find

$$\sigma^2_V = \frac{\gamma^2 e_1^2 + e_2^2}{(N-1)(\gamma - 1)^2},$$

which is identical to the result obtained from regression. Thus, the techniques are almost the same. However, the best estimator technique is more transparent, and the cause of the instability is more easily recognized and corrected with this technique.
In the previous analysis I left out a condition — \( a \) and \( 1 - a \) must both be non-negative. In this case, the solution (20) is only valid when
\[
e_1^2 \geq (\gamma - 1)\sigma^2, \tag{21}
e_2^2 \geq -\gamma(\gamma - 1)\sigma^2. \tag{22}
\]
Applying this condition, \( \sigma^2 \) is minimized with
\[
a = \begin{cases} 
0 & \gamma < 1, \\
1 & \gamma > 1,
\end{cases}
\tag{23}
in the limit \( e_1, e_2 \to 0 \). I then obtain
\[
V = \begin{cases} 
\gamma \bar{v} & \gamma < 1, \\
\bar{v} & \gamma > 1,
\end{cases}
\tag{24}
\]
and
\[
\sigma^2_V = \begin{cases} 
\gamma^2\sigma^2 + e_2^2 & \gamma < 1, \\
\sigma^2 + e_1^2 & \gamma > 1.
\end{cases}
\tag{25}
\]
Thus, the systematic error is not amplified with this procedure, and the estimate of \( \sigma^2_V \) is not artificially small.

The crucial point is the non-negativity of \( a \) and \( 1 - a \). Mathematically, this can be written as
\[
\forall i: \frac{\partial f_i}{\partial y_i} \geq 0. \tag{26}
\]
This general requirement for a stable fit is that, given a perturbation in the data, the function does not move locally against the direction of the perturbation. It is intuitively obvious, though I am not sure whether it has been rigorously demonstrated.

The partial derivative is calculated as follows. The general fitting condition of minimizing \( \chi^2 \) can be written as
\[
\forall a: \sum_{j,k} (C^{-1})_{jk} \frac{\partial f_j}{\partial \alpha_a} (f_k - y_k) = 0, \tag{27}
\]
where \( \{\alpha\} \) is the set of fitting parameters. If \( y_i \to y_i + \delta y_i \), we must have now
\[
\forall a: \sum_{j,k,b} (C^{-1})_{jk} \left\{ \frac{\partial f_j}{\partial \alpha_a} \frac{\partial f_k}{\partial \alpha_b} + \frac{\partial^2 f_j}{\partial \alpha_a \partial \alpha_b} (f_k - y_k) \right\} \delta \alpha_b - \sum_j (C^{-1})_{ij} \frac{\partial f_j}{\partial \alpha_a} \delta y_i = 0. \tag{28}
\]
This can be written more compactly in matrix form:
\[
\delta \alpha_b = \sum_a (M^{-1})_{ab} K_{ai} \delta y_i, \tag{29}
\]
\[
M_{ab} = \sum_{j,k} (C^{-1})_{jk} \left\{ \frac{\partial f_j}{\partial \alpha_a} \frac{\partial f_k}{\partial \alpha_b} + \frac{\partial^2 f_j}{\partial \alpha_a \partial \alpha_b} (f_k - y_k) \right\}, \tag{30}
\]
\[
K_{ai} = \sum_j (C^{-1})_{ij} \frac{\partial f_j}{\partial \alpha_a}. \tag{31}
\]
Finally, I obtain

\[ \delta f_i = \sum_b \frac{\partial f_i}{\partial \alpha_b} \delta \alpha_b, \]  
\[ = \sum_{a,b} \frac{\partial f_i}{\partial \alpha_b} (M^{-1})_{ab} K_{ai} \delta y_i, \]  

and the partial derivative is

\[ \frac{\partial f_i}{\partial y_i} = \sum_{a,b} \frac{\partial f_i}{\partial \alpha_b} (M^{-1})_{ab} K_{ai}. \]  

For the fit to a constant \( V \), \( \partial f_i / \partial V = 1 \), so

\[ \frac{\partial f_i}{\partial y_i} = \frac{\sum_j (C^{-1})_{ij}}{\sum_{j,k} (C^{-1})_{jk}}. \]  

The denominator is never negative, as it is equal to a sum of eigenvalues of \( C^{-1} \) (with all weights non-negative), and all eigenvalues of \( C^{-1} \) are non-negative. Thus, the stability condition for this regression is

\[ \forall i : \sum_j (C^{-1})_{ij} \geq 0, \]  

which is trivially satisfied for uncorrelated data (\( C \) is then diagonal). If this condition is violated, then the best estimator should be used instead of the regression, to obtain the variance in the fit parameters.

The best estimator technique can also be used to fit lines and more complicated curves to data. For a line, first fit \( y = ax + b \) to all independent sets of points \( ij \) to obtain

\[ a_{ij} = \frac{y_i - y_j}{x_i - x_j}, \]  
\[ b_{ij} = \frac{x_i y_j - x_j y_i}{x_i - x_j}. \]  

Then construct linear estimators for the quantities \( a \) and \( b \),

\[ a = \sum_{i \neq j} k_{ij} a_{ij}, \]  
\[ b = \sum_{i \neq j} l_{ij} b_{ij}, \]  

with the constraints

\[ \sum_{i \neq j} k_{ij} = \sum_{i \neq j} l_{ij} = 1. \]  

Finally, minimize the variance in \( a \) and \( b \), to obtain the values and variances of both, but with the conditions

\[ \forall ij : k_{ij}, l_{ij} > 0. \]  

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In general the procedure is not worth the effort required, as the fit parameters are identical to those obtained with regression.

I have shown that covariance matrix regression should be supplemented by a test for the stability of the regression. When the regression is unstable, the fit parameters can be altered in an uncontrolled fashion. These alterations can sometimes be ruled out by a $\chi^2$ test; however, for arbitrarily small $\chi^2$, if the data set is small and fluctuations are large, the apparent errors in fit parameters can be much smaller than the difference between their apparent values and the best estimators for these values.

The alternative to using covariance matrix regression is to fit all possible sets of points (as many points per set as there are fit parameters) to obtain all possible linearly independent sets of the fit parameters, and use the linear combinations of the values obtained in this way (with no negative multipliers) that have the lowest variances as the best estimators of the fit parameters. This is computationally more cumbersome, but is the more rigorous procedure so it may be simplest to use this in the first place rather than attempting covariance matrix regression first.

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