On the repeated inversion of a covariance matrix

M. de Jong
NWO-I, Nikhef, PO Box 41882, Amsterdam, 1098 DB Netherlands
Leiden University, Leiden Institute of Physics, PO Box 9504, Leiden, 2300 RA Netherlands

August 28, 2017

Abstract

In many cases, the values of some model parameters are determined by maximising the likelihood of a set of data points given the parameter values. The presence of outliers in the data and correlations between data points complicate this procedure. An efficient procedure for the elimination of outliers is presented which takes the correlations between data points into account.

1 Introduction

In general, the values of some model parameters are optimally determined by maximising the likelihood of a set of data points given the parameter values (see e.g. [1]). In this, a data point that has too low a probability to match the model can be considered an outlier. The presence of such outliers in the data can readily be accommodated in the probability density function of the data points. It is, however, not straightforward to also take the correlations between the data points into account. If the underlying probability density functions are normal distributions, both the uncorrelated and correlated uncertainties of the data points can be incorporated in a single matrix. The values of the model parameters can then be determined by minimising the $\chi^2$:

$$\chi^2 = \epsilon^T V^{-1} \epsilon$$  \hspace{1cm} (1)

where $\epsilon$ and $\epsilon^T$ are the $(N \times 1)$ and $(1 \times N)$ vectors containing the distances between the model and the data points and $V$ is a $(N \times N)$ matrix. The elements of $V$ are set as follows.

$$V_{ii} = (\sigma_i)^2$$  \hspace{1cm} (2)

$$V_{ij} = \sum_k \frac{\partial \epsilon_i}{\partial u_k} \frac{\partial \epsilon_j}{\partial u_k} (\delta u_k)^2$$  \hspace{1cm} (3)

where $\sigma_i$ refers to the uncorrelated uncertainty of data point $i$ and $u_k$ to some correlation parameter which itself has an uncertainty $\delta u_k$. The terms in the summation of equation (3) are commonly referred to as the covariances of the data points. The matrix $V$ is therefore often called the covariance matrix. By construction, the matrix $V$ is symmetric and can thus be inverted using an LDU decomposition. The computation of $V^{-1}$ then requires $O(N^3)$ operations.
The presence of outliers cannot easily be incorporated in the covariance matrix. So, it is desirable to remove the outliers and repeat the fit. For this, a criterion is required to identify an outlier. A common criterion is based on the value of the so-called standard deviation, $D$:

$$D_k \equiv \frac{|\epsilon_k|}{\sigma_k}$$  \hspace{1cm} (4)

A typical maximal allowed value of $D$ is $D_{\text{max}} = 3$ which—in the absence of correlations—corresponds to a probability to keep a good data point of about 0.997. The removal of outliers could simply proceed by removing the data point with the largest $D$ and repeating the fit until there are no more data points with $D > D_{\text{max}}$.

In case the correlations between the data points are strong, this procedure may no longer be adequate. In this scenario, the absolute values of some off-diagonal elements of $V$ are comparable to (or even larger than) the values of the diagonal elements. The standard deviation is then no longer a good criterion because the distances and covariances of the other data points should also be taken into account. A brute force procedure to identify outliers is to 1) remove data point $k$, 2) determine $V''$, 3) invert $V''$ and 4) minimise $\chi^2$, for each data point $k$. In this, $V''$ corresponds to the $(N-1) \times (N-1)$ covariance matrix. The change in $\chi^2$ is then a good criterion to identify an outlier, i.e:

$$D_k \equiv \sqrt{\chi^2 - \chi_k^2}$$  \hspace{1cm} (5)

where $\chi_k^2$ corresponds to the $\chi^2$ of the fit after removal of data point $k$. As each inversion of $V''$ requires $O((N-1)^3)$ operations, this way of eliminating outliers requires $O(N^4)$ operations. For a large number of data points, the number of operations needed to eliminate outliers may become too excessive.

An alternative exists, based on the fact that the removal of data point $k$ is equivalent to setting the corresponding uncertainty $\sigma_k$ to infinity. By doing so, the $(N \times N)$ covariance matrix $V''$ can be decomposed as follows:

$$V' = V + g \delta_{k,k}$$  \hspace{1cm} (6)

In this, $g$ is some arbitrary large value; in any case much larger than $\sigma_k$. The matrix $\delta_{i,j}$ has 1 at row $i$ and column $j$ and 0 everywhere else. To repeat the fit without data point $k$, it is required to invert matrix $V'$. As a first step, the known inverse of the original matrix $V$ is considered. This is possible because $V^{-1}$ and $V'$ have the same dimensions.

$$V' \times V^{-1} = (V + g \delta_{k,k}) \times V^{-1}$$  \hspace{1cm} (7)

$$= VV^{-1} + g \delta_{k,k}V^{-1}$$  \hspace{1cm} (8)
\[
I + g \begin{pmatrix}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0 \\
V_{k,1}^{-1} & V_{k,k}^{-1} & \cdots & V_{k,N}^{-1}
\end{pmatrix} \leftarrow \text{row } k
\]

(9)

\[
\equiv A
\]

(10)

where \(I\) is the identity matrix. It is obvious that the inverse of matrix \(V'\) is equal to the product \(V^{-1}A^{-1}\). Consequently, the problem of inverting \(V'\) is reduced to inverting matrix \(A\). The inverse of matrix \(A\) is trivial, namely:

\[
A^{-1} = I - \frac{g}{1 + gV_{k,k}} \begin{pmatrix}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0 \\
V_{k,1}^{-1} & V_{k,k}^{-1} & \cdots & V_{k,N}^{-1}
\end{pmatrix} \leftarrow \text{row } k
\]

(11)

Now, one can let go \(g \rightarrow \infty\) and multiply \(V^{-1}\) and \(A^{-1}\) to obtain the inverse of matrix \(V'\). As can be seen from equation (11) the product of \(V^{-1}\) and \(A^{-1}\) requires \(O(N^2)\) operations. Hence, this way of eliminating outliers only requires \(O(N^3)\) operations which actually is equal to the number of operations needed to invert the covariance matrix for the first fit. It is interesting to note that no additional memory is required for the computation of \(V'^{-1}\).

A further reduction in the number of operations is possible when the outcome of the first fit is retained. In that case, the distance \(\epsilon_i\) between the model and data point \(i\) stays the same. The \(\chi^2\) without data point \(k\) can then be expressed as:

\[
\chi^2_k = \sum_{i=1}^{N} \sum_{j=1}^{N} \epsilon_i V_{i,j}^{-1} \epsilon_j
\]

(12)

\[
= \sum_{i=1}^{N} \sum_{j=1}^{N} \epsilon_i (V^{-1}A^{-1})_{i,j} \epsilon_j
\]

(13)

\[
= \chi^2 - \frac{1}{V_{k,k}^{-1}} \left( \sum_{j=1}^{n} V_{k,j}^{-1} \epsilon_j \right)^2
\]

(14)

As can be seen from equation (14) the distances and covariances of the other data points are taken into account but the inverse of \(V'\) is no longer required. As a result, the summation takes only \(O(N)\) operations and the elimination of outliers \(O(N^2)\) operations.
2 Conclusions

An efficient method is presented to eliminate outliers from a set of data points which takes the correlations between the data points into account. The number of operations needed for this procedure is the same as that needed for the inversion of the covariance matrix.

References

[1] W.J. Metzger. *STATISTICAL METHODS IN DATA ANALYSIS*. Katholieke Universiteit Nijmegen, the Netherlands, 1996. HEN-343.