Combining Experiments with Systematic Errors

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Abstract

We consider two methods of fitting parameters to datasets with systematic errors. Such a procedure is needed to combine results from different experiments where the elements within each dataset share a common systematic uncertainty. We show the methods are equivalent.

1. The Problem

Consider the fitting of a function $f(x; a)$ to data from several experiments, where points within an experiment share a common uncertainty, reported by each experiment as its systematic error.

This situation is frequently encountered. Combination of datasets from different experiments is increasingly important, and techniques are being proposed to enable it [1]. For example, it arises in fitting Regge theory predictions to results from several scattering experiments [2] where particle counts were recorded in similar detectors at different angles. Within a set of experimental results, each measured differential cross section has a statistical Poisson error, but there is also an overall uncertainty on the detector efficiency and the beam current common to all results of this experiment, but not shared with others.

The situation is illustrated in Figure 1: the two (simulated) experiments, shown as circles and squares, each have sizeable systematic uncertainties. The simple best fit through the complete dataset, shown as the dashed line, clearly has the wrong slope. The dotted line, drawn as described later, clearly matches the data better.
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Figure 1: Results from two experiments, shown as circles and squares, with only statistical errors shown. Points from the same experiment share a systematic offset. The dashed line of best fit is clearly wrong. The dotted line is the result of including the systematic uncertainties.

It should be stressed that the systematic errors discussed here are well-behaved ‘known unknowns’. The two experiments in the figure have a quoted systematic error of 5.0, and the circles apparently have a common upward fluctuation (or the squares a downward one, or some other combination) which is entirely compatible with this.

2. Two methods for solution

To establish notation: suppose that there are \( N \) experiments, with experiment \( r \) having \( n_r \) measured values which share a systematic error \( S_r \). (We will use \( r \) as an index over the experiments and \( i, j, k \) for the measurements.) We wish to fit the parameter(s) \( a \) of a function \( y = f(x; a) \) to a set of measurements \( \{x_i, y_i\} \), where the \( y_i \) have associated statistical errors \( \sigma_i \). For convenience we write \( \Delta_i = y_i - f(x_i; a) \).
If it were not for the systematic errors, one would write

$$\chi^2 = \sum_i \frac{\Delta_i^2}{\sigma_i^2}. \tag{1}$$

Minimising this quantity gives the black line in the figure. Two approaches can be taken to adapt this.

The first method is to use the inverse of the full covariance matrix in the $\chi^2$ formalism.

$$\chi^2 = \sum_i \sum_j \Delta_i V^{-1}_{ij} \Delta_j \tag{2}$$

where the matrix $V$ includes the statistical error term $\sigma_i^2$ along the diagonal, and a systematic term $S_r^2$ between all data points common to a particular experiment [3].

The second method is to introduce new variables $z_r$, the actual offsets for each experiment, and include them in the prediction, while adding a term to the total $\chi^2$ to account for the variation of the $z_r$ within their errors.

$$\chi^2 = \sum_r \sum_i \left( \frac{(\Delta_i - z_r)^2}{\sigma_i^2} \right) + \sum_r \left( \frac{z_r}{S_r} \right)^2, \tag{3}$$

where the summation over $i$ covers the data within experiment $r$. This has the disadvantage of increasing the number of parameters in the minimisation, but the advantages that it does not require a matrix inversion, and that estimates for the offsets $z_r$ are obtained explicitly; these may be of interest if one wishes to check that they are compatible with their quoted errors $S_r$.

3. The equivalence of the two methods

Despite their different approaches, these methods yield identical results, as will now be demonstrated.

Consider the first method. The inversion of the matrix $V$ can be performed algebraically. If the data are grouped together according to their experiment, $V$ is block-diagonal, each block having the form (if, for illustration, all $\sigma_i$ are the same):

$$V_r = \begin{pmatrix} \sigma^2 + S_r^2 & S_r^2 & S_r^2 & \ldots \\ S_r^2 & \sigma^2 + S_r^2 & S_r^2 & \ldots \\ S_r^2 & S_r^2 & \sigma^2 + S_r^2 & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{4}$$

The inverse of $V$ is also block diagonal in the individual inverse matrices $V_r^{-1}$, and so Equation 2 can be written

$$\chi^2 = \sum_r \sum_i \sum_j \Delta_i (V_r^{-1})_{ij} \Delta_j \tag{5}$$

where the sums over $i$ and $j$ run over the measurements of the experiment $r$.

Introducing the matrix $U$ for which all members are unity, and noting that for an $n \times n$ square matrix, $U^2 = nU$, Equation 2 may be written as $V_r = \sigma^2 I + S_r^2 U$, and $V_r^{-1}$
is just:

\[ V_r^{-1} = \frac{1}{\sigma^2} I - \left( \frac{S_r^2}{\sigma^2 (\sigma^2 + n_r S_r^2)} \right) U \]  

(6)

If the \( \sigma_i \) are different then the situation is not quite so elegant, but the inverse is still writeable in closed form as

\[ (V_r^{-1})_{ij} = \frac{\delta_{ij}}{\sigma_i^2} - \left( \frac{1}{\sigma_i^2} + \sum_k \frac{1}{\sigma_k^2} \right) \left( \frac{1}{\sigma_i^2} \right) \]  

(7)

as can be seen by multiplying out this expression and \( (V_r)_{ij} = \delta_{ij} \sigma_i^2 + S_r^2 \).

The \( \chi^2 \) to be minimised in the first method is thus

\[ \chi^2 = \sum_r \sum_i \frac{\Delta_i^2}{\sigma_i^2} - \sum_r \left( \frac{1}{\sigma_i^2} + \sum_k \frac{1}{\sigma_k^2} \right) \sum_i \sum_j \frac{\Delta_i \Delta_j}{\sigma_i^2 \sigma_j^2} . \]  

(8)

For the second method the expression for \( \chi^2 \) is given by Equation 3. To find the minimum the differentials are set to to zero, and the resulting system of simultaneous equations partially decouples. The differential for one of the \( z_r \) is

\[ \frac{\partial \chi^2}{\partial z_r} = -2 \sum_j \frac{\Delta_j - z_r \sigma_j^2}{\sigma_j^2} + 2 z_r \sigma_j^2 S_r^2 \]  

(9)

which gives the estimate of \( z_r \) for a particular \( a \), writing, for convenience, \( \zeta_r = \frac{1}{\sigma_i^2 + \sum_k \frac{1}{\sigma_k^2}} \)

\[ \hat{z}_r = \zeta \sum_j \frac{\Delta_j}{\sigma_j^2} \]  

(10)

Inserting Equation 10 into Equation 3 gives

\[ \chi^2 = \sum_r \left( \sum_i \frac{\Delta_i^2}{\sigma_i^2} - 2 \sum_i \frac{\Delta_i}{\sigma_i^2} \sum_j \frac{\Delta_j}{\sigma_j^2} + \left( \sum_k \frac{1}{\sigma_k^2} + \frac{1}{\sigma_i^2} \right) \zeta^2 \sum_i \sum_j \frac{\Delta_i \Delta_j}{\sigma_i^2 \sigma_j^2} \right) \]  

(11)

which reduces to the expression in Equation 8.

The two methods lead to the same quantity to be minimised to give the result. Although their mathematics is apparently different, the statistical assumptions are consistent and the same end result ensues.

In the example shown in Figure 1, either method gives slope of 1.053 and a constant of 2.435. This is the dotted line shown, and clearly represents a good fit. (Incidentally the R optim function was used for the minimisation [4], with the BFGS gradient method. \( S \) and \( \sigma \) are 5.0 and 0.5 respectively.)

The extra parameters of Method 2 increase the difficulty of the minimisation. Also if, as is usual, the function includes an additive constant term, the search space now includes a direction in which a change in this term can be balanced by an opposite shift in the the mean \( z \). In this direction \( \chi^2 \) changes slowly, through the \( 1/S^2 \) terms, whereas the change in any orthogonal direction is, assuming that there are many more datapoints than datasets, much larger. This causes a problem of the Rosenbrock’s Valley type [5]. R’s default Nelder-Mead method for R’s optim function does not perform reliably.
the second method is used, then even if the minimiser reports ‘successful convergence’, the result should be confirmed with more than the usual care. In a particular analysis it may be preferable to simplify the minimisation of the $\chi^2$ of Equation 3 by treating it as a problem solely in the $a$ parameters, with the $z_i$ at every step being given explicitly by Equation 10.

4. Conclusion

In combining datasets from experiments with systematic uncertainties, one may either use the full covariance matrix in the $\chi^2$, or introduce the offsets as additional parameters: the methods are equivalent.

References

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