Appunti della Lezione:
Fit con incertezze in ascissa ed ordinata

Least Squares Fitting when Both Variables have Errors

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When both the dependent and independent variables have associated errors or uncertainties, conventional least-squares fitting routines are not applicable. Instead, a more general minimum variance technique employing numerical minimisation such as that used in MINUIT [1] is the natural route to follow. However, with many data points, such an approach rapidly leads to a very large number of variable parameters, a situation which can lead to problems with the fitting routines. In this report, an effective variance method which approximates the more exact technique is described. Such an approximation holds very well for most applications of physical interest. Finally, the approximation involved in adapting this effective variance technique to a conventional fitting routine is described.

INTRODUCTION:

Many measurements in physics are characterised by errors in **both** the independent and dependent variables. However, the conventional least squares techniques for fitting data assume that the measurements of the independent variable are **exact**, with no uncertainty. In such cases, all the uncertainty is considered to apply only to the dependent variable. In fact, it is difficult to find in the standard reference books used by nuclear and particle physicists descriptions of techniques relevant to the more general case. In the Particle Properties Data Booklet [2], for example, this particular class of fitting problem is completely ignored. In his classic treatment of errors for physicists, Bevington [3] only offers an extremely crude method for treating the situation where errors occur in the independent variable as well as the dependent variable:

> "We are not always justified in ascribing all the uncertainties to the dependent parameter. Sometimes the uncertainties in the determinations of both quantities x and y are nearly equal. But our fitting procedure will still be fairly accurate if we combine the uncertainties of both quantities and assign them to the dependent variable alone. This is the assumption we will generally make. We will proceed with our calculations on the basis that we need consider uncertainties in the dependent quantity only, but we will understand that the corresponding fluctuations were originally derived from unncertainties in the determinations of both quantities.
>
> In those cases where the uncertainties in the determination of the independent quantity are considerably greater than those of

the dependent quantity, we might benefit from redefining which quantity we consider as dependent and which as independent."

Appropriate methods for dealing with errors in both variables have been described, however. The general nuclear techniques textbook by Leo [4], for example, refers to the *effective variance method* for treating such problems. In the rest of this report, I will refer to the discussions of the *effective variance method* presented by Orear [5] and Lybanon [6].

MINIMUM VARIANCE: GENERAL

When there is uncertainty associated with the value of the independent variable, then the "best values" for these data points must also be determined by the fitting routine, in addition to the fitted parameters describing the functional relationship between the two variables. Thus, for each **true** value x_j^0 there will be a measured x_j Gaussian-distributed about x_j^0 with a standard deviation δx_j, and similarly a measured y_j Gaussian-distributed about $y_j^0 = f(x_j^0)$ with standard deviation δy_j. If there are m parameters α_i to be determined in the function $f(x)$, and n sets of measured pairs of (x_j, y_j), then the chi-square, χ^2, is found by minimising the weighted sum of the squared deviations:

$$S(\alpha) = \sum_{j=1}^{n} \left[\left(\frac{x_j - x_j^0}{\delta x_j} \right)^2 + \left(\frac{y_j - f(x_j^0}{\delta y_j} \right)^2 \right] \qquad (1)$$

This is an obvious extension of the usual definition for the χ^2 when only the dependent variable is characterised by measurement errors.

In this case, in addition to the m values of α_i, there are n values of x_j^0, giving a total of $(m+n)$ unknowns. The total number of experimental points consists of the n values of x_j together with the n values of y_j. Thus the number of degrees of freedom are $[2n - (m+n)] = (n-m)$, which in fact is exactly the same as it would be if only the dependent variable was characterised by errors!

The minimisation of equation 1 has to be performed for the n values of x_j^0 as well as for the m values of α_i. An obvious approach is the employment of MINUIT with minimisation carried out for all $m+n$ parameters simultaneously. However, if there are many data points, *the number of parameters* involved in the minimisation can become a problem, leading to difficulties with the fitting routine. The standard (default) version of MINUIT, for example, can accommodate **up to** 35 variable (although, with some effort, the MINUIT code can be redimensioned for more parameters).

Interestingly, an **approximate** method exists for carrying out the minimisation of equation 1 *without* the necessity of including the independent variables as parameters, the so-called *effective variance method.*

EFFECTIVE VARIANCE: GENERAL

In the effective variance method, the number of variables which have to be handled is reduced considerably, (from $m + n$ to just m). This is the technique described, for example, by Orear [5], a generalisation of an earlier approach presented by Barker and Diana [7]. As this method still involves a non-linear minimisation, numerical techniques such as use of MINUIT must still be employed. However, an approximate solution of this effective variance method can be obtained using a standard least squares fit routine (designed for the case where only the dependent variable has errors), an example being the **fit** routine in ROOT [8]. The user should be warned, however, that the "solution" obtained by this latter method is only approximate, and is not as "good" as that obtained using MINUIT.

The effective variance method essentially relies on the adequacy of being able to approximate the function $f(x)$ by a *linear* function in the neighbourhood of each experimental point (ie, within a range of $\delta x_j, \delta y_j$ of each x_j, y_j). In the region around (x_j, y_j), the best value of x_j^0 is found by minimising the value of the following equation with respect to x_j^0:

$$r^2(x_j^0) = \frac{(x_j - x_j^0)^2}{(\delta x_j)^2} + \frac{(y_j - f(x_j^0))^2}{(\delta y_j)^2}$$

That is:

$$\frac{(x_j - x_j^0)}{(\delta x_j)^2} + \frac{(y_j - f(x_j^0))}{(\delta y_j)^2} f'(x_j^0) = 0$$

If $f(x)$ is linear, then this latter equation can be solved for x_j^0 in terms of the known quantities: $x_j, y_j, \delta x_j, \delta y_j$ and the two parameters describing the linear relationship $f(x)$. Substituting these solutions for x_j^0 into equation 1 yields, after simplification, the *effective variance* expression:

$$S(\alpha) = \sum_{j=1}^{n} \left(\frac{y_j - f(x_j)}{\delta_j} \right)^2, \qquad (2)$$

where $(\delta_j)^2 = (f_j')^2 (\delta x_j)^2 + (\delta y_j)^2$, with f_j' the differential of $f(x)$ at x_j [5] (here, it is assumed that $f'(x_j^0) \approx f'(x_j)$). By means of this approximation, the problem is transformed into one involving a summation over deviations in the **dependent** variable, only. This expression no longer depends on the parameters, x_j^0. The penalty for this is the requirement that the differential of $f(x)$ be available. Equation 2 differs from the one used in the usual minimimum variance method in the modification to the weighting (the denominator of equation 2), a quantity which is no longer independent of the variable parameters, but now depends on them through the differential: $f'(x)$. It is this non-linearity which is responsible for the necessity of using a numerical technique such as MINUIT for the minimisation. However, Equation 2 can be solved in a very straightforward way using MINUIT. In this case, only the m parameters α_i are varied.

If the "best" values, x_j^0 are also desired, the whole procedure of solving equation 1 by, say, MINUIT, is **not** required. Instead, the effective variance

method can be used to solve for the parameters, α_i, and then these used as fixed parameters when minimising equation 1. In this case, the **only** parameters allowed to vary are the **desired** x_j^0! (Since each of the terms in the summation of equation 1 contains a **single** x_j^0, the result is the same as that which would result if they were all allowed to vary).

An even simpler (but not as accurate) approximation for the solution of equation 2 can be obtained [5] through the use of standard minimum variance routines such as the **fit** function in ROOT. In this method, the $S(\alpha)$ of equation 2 is minimised iteratively. In each iteration, $(\delta_j)^2$ is held constant, with the value for f_j' evaluated in terms of the α_i resulting from the fit of the previous iteration. Such a technique converges to a solution which is generally quite a good approximation to the "correct" solution. In fact, in his original paper, Orear [5] believed that such an iterative process would indeed converge to the "correct" solution. However, Lybanon [6] subsequently pointed out that such a process does *not* converge, in general, to the "correct" solution.

EXPLICIT EXAMPLE:

As a numerical example, consider the following set of data which is to be fit by a linear function of x: $y = a + bx$.

x	δx	y	δy
1.0	0.1	1.0	0.2
2.5	0.2	2.4	0.2
3.0	0.2	3.0	0.3
4.6	0.6	6.1	0.1
5.4	0.2	5.7	0.2

Table 1: Values and associated uncertainties

The various procedures which could be followed for fitting this data are now described in detail:

1. **Standard minimum variance: [Errors on dependent variable, only]**
   First, a **fit** was performed (using ROOT), with $(\delta_j)^2$ taken to be equal to $(\delta y_j)^2$ (ie, disregarding the errors in x_j, the δx_j). The values of the resulting parameters a and b and their errors are given in the first column of results listed in Table 2. Graphically, this solution is shown as the red curve in Fig.1.

2. **Full Minuit fit**:
   In this case, MINUIT was used to minimise the $S(\alpha)$ of equation 1. In this case, the minimisation involved **seven** parameters, the two α_i, (a and b), and the five values of x_j^0. For the initial estimates of these parameters, the x_j^0 were set equal to x_j, and the parameters a and b were set to the values resulting from the previous "minimum variance" solution, the values given in the first column of Table 2. Results for

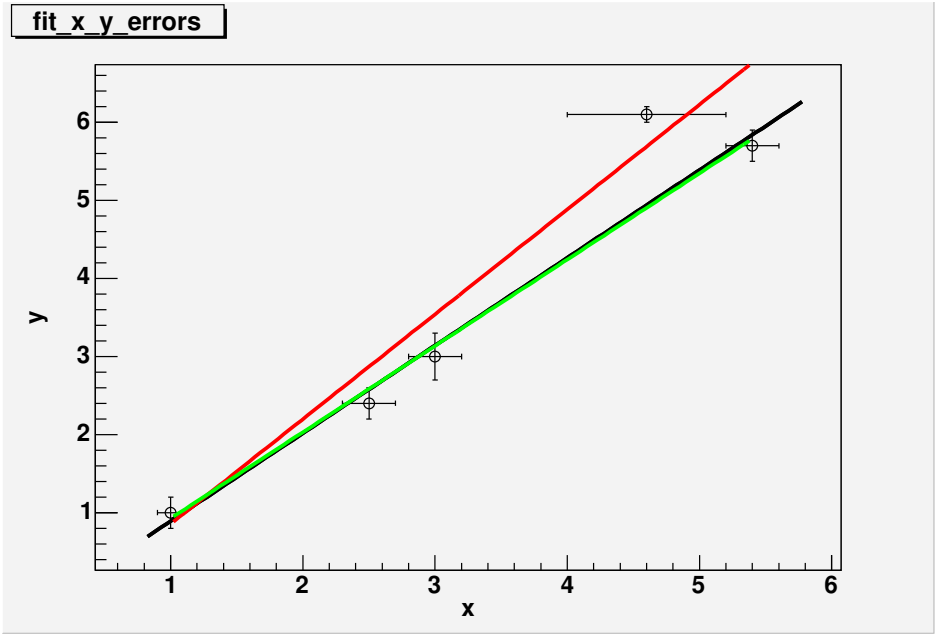

Figure 1: Sample Fits

this fit are given in the second column of Table 2, and the resulting curve is shown as black line in Fig.1.

3. **Effective Variance Method: "Iterative fit" Approach**

In this case, an approximate solution to the minimisation of the $S(\alpha)$ of equation 2 was obtained by the iterative technique referred to earlier. This was done by writing an appropriate executable command macro for ROOT using, as input, the results from a simple minimum variance fit as illustrated in the following:

```
.....
name1 = new TGraphErrors(n, x, y, errx, erry);
name2 = new TGraphErrors(n, x, y, noerrx, erry);
TF1 *fit = new TF1("fitlineare","[0]+[1]*x",x[0],x[n-1]);
name1->Fit("fitlineare");
fit->DrawCopy("same");
name2->Fit("fitlineare");
fit->SetLineColor(2);
fit->DrawCopy("same");
a = fit->GetParameter(0);
b = fit->GetParameter(1);
chi2 = fit->GetChisquare();
cout<<chi2<<endl;
while ((fabs(chi2-chi2old)/chi2)>0.001) {
chi2old = chi2;
for(Int_t i=0; i<n; i++){
errynew[i] = sqrt(erry[i]**2+(b*errx[i])**2);
}
```

```
delete name2;
name2 = new TGraphErrors(n, x, y, noerrx, errynew);
name2->Fit("fitlineare");
a = fit->GetParameter(0);
b = fit->GetParameter(1);
chi2 = fit->GetChisquare();
cout<<(fabs(chi2-chi2old)/chi2old)<<endl;
}
.....
```

The resulting values and errors are listed in the third column of Table 2 and the function characterising this solution is illustrated by the green curve in Fig.1. Although convergence was obtained fairly quickly (five iterations), and the results were "close" to the more accurate ones (column 2 Table 2), this iterative "solution" differs slightly from the one obtained by minimising the whole $S(\alpha)$ simultaneously, as expected [6].

	Example 1		**Example 2**		**Example 3**	
α_i	χ^2		χ^2		χ^2	
	54.43		3.82		2.74	
	Value	Error	Value	Error	Value	Error
a	-0.48	0.21	-0.23	0.26	-0.17	0.28
b	1.34	0.05	1.12	0.08	1.10	0.09

Table 2: Results of fitting procedures

ACKNOWLEDGEMENTS

These notes developed as a result of my frustration with trying to find simple techniques described in the literature for fitting data of the kind described. I was even forced to develop much of this material myself! Then, Fraser Duncan showed me the references to the works of Orear (and others) in the textbook by Leo [4]. However, since the American Journal of Physics is not a standard source of reference material for our graduate students, I felt it might be helpful to others to summarize here the results of this search. Thus, for Fraser's help, I am most grateful.

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