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TO THE METHOD OF LEAST SQUARES

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Peter Cziffra and Michael J. Moravcsik

June 5, 1959

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ABSTRACT

This report, a revised and corrected version of UCRL-8523, gives a short and practical summary of curve fitting by the method of least squares. The purpose is to list and roughly justify the formulae used in finding the best fitting curve, the errors, and the quantities which describe the goodness of the fit.
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INTRODUCTION

This report gives a short and practical summary of curve fitting by the method of least squares. The purpose is to list and roughly justify the formulae used in finding the best-fitting curve, the errors, and the quantities which describe the goodness of the fit. The contents are therefore well known to statisticians, but apparently very poorly known to physicists, although the problem in question arises very often in everyday analysis of data. For more details as well as for a mathematically more satisfactory treatment the reader is referred to textbooks on statistics. This report, however, is self-contained, and explicitly utilitarian in tone.

1. NOTATION AND DEFINITIONS

The experimental point is denoted by

\[ y(x_i) \equiv y_i, \quad i = 1, \ldots, N. \]  

(1.1)

This is usually the average of a series of measurements of \( y \) at the point \( x_i \).

The uncertainty (experimental) in \( y_i \) is

\[ \xi_i \equiv \xi(x_i). \]  

(1.2)

This is the experimentally determined estimate of the standard deviation. We assume throughout that \( x_i \) is measured exactly, or at least with an error which is negligible compared to that of \( y_i \), or that \( x_i \) is a pre-assigned (intended) rather than a measured value.

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*This work was done under the auspices of the U. S. Atomic Energy Commission*
We approximate the experimental points by the series of degree n:

\[ f(x_i) = \sum_{k=0}^{n} a_k \phi_k(x_i). \]  

(1.3)

The functions \( \phi_k(x) \) may be any set of linearly independent functions of \( x \). Most simply we may set \( \phi_k(x) = x^k \), which would give us a polynomial of degree \( n \). Other possible choices are, for instance, Legendre polynomials, Tschebycheff polynomials, \( \phi_k(x) = \sin kx \), etc.

The residual for this function is

\[ r(x_i) \equiv r_i = y_i - f(x_i) = y_i - \sum_{k=0}^{n} a_k \phi_k(x_i). \]  

(1.4)

Weights used here are:

\[ w_i = \frac{1}{\zeta_i^2} > 0. \]  

(1.5)

The "real" or "true" values of the \( y_i \) are denoted by

\[ Y(x_i) \equiv Y_i. \]  

(1.6)

The \( Y_i \) are the exact unknowable values which the average of the \( y_i \) would approach if an infinite number of measurements could be made of them.

Standard deviation (true) or variance is

\[ \sigma(x_i) \equiv \sigma_i \equiv \"true\" \text{ value of } \zeta_i \]  

(1.7)

The series of degree \( n \) approximating \( Y(x_i) \) is

\[ F(x_i) = \sum_{k=0}^{n} A_k \phi_k(x_i) \]  

(1.8)

The residual for this series is

\[ R(x_i) \equiv R_i = Y_i - F(x_i). \]  

(1.9)

The "true" error in \( y_i \) is

\[ E(x_i) \equiv E_i = Y_i - y_i. \]  

(1.10)
We define for the "experimental" approximating function

\[ q = \sum_{i=1}^{N} w_i [y_i - f(x_i)]^2 = \sum_{i=1}^{N} w_i r_i^2. \]  

(1.11)

We define for the "true" approximating function

\[ Q = \sum_{i=1}^{N} w_i [Y_i - F(x_i)]^2 = \sum_{i=1}^{N} w_i R_i^2(x_i). \]  

(1.12)

We will set

\[ \frac{\sigma_i^2}{\xi_i^2} = \rho^2 \]

for all \( i \), where we have

\[ \rho^2 = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^2}{\xi_i^2}. \]  

(1.13)

"Experimental" quantities are lower-case:

\[ y_i, x_i, \xi_i, f(x_i), a_k r(x_i), w_i, q. \]

"True" quantities are upper-case (except \( \sigma_i \)):

\[ Y_i, F(x_i), A_k, R(x_i), Q, E(x_i). \]

We wish to reassure the reader that the "true" quantities are used merely for mathematical purposes, and that a knowledge of them is not necessary for the use of the results of this article.
2. STATEMENT OF THE PROBLEM

The basic problem is as follows. For each abscissa \( x_i \) \((i = 1 \ldots N)\) we are given an experimental value of the ordinate \( y_i \), with experimental uncertainty \( \xi_i \). We wish to construct a curve of a given type, i.e., with a given \( \phi_k(x) \) or of a given degree, in such a way that this curve most closely approximates the data.

To solve the problem, we assume that the measured values \( y_i \) have a Gaussian (normal) distribution around the "true" value \( Y_i \), with standard deviation \( \sigma_i \). Thus the probability that for an experimentally determined \( y_i \) the "true" value \( Y_i \) lies between \( Y_i \) and \( dY_i \) is

\[
P(Y_i) dY_i = \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left( -\frac{(Y_i - y_i)^2}{2 \sigma_i^2} \right) dY_i.
\]

Thus the best (most probable) guess of the \( Y_i, i = 1 \ldots N \) is obtained when

\[
P = \prod_{i=1}^{N} P(Y_i) = \prod_{i=1}^{N} \left( \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left( -\frac{(Y_i - y_i)^2}{2 \sigma_i^2} \right) \right)
\]

\[
= \prod_{i=1}^{N} \left( \frac{1}{\sigma_i \sqrt{2\pi}} \right) \exp \left( -\sum_{j=1}^{N} \frac{(Y_j - y_j)^2}{2 \sigma_j^2} \right),
\]

is a maximum, or--what amounts to the same thing--when

\[
\sum_{i=1}^{N} \frac{(Y_i - y_i)^2}{\sigma_i^2}
\]

is a minimum. Now, we wish to determine the values of \( a_k \) in Eq. (1.3) so that \( f(x_i) \) is the most probable estimate of the \( Y_i \). From Eq. (2.3) this will occur when

\[
q = \sum_{i=1}^{N} w_i (y_i - f(x_i))^2 = \sum_{i=1}^{N} w_i y_i (y_i - f(x_i))
\]

is a minimum. Here we have used \( \xi_w, (w_i = \xi_i^2) \) as the best available estimate of \( \sigma_i \). Equation (2.4) is Legendre's principle of least squares.
3. OBTAINING THE COEFFICIENTS OF \( f(x) \)

We want to minimize

\[
q = \sum_{i=1}^{N} \left( \sum_{k=0}^{n} a_k \phi_k(x_i) - y_i \right)^2 
\]

or we want to satisfy

\[
\frac{\partial q}{\partial a_{\ell}} = 2 \sum_{i=1}^{N} \left( \sum_{k=0}^{n} a_k \frac{\phi_k(x_i) \phi_{\ell}(x_i)}{\xi_i^2} \right) \phi_{\ell}(x_i) = 0
\]

for all \( \ell = 0 \ldots n \).

Thus we get a set of linear equations

\[
\sum_{k=0}^{n} a_k \left( \sum_{i=1}^{N} \frac{\phi_k(x_i) \phi_{\ell}(x_i)}{\xi_i^2} \right) = \sum_{i=1}^{N} \frac{y_i \phi_{\ell}(x_i)}{\xi_i^2}, \quad \ell = 0 \ldots n.
\]

These are called the normal equations for the least-square-fitting procedure. These equations can also be written as a matrix equation,

\[
h a = g.
\]

where

\[
h_{k\ell} = \sum_{i=1}^{N} \frac{\phi_k(x_i) \phi_{\ell}(x_i)}{\xi_i^2}, \quad g_{\ell} = \sum_{i=1}^{N} \frac{y_i \phi_{\ell}(x_i)}{\xi_i^2}.
\]

The solution can therefore be written as

\[
a_k = \sum_{\ell=0}^{n} (h^{-1})_{k\ell} g_{\ell} = \sum_{\ell=0}^{n} (h^{-1})_{k\ell} \sum_{i=1}^{N} \frac{y_i \phi_{\ell}(x_i)}{\xi_i^2}.
\]

The matrix \( h \) is symmetric. If the \( \phi_{\ell}(x_i) \) are orthogonal, \( h \) is a diagonal matrix.
4. ERRORS IN THE COEFFICIENTS

The "true" error in the \( y_i \) is given by \( E_i = Y_i - y_i \). From Eq. (2.1) the probability that \( E_i \) lies between \( E_i \) and \( E_i + dE_i \) is given by

\[
P(E_i)dE_i = \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left[ -\frac{E_i^2}{2\sigma_i^2} \right] dE_i. \tag{4.1}
\]

Thus, if we make a very large number of measurements of \( y_i \), we find for the average value of \( E_i^2 \),

\[
\overline{E_i^2} = \frac{1}{\sigma_i \sqrt{2\pi}} \int_{-\infty}^{\infty} E_i^2 \exp \left[ -\frac{E_i^2}{2\sigma_i^2} \right] dE_i = \sigma_i^2 \tag{4.2}
\]

and for \( i \neq j \),

\[
\overline{E_i E_j} = \int_{-\infty}^{\infty} \frac{dE_i}{\sigma_i \sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{dE_j}{\sigma_j \sqrt{2\pi}} E_i E_j \exp \left[ -\frac{1}{2} \left( \frac{E_i^2}{\sigma_i^2} + \frac{E_j^2}{\sigma_j^2} \right) \right] = 0. \tag{4.3}
\]

The bar over the variables denotes an average over a very large number of measurements.

Let the "true" series fitting the "true" data \( Y_i \) be given by

\[
F(x_i) = \sum_{k=0}^{n} A_k \phi_k(x_i).
\]

We can then define the uncertainty in the coefficient of \( f(x) \) to be

\[
\sqrt{\left( a_k - A_k \right)^2} \right)^{1/2} \tag{4.4}
\]
Now, from Eq. (3.6),

\[
a_k = \sum_{\ell=0}^{n} (h^{-1})_{k\ell} \sum_{i=1}^{N} \frac{y_i \phi_\ell (x_i)}{\zeta_i^2}.
\]  

(4.4)

Since \( h^{-1} \) does not depend on the \( y_i \), being dependent only on the \( x_i \) and \( \zeta_i \), we find

\[
A_k = \sum_{\ell=0}^{n} (h^{-1})_{k\ell} \sum_{i=1}^{N} \frac{Y_i \phi_\ell (x_i)}{\zeta_i^2}.
\]  

(4.5)

Hence we have

\[
(a_k - A_k)^2 = \sum_{\ell=0}^{n} (h^{-1})_{k\ell} \sum_{i=1}^{N} \frac{\phi_\ell (x_i^2)}{\zeta_i^2} E_i.
\]  

(4.6)

Let us denote temporarily

\[
\overline{\phi_k} (x_i) = \sum_{\ell=0}^{n} (h^{-1})_{k\ell} \phi_\ell (x_i).
\]  

(4.7)

Then we have

\[
(a_k - A_k)^2 = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{1}{\zeta_i^2} \frac{1}{\zeta_j^2} \overline{\phi_k} (x_i) \overline{\phi_k} (x_j) E_i E_j.
\]  

(4.8)

Taking the average of both sides, using Eqs. (4.2) and (4.3) gives us

\[
\overline{(a_k - A_k)^2} = \sum_{i=1}^{N} \left( \frac{\phi_k^2 (x_i)}{\zeta_i^2} \right) \left( \frac{\sigma_i^2}{\zeta_i^2} \right).
\]  

(4.9)
The $\xi_i$ are supposed to be the best possible experimental estimates of the $\sigma_i$. It is therefore not unreasonable to assume that $\sigma_i^2/\xi_i^2$ does not vary much with $i$, and to replace it by its average value

$$\rho^2 = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_i^2}{\xi_i^2}.$$ 

We can thus write Eq. (4.7) as

$$(a_k - A_k)^2 = \rho^2 \sum_{i=1}^{N} \left( \frac{\phi_k^2(x_i)}{\xi_i^2} \right). \quad (4.10)$$

Now we have

$$\sum_{i=1}^{N} \frac{\phi_k^2(x_i)}{\xi_i^2} = \sum_{i=1}^{N} \frac{1}{\xi_i^2} \sum_{l=0}^{n} (h^{-1})_{lk} \phi_l(x_i) \sum_{m=0}^{n} (h^{-1})_{mk} \phi_m(x_i)$$

$$= \sum_{l=0}^{n} (h^{-1})_{lk} \sum_{m=0}^{n} (h^{-1})_{mk} \sum_{i=1}^{N} \frac{1}{\xi_i^2} \phi_l(x_i) \phi_m(x_i)$$

$$= \sum_{l=0}^{n} (h^{-1})_{lk} \sum_{m=0}^{n} (h^{-1})_{mk} h_{lm} \quad \text{by (3.5)}$$

$$= \sum_{l=0}^{n} (h^{-1})_{lk} \delta_{lk} = (h^{-1})_{kk}, \quad (4.11)$$

so that we obtain

$$(a_k - A_k)^2 = \rho^2 (h^{-1})_{kk}. \quad (4.12)$$

This is as far as we can go without further assumptions, because $\rho^2$ is not a directly measurable quantity.
In order to estimate \( p \) we proceed as follows:

\[
E_1 = Y_1 - y_1 ,
\]

and therefore

\[
E_1 + r_1 = F(x_1) + R_1 ,
\]

where

\[
r_1 = y_1 - f(x_1) \quad \text{and} \quad R_1 = Y_1 - F(x_1).
\]

Thus we have

\[
E_1 + r_1 = \sum_{k=0}^{n} (A_k - a_k) \phi_k(x_1) + R_1
\]

\[
= \sum_{k=0}^{n} \phi_k(x_1) \sum_{j=1}^{N} \frac{\Phi_k(x_1)}{\xi_j} E_j + R_1 ,
\]

Multiplying both sides by \( r_i / \xi_i^2 \) and summing over \( i \), we get

\[
\sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i E_i + \sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i^2 = \sum_{i=1}^{N} \sum_{j=0}^{n} \sum_{j=1}^{N} \frac{1}{\xi_i^2} \frac{1}{\xi_j^2} r_i \phi_k(x_j) E_j
\]

\[
+ \sum_{i=1}^{N} \frac{r_i R_i}{\xi_i^2}
\]

From Eq. (3.2) we see immediately

\[
\sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i \phi_k(x_i) = 0 ,
\]
whereupon Eq. (4.14) becomes

$$\sum_{i=1}^{N} \frac{1}{\xi_i} r_i E_i + \sum_{i=1}^{N} \frac{1}{\xi_i} r_i^2 = \sum_{i=1}^{N} \frac{r_i R_i}{\xi_i}. \quad (4.16)$$

Multiplying Eq. (4.13) by $E_i/\xi_i^2$ and summing over $i$, we get

$$\frac{E_i^2}{\xi_i^2} + \frac{r_i E_i}{\xi_i^2} = \sum_{k=0}^{n} \sum_{j=0}^{N} \sum_{i=1}^{N} \phi_k(x_i) \phi_k(x_j) \frac{E_i E_j}{\xi_i^2 \xi_j^2} + \sum_{i=1}^{N} \frac{E_i R_i}{\xi_i^2}. \quad (4.17)$$

Eliminating $\sum \frac{1}{\xi_i} r_i E_i$ between Eqs. (4.16) and (4.17), we obtain

$$\sum_{i=1}^{N} \frac{E_i^2}{\xi_i^2} + \sum_{i=1}^{N} \frac{r_i R_i}{\xi_i^2} = \sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i^2 = \sum_{k=0}^{n} \sum_{j=1}^{N} \sum_{i=1}^{N} \phi_k(x_i) \phi_k(x_j) \frac{E_i E_j}{\xi_i^2 \xi_j^2} + \sum_{i=1}^{N} \frac{E_i R_i}{\xi_i^2}. \quad (4.18)$$

Let us now take the average of both sides of Eq. (4.18) on the basis of the normal distribution of the $y_i$. We note $\bar{y}_i = y_i$, so the $\bar{r}_i = R_i$, and $E_i = 0$. Using these results as well as Eqs. (4.2) and (4.3), we get for Eq. (4.18),

$$\sum_{i=1}^{N} \frac{\sigma_i^2}{\xi_i^2} + \sum_{i=1}^{N} \frac{R_i^2}{\xi_i^2} - \sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i^2 = \sum_{k=0}^{n} \sum_{i=1}^{N} \frac{\phi_k(x_i) \phi_k(x_i) \sigma_i^2}{\xi_i^2 \xi_i^2} + \sum_{i=1}^{N} \frac{E_i R_i}{\xi_i^2}. \quad (4.19)$$

From the definition of $\rho^2$ we have $\sum \frac{E_i^2}{\xi_i^2} = N \rho^2$, and setting...
\[
\frac{\sigma_i^2}{\xi_i^2} = \rho^2 \text{ on the left-hand side of Eq. (4.19), we get}
\]
\[
N \rho^2 + \sum_{i=1}^{N} \frac{R_i^2}{\xi_i^2} = \sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i^2 = \rho^2 \sum_{k=0}^{n} \sum_{i=1}^{N} \frac{\phi_k(x_i) \overline{\phi_k(x_i)}}{\xi_i^2}. \tag{4.20}
\]

However, we have
\[
\sum_{i=1}^{N} \frac{\phi_k(x_i) \overline{\phi_k(x_i)}}{\xi_i^2} = \sum_{i=1}^{N} \frac{\phi_k(x_i)}{\xi_i^2} \sum_{l=0}^{n} (h^{-1})_{kl} \phi_l(x_i)
\]
\[
= \sum_{k=0}^{n} (h^{-1})_{kl} h_{kl} = 1
\]

and
\[
\sum_{k=0}^{n} \sum_{i=1}^{N} \frac{\phi_k(x_i) \overline{\phi_k(x_i)}}{\xi_i^2} = \sum_{k=0}^{n} 1 = n + 1,
\]

so that Eq. (4.20) becomes
\[
\rho^2 = \frac{1}{N - n - 1} \left[ \sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i^2 - \sum_{i=1}^{N} \frac{1}{\xi_i^2} R_i^2 \right]. \tag{4.21}
\]

We may approximate the first term on the right by the actually observed residuals, in which case we obtain
\[
\rho^2 \approx \frac{1}{N - n - 1} \left[ q - \sum_{i=1}^{N} \frac{R_i^2}{\xi_i^2} \right]. \tag{4.22}
\]
If we have \( R_i = 0 \) for all \( i \) — that is, if there is an underlying physical law which obeys a series of degree \( n \),

\[
Y_i = \sum_{k=0}^{n} A_k \phi_k(x_i),
\]

we get \( \rho^2 = q/(N - n - 1) \). For \( R_i \neq 0 \) we see from Eq. (4.22) that \( q/(N - n - 1) > \rho^2 \); thus, in setting \( \rho^2 = q/(N - n - 1) \) in Eq. (4.10) we are making a conservative estimate of \( \rho^2 \) and also in some measure taking into account the poorness of the fit. The error in the coefficients may consequently be written

\[
(\Delta a_k)^2 = (a_k - A_k)^2 = \frac{(h^{-1})_{kk} q}{N - n - 1}
\]

\[
= \frac{(h^{-1})_{kk}}{N - n - 1} \sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i^2.
\]

5. ERROR AT ANY GIVEN POINT

The error at any given point is given by

\[
\Delta^2(x) = \left[ F(x) - f(x) \right]^2 = \left[ \sum_{k=0}^{n} (A_k - a_k) \phi_k(x) \right]^2
\]

\[
= \sum_{k=0}^{n} \sum_{\ell=0}^{n} (A_k - a_k)(A_\ell - a_\ell) \phi_k(x) \phi_\ell(x).
\]

Using Eqs. (4.6) and (4.7), we can write this as

\[
\Delta^2(x) = \sum_{k=0}^{n} \sum_{\ell=0}^{n} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{1}{\xi_i^2} \frac{1}{\xi_j^2} E(x_i)E(x_j) \phi_k(x_i) \phi_\ell(x_j) \phi_k(x) \phi_\ell(x).
\]

(5.2)
Again assuming, as in Section 4, the randomness of the distribution in \( \gamma_i \), we get

\[
\Delta^2(x) = \rho^2 \sum_{k=0}^{n} \sum_{f=0}^{n} \phi_k(x) \phi_f(x) \sum_{i=1}^{N} \frac{1}{\xi_i} \Phi_k(x_i) \Phi_f(x_i).
\]  

(5.3)

But we have

\[
\sum_{i=1}^{N} \frac{1}{\xi_i} \Phi_k(x_i) \Phi_f(x_i) = \sum_{i=1}^{N} \frac{1}{\xi_i} \sum_{p=0}^{n} (h^{-1})_{pk} \phi_p(x_i) \sum_{q=0}^{n} (h^{-1})_{qf} \phi_q(x_i)
\]

\[
= \sum_{i=1}^{n} \sum_{p=0}^{n} \sum_{q=0}^{n} \frac{1}{\xi_i} \phi_p(x_i) \phi_q(x_i) (h^{-1})_{pk} (h^{-1})_{qf}.
\]

(5.4)

so that we may write

\[
\Delta^2(x) = \rho^2 \sum_{k=0}^{n} \sum_{f=0}^{n} (h^{-1})_{fk} \phi_k(x) \phi_f(x).
\]  

(5.5)

Again, assuming that (a) the "true" function \( F(x) \) is an ideally good approximation to \( Y_i \), i.e. \( R_i \approx 0 \), and (b) the sum of the squares of the average values of the weighted residuals can be approximated by the sum of the squares of the observed values of the residuals, we get

\[
\Delta^2(x) = \frac{1}{N - n - 1} \left( \sum_{i=1}^{N} \frac{x^2(x_i)}{\xi_i^2} \right) \left[ \sum_{k=0}^{n} \sum_{f=0}^{n} (h^{-1})_{fk} \phi_k(x) \phi_f(x) \right].
\]  

(5.6)
6. SOME PROPERTIES OF THE ERRORS

A. The Average Error of the Fitting Function at the Points of Observation

If we set $x = x_i$ in Eq. (5.5), divide by $\zeta_i^2$, and sum over $i$, we obtain

$$\sum_{i=1}^{N} \frac{\Delta^2(x_i)}{\zeta_i^2} = \rho^2 \sum_{i=1}^{N} \frac{1}{\zeta_i^2} \sum_{k=0}^{n} \sum_{l=0}^{n} (h^{-1})_{lk} \phi_k(x_i) \phi_l(x_i)$$

and therefore

$$\left( \frac{\Delta^2(x_i)}{\zeta_i^2} \right)_{av} = \rho^2 \sum_{k=0}^{n} \sum_{l=0}^{n} (h^{-1})_{lk} = (n + 1) \rho^2,$$  \hspace{1cm} (6.1)

and therefore

$$\left( \frac{\Delta^2(x_i)}{\zeta_i^2} \right)_{av} = \frac{n + 1}{N} \rho^2 = \frac{n + 1}{N} \frac{1}{N-n-1} \sum_{i=1}^{N} \frac{r^2(x_i)}{\zeta_i^2}. \hspace{1cm} (6.2)$$

Here $av$ refers to averaging over the points of observation. The extreme right-hand side holds under the conditions that make Eq. (4.26) and Eq. (5.6) possible. Thus if $\rho^2$ is unity (see Section 7), the average error of the fitting curve is always less than the error of the observation at that point, because we require $n + 1 \leq N$ for a meaningful fit.

B. The Average Error over an Interval

This average is given by

$$\Delta^2(x) = \frac{1}{x_1 - x_2} \int_{x_1}^{x_2} \Delta^2(x) \, dx = \frac{1}{N-n} \left( \sum_{i=1}^{n} \frac{r^2(x_i)}{\zeta_i^2} \right) \frac{1}{x_2 - x_1}$$

and

$$\sum_{k=0}^{n} \sum_{l=0}^{n} (h^{-1})_{lk} \int_{x_1}^{x_2} \phi_k(x) \phi_l(x) \, dx, \hspace{1cm} (6.3)$$
which in case of polynomial functions can be written as

\[ \Delta^2(x) = \frac{1}{N - n - 1} \left( \sum_{i=1}^{N} \frac{r^2(x_i)}{\xi_i^2} \right) \frac{1}{n} \sum_{k=0}^{n} \sum_{l=0}^{n} (h^{-1})_{k,l} (x_{l+k+1} - x_1)^2. \]  

(6.4)

7. GOODNESS-OF-FIT CRITERIA

The error in the fitting series, as given by Eq. (5.6) is composed of two factors. One of them, namely

\[ \sum_{k=0}^{n} \sum_{l=0}^{n} (h^{-1})_{k,l} \phi_k(x) \phi_l(x), \]  

(7.1)

gives the contribution of the statistical errors of the experiment. This expression is independent of \( y \), and is determined only by the experimental errors \( \xi_i \) and the abscissae and basic functions we use for fitting.

For the other factor in Eq. (5.6), we have

\[ \frac{1}{N - n - 1} \sum_{i=1}^{N} \frac{r^2(x_i)}{\xi_i^2} = \frac{1}{N - n - 1} q, \]  

(7.2)

which, once we have assumed that the "true" values \( Y \), are ideally fitted by the "true" function \( F(x) \), gives an indication of the goodness of the set of data under consideration. In particular, it can tell us whether the set of data is an "unlikely" one or not. If it is a very unlikely set, one might suspect some systematic error in the measurement.

In practice, however, often it is not known for certain whether \( F(x) \) indeed gives an ideal fit to \( Y \). If not, and the minimum value of \( Q \) is not 0, this will also show up in Eq. (7.2). Thus it is in fact difficult to tell whether this is the case or whether there is a systematic error in the experiment.

The goodness-of-fit criteria are concerned with the quantity in Eq. (7.2). We discuss two tests for such fit, the so-called chi-square test and the so-called F test.
A. The Chi-Square \( \chi^2 \) Test

In Section 4, Eq. (4.21), we showed that for \( y_i \) which are distributed normally about the \( Y_i \), we have

\[
q = \sum_{i=1}^{N} \frac{r_i^2}{\xi_i^2} = (N - n - 1)\rho^2 + \sum_{i=1}^{N} \frac{1}{\xi_i^2} R_i^2. \tag{7.3}
\]

If the \( \xi_i \) are good estimates of the \( \sigma_i \), then \( \rho^2 \approx 1 \). If in addition the \( R_i \approx 0 \), which would be the case for a good fit, then we would expect

\[
q = \sum_{i=1}^{N} \frac{1}{\xi_i^2} r_i^2 \approx N - n - 1. \tag{7.4}
\]

For a poor fit, \( R_i^2 \) is greater than zero, so that we would expect \( q > N - n - 1 \).

It can be shown that for normally distributed \( y_i \), with \( R_i \) 0 and \( \xi_i = \delta_i \), the statistic \( q \) obeys what is known as a chi-square \( \chi^2 \) distribution. That is, the probability that \( q \) lies between \( q \) and \( q + dq \) is given by

\[
P_{M}(q) dq = \frac{1}{2^{M/2} \Gamma(M/2)} e^{-q/2} q^{(M-2)/2} dq, \tag{7.5}
\]

where \( M = N - n - 1 \) is the number of degrees of freedom of the distribution. A simple integration shows

\[
\bar{q} = \int_{0}^{\infty} q P_{M}(q) dq = M, \tag{7.6}
\]

in agreement with Eq. (7.4). In order to find the degree of the series which best fits the data, one calculates \( q/M \) for \( n = 1, 2, 3, \ldots \), etc. In general, \( q/M \) as a function of \( n \) will first decrease, then level off to a plateau, and finally perhaps slowly increase. The best series is thus the one with the smallest \( n \) at which the plateau begins.

Sometimes the plateau will not occur at \( q/M \approx 1 \), but at some higher value. If this value is so high as to be improbable it may be concluded either that the \( R_i \) are not small, or that there is some internal inconsistency
in the data. The probability \( p \) that \( q \) be larger than a given value \( q_0 \) is, for \( 0 < p < 1 \),

\[
\int_{q_0}^{\infty} P_M(q')dq' = p.
\]

A brief table of \( p \), \( q_0 \), and \( M \) is given in the Appendix.

Another thing that can lead to values of \( q/M \) differing significantly from one is a poor estimate of the uncertainty \( \xi_i \). For instance, two unwarranted rejection of data would make \( \xi_i \) too small, resulting in a large \( p^2 \). On the other hand, estimates of \( \xi_i \) that are too conservative would make \( p^2 \) small, so that for \( R \approx 0 \), \( q/M \) would be considerably less than one.

Supplementing the \( \chi^2 \) test one can also use the \( F \) test, which is discussed next.

B. The \( F \) Test

Strictly speaking the \( F \) test was designed to solve the following problem. Suppose we are given a set of normally distributed variables \( y_i \), of which it is known that the true values \( Y_i \) obey a relation of the form

\[
Y_i = \sum_{k=0}^{n} A_k \phi_k(x_i),
\]

where \( n \) is unknown. For a given \( n \), what is the probability, on the basis of the available data, that \( A_i = 0 \)? In most practical cases we do not know whether the \( Y_i \) values obey a relation of the above form; as a matter of fact, in many cases (e.g., scattering cross-sections in nuclear physics) the underlying physical law may be an infinite series. However, even though the test is not rigorously applicable it may still be used to indicate the degree of the series that best fits the data. Let the data be fitted with a series of degree \( n \) and with a series of degree \( n-1 \); let \( q_n \) and \( q_{n-1} \) be the respective weighted sums of the residuals. We form the statistic

\[
S_M = \frac{M}{q_n} (q_{n-1} - q_n),
\]

(7.8)
where $M = N - n - 1$. Under the conditions stated above $q_n$ obeys a $\chi^2$ distribution with $M$ degrees of freedom; similarly $q_{n-1}$ and $q_n$ obeys a $\chi^2$ distribution with one degree of freedom. Now the distribution of the ratio of two $\chi^2$ variables divided by their degrees of freedom is called a Fisher $F(m_1, m_2)$ distribution, where $m_1$ and $m_2$ are the degrees of freedom of the variables in the numerator and denominator, respectively. In our case we have $m_1 = 1$, $m_2 = M$, so that $S_M$ has an $F(1, M)$ distribution. If $P_M(F)$ is the $F(1, M)$ distribution, then the probability $a$ for $S_M \geq F_a(M)$ is given by

$$a = \int_{F_a(M)}^{\infty} P_M(F) \, dF,$$

(7.9)

The $F$ test now states that for $S_M \geq F_a(M)$ one may assume $\lambda_n \neq 0$ with a probability $a$ of being wrong in this assumption. Thus if $S_M$ corresponds to an $F_a(M)$ with $a = 0.75$ there is a 75\% chance of being right if we assume $\lambda_n = 0$. A Table of $F_a(M)$ is given in the Appendix.

The $F$ test must always be used in concert with the $\chi^2$ test. For suppose the $F$ test indicates that with a high probability $\lambda_n = 0$, it is still possible that $\lambda_{n+1}, \lambda_{n+2}, \ldots$ are not zero. However, if in that case we terminate the series at $n-1$, the $\chi^2$ test indicates that a good fit has not yet obtained.
8. EXAMPLE

Consider the set of numbers given at the left. By use of an IBM-650 computer these were fitted with the function

\[ f(x) = \sum_{k=0}^{n} a_k x^k \]

for \( n = 1, 2, 3, 4, 5 \). The results are shown below.

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We see immediately that the \( \chi^2 \) test selects \( n = 3 \) as giving the best fit. The \( F \) test corroborates this selection, because \( S_M = 0.02748 \) for \( M = 9 \) corresponds, according to the table in the Appendix, to \( t_\alpha \approx 0.85 \). Thus in terminating the series at \( n = 3 \) we have approximately an 85% chance of being right.

ACKNOWLEDGEMENT

We are grateful to Drs. William Frazer, Edward Kaplan, and Jay Orear for helpful discussions, comments, and criticism.
## APPENDIX

**Distribution of \( \chi^2 \)**

Values of \( q_0 \) for given \( M \) and \( p \)

\[
\int_{q_0}^{\infty} p_M (\chi^2) \, d\chi^2 = p
\]

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Distribution of F:

Values of $F_a(M)$ for given $M$ and $a$:

\[ \int_{F_a(M)}^\infty P_M(F) \, dF = a \]

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REFERENCES


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