Some aspects of the general least-squares problem for data fitting

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Publication date:
1971

Document Version
Publisher's PDF, also known as Version of record

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Title and author(s)

Some Aspects of the General Least-Squares Problem for Data Fitting

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Date August 1971

Department or group

Reactor Physics Department

Group's own registration number(s)

16 pages + 0 tables + 0 illustrations

Abstract

A presentation is given of formulas and methods applicable to the general least-squares problem for data fitting. An iterative procedure of the Marquardt type is described for models that are nonlinear in the parameters. For partially nonlinear models it is shown that the iterative procedure may be confined to the space of nonlinear parameters. Constraints of certain simple types are included in the formalism. Based on ideal assumptions, a statistical analysis is given of the least-squares solution for the parameters.

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CONTENTS

1. Introduction

This paper deals with the general least-squares problem and presents a collection of formalisms and methods that have proved successful for data fitting of various types. Most of the principles described are certainly not new (an exception, as far as the author is aware, is sec. 4); they can be found scattered in the literature of statistics and numerical analysis. However, the author felt that a unified treatment of the statistical as well as the computational aspects would be valuable.

2. The General Least-Squares Problem with Constraints

Let a mathematical model be given,

$$y = f(x;b) \tag{1}$$

where x and y are the independent and the dependent variable respectively, and b is a parameter vector with k components,

$$b = (b_1, \ldots, b_k)^T \tag{2}$$

(T stands for transpose)

subject to the following m constraints

$$K_l(b) = 0 \quad (l = 1, \ldots, m) \tag{3}$$

(Constraints of the very simple type

$$b_j = b_{jo} \tag{4}$$

are not included in (3); instead the parameter is deleted from the parameter list).

Further, let a data sample (x_i, y_i) $(i = 1, \ldots, n)$ be given. According to the least-squares principle, we will find b so that

$$\Phi = \sum_{i=1}^{n} w_i (y_i - f(x_i;b))^2 \tag{5}$$

is minimized under the constraints (3). The w_i are the weights of the data

points; appropriate weighting will be discussed later, but here we need only assume that the weights are fixed numbers accompanying our sample.

Of course, if some of the b_j occur symmetrically in (1) and (3), several permuted b-solutions may exist. On the other hand, there may for finite b be no minimum solution at all. Or, a local minimum might exist without being a global one. It is a very difficult problem to state conditions for the existence and uniqueness of minimum solutions. Here, we disregard these complications and postulate that a usable solution b to our problem exists and can be determined by the subsequent equations.

We use the method of Lagrange and consider the functional

$$\psi = \Phi + 2 \sum_{l=1}^{m} \mu_l K_l(b) \tag{6}$$

where $2\mu_l$ are Lagrange multipliers. The minimizing b is the first part of the composite vector (b, μ) satisfying the following k+m equations obtained by zeroing $\partial\psi/\partial b_j$ and $\partial\psi/\partial\mu_l$:

$$\left.\begin{aligned} &\sum_{i=1}^{n} w_i(y_i - f_i)\frac{\partial f_i}{\partial b_j} - \sum_{l=1}^{m} \mu_l \frac{\partial K_l}{\partial b_j} = 0 \\ &K_l(b) = 0 \quad (l = 1, \ldots, m) \end{aligned}\right\} \tag{7}$$

where f_i has been written for $f(x_i; b)$.

The discussion of how to compute the solution b of (7) for special constraints is postponed until secs. 4-5; at this point we assume that a solution has already been obtained, and we shall examine its statistical behaviour.

3. Statistical Analysis of the Least-Squares Solution

Let y_i show statistical fluctuations around their mean values η_i, whereas x_i (and w_i) are fixed. Then the solution b of the system (7) will also be a random variable with a distribution that can be found under certain restrictive assumptions.

In the first place, the fluctuations $y_i - \eta_i$ must be small. Let the solu-

tion corresponding to an arbitrary sample (x_i, y_i, w_i) be (b, μ) and that corresponding to the "mean-value sample" (x_i, η_i, w_i) be (b_o, μ_o). Then $b-b_o$ (and $\mu - \mu_o$) is small, and we may assume that our model (1) and the constraints (3) are locally linear in a domain S including b and b_o:

$$f(x_i ; b) = f(x_i ; b_o) + \sum_{j=1}^{k} \frac{\partial f_i}{\partial b_j} (b_j - b_j^o)$$

$$\sum_{j=1}^{k} \frac{\partial K_l}{\partial b_j} (b_j - b_j^o) = 0 \qquad (8)$$

where $\partial f_i / \partial b_j$ and $\partial K_l / \partial b_j$ may be considered constant in S. The next assumption is that (1) is an ideal model of our sample, i. e.

$$f(x_i ; b_o) = \eta_i \qquad (9)$$

Then (7) becomes a linear system of the order k + m with $(\delta b, \delta \mu)$ $(b - b_o, \mu - \mu_o)$ as the unknown,

$$\begin{array}{c} \\ k \\ m \end{array} \begin{array}{c} \begin{array}{cc} k & m \end{array} \\ \left[\begin{array}{c|c} P^T W P & R^T \\ \hline R & \theta \end{array}\right] \end{array} \left[\begin{array}{c} \delta b \\ \hline \delta \mu \end{array}\right] = \left[\begin{array}{c} \delta v \\ \hline e \end{array}\right] \qquad (10)$$

where $p_{ij} = \frac{\partial f_i}{\partial b_j}$, $w_{ij} = \delta_{ij} w_i$, $r_{lj} = \frac{\partial K_l}{\partial b_j}$, $\delta v_j = \sum_{i=1}^{n} w_i (y_i - \eta_i) \frac{\partial f_i}{\partial b_j}$ (11)

(δ_{ij} is the Kronecker delta)

Here, and in the following, θ is written for a zero matrix. The matrix of the system (10) will be denoted H. Introduction of the vector $\delta y = (y_1 - \eta_1, \ldots, y_n - \eta_n)^T$ yields

$$\delta v = P^T W \, \delta y \qquad (12)$$

and $$\delta b = K \, \delta y \qquad (13)$$

with $$K = Q P^T W \qquad (14)$$

where Q is obtained by deletion of the last m rows and columns from the symmetric matrix H^{-1},

$$H^{-1} = \begin{array}{c} \\ k \\ \\ m \end{array} \begin{array}{c} \begin{array}{cc} k & \quad m \end{array} \\ \left[\begin{array}{c|c} Q & S^T \\ \hline S & T \end{array}\right] \end{array} \tag{15}$$

Hence δb is related to y simply by a linear transformation. As δy has zero mean, so has δb, i.e. b is an unbiased estimate of b_o. Further, according to statistical theory [3], the var-cov matrix M of b (or δb) is connected to the var-cov matrix V of y (or δy) by the equation

$$M = K V K^T \tag{16}$$

(in particular, if y has a multi-normal distribution, so has b). Let us now assume that y_i are independent. Then V is diagonal,

$$v_{ij} = \delta_{ij} \sigma_i^2 , \tag{17}$$

σ_i^2 being sample variances assumed known.

Further, let us make a special choice of the weights,

$$w_i = \frac{1}{\sigma_i^2} \tag{18}$$

This weighting is sometimes referred to as "statistical weighting" [1]. It has a double advantage: it ensures that the data points with the largest variances will have small influence on the fit and vice versa, and it permits a relatively simple statistical analysis of the results. From (18), (14) and (16) we get $V = W^{-1}$ and $M = QP^T WW^{-1} WPQ$, or

$$M = Q P^T W P Q \tag{19}$$

(in the case of no constraints, $Q = (P^T WP)^{-1}$, and hence $M = Q$).

Next we shall consider the statistical distribution of Φ_{min}, the minimum value of Φ. From (5) and (8) we have

$$\Phi_{min} = \sum_{i=1}^{n} w_i (y_i - \eta_i - \sum_{j=1}^{k} \frac{\partial f_i}{\partial b_j} (b_j - b_j^o))^2 \qquad (20)$$

or

$$\Phi_{min} = (\delta y - P \delta b)^T W (\delta y - P \delta b) \qquad (21)$$

From (13) and (14),

$$\Phi_{min} = \delta y^T B \, \delta y \ , \qquad (22)$$

expressing Φ_{min} as a quadratic form in δy with the matrix

$$B = (I_n - PQP^T W)^T W (I_n - PQP^T W) \qquad (23)$$

($I_n \equiv$ unit matrix of the order n),

or

$$B = W^{1/2} (I_n - W^{1/2} PQP^T W^{1/2})^2 W^{1/2} \qquad (24)$$

At this point we introduce the substitution

$$\delta y = W^{-1/2} u \qquad (25)$$

and from now on we assume that δy_i are not only independent, but also normal; then u becomes multi-normal with the var-cov matrix I_n. By means of (25) Φ_{min} is expressed as a quadratic form in u,

$$\Phi_{min} = U^T C u \qquad (26)$$

with the matrix $C = W^{-1/2} B W^{-1/2} = (I_n - W^{1/2} PQP^T W^{1/2})^2 \qquad (27)$

Presently it will be shown that C has n-k+m eigenvalues equal to unity and k-m equal to zero. Consequently, there exists an orthogonal transformation $u = Vz$ that transforms Φ_{min} into a sum of the squares of n-k+m independent and (0, 1)-normal variables z_i,

$$\Phi_{min} = \sum_{1}^{n-k+m} z_i^2 \qquad (28)$$

so that[3] Φ_{min} has a χ^2-distribution with $q = n-k+m$ degrees of freedom. Its mean and variance are q and 2q. If q is large, the distribution of Φ_{min} is approximately normal $(q, \sqrt{2q})$. (Fisher recommends[3] to consider $\sqrt{2\Phi_{min}}$ as normally distributed $(\sqrt{2q-1}, 1)$ if q is large).

Still it remains to prove that C (eq. (27)) has q eigenvalues = 1, and n-q eigenvalues = 0,

$$\lambda_1(C) = \ldots = \lambda_q(C) = 1, \quad \lambda_{q+1}(C) = \ldots = \lambda_n(C) = 0 \tag{29}$$

Writing $E \equiv W^{1/2} P Q P^T W^{1/2}$ we observe that $\lambda((I_n-E)^2) = \lambda^2(I_n-E)$, it is sufficient for our purpose to show that

$$\lambda_1(E) = \ldots = \lambda_q(E) = 0, \quad \lambda_{q+1}(E) = \ldots = \lambda_n(E) = 1 \tag{30}$$

From $HH^{-1} = I_{k+m}$ (cf. (10) and (15)) we derive the equations

$$RQ = \theta \tag{31}$$

$$P^T W P Q = I_k - R^T S \tag{32}$$

$$SR^T = I_m \tag{33}$$

From (31) it is clear that Q and hence E have the rank k-m. This proves the first part of (30). Assuming now $\lambda(E) \neq 0$, we see by premultiplying $Ex = \lambda(E) \cdot x$ by $P^T W^{1/2}$ that

$$\lambda(E) = \lambda(P^T W P Q) \tag{34}$$

so the problem is reduced to find the eigenvalues $\neq 0$ of $P^T W P Q$. If we look at the term $R^T S$ in (32), this matrix has the rank m and consequently k-m zero eigenvalues and m non-zero eigenvalues. Its eigenvalue equation $R^T S x = \lambda(R^T S) x$ where $Sx \neq 0$) is premultiplied by S and gives when (33) is used $\lambda(R^T S) = 1$. It follows from (32) that all nonzero eigenvalues of $P^T W P Q$ are 1, whereby (34) and the second part of (30) are proved.

4. Semi-linear Least Squares Technique

We now turn to the computational aspects of the least-squares data fitting problem.

If the model (1) is nonlinear in b, an iterative solution method is necessary; we chose the Gauss - Newton method [1] with the diagonal modification proposed by Marquardt [2].

If $b = (\alpha, \beta)$, and $f(x; b)$ is nonlinear in β, but linear in α, it is possible to confine the iterations to the subspace of the nonlinear parameters and compute conditional solutions for α after each β-iteration. This device results as a rule in a considerable saving of iterations at the expense of a slight increase in the cost per iteration. Consider the model

$$y = f(x; \alpha, \beta) = \sum_{j=1}^{k_\alpha} a_j \, u_j(x; \beta) \tag{35}$$

where α has k_α and β k_β components, and let us assume that the m constraints (cf. (3)) are confined to α and are linear:

$$K\alpha = \delta \tag{36}$$

where $K = K_{mk_\alpha}$ (constraints on the nonlinear components are consequently restricted to the simple type (4)).

In sec. 5 we shall discuss the iterations in the β-space, but for the moment we consider β as fixed (to the value after a β-iteration), and shall minimize Φ (cf. (5)) by varying α under the constraints (36). As in sec. 2 we use Lagrange's method and consider

$$\Psi = \Phi + 2 \sum_{l=1}^{m} \mu_l \left(\sum_{j=1}^{k_\alpha} k_{lj} a_j - \delta_l \right) \tag{37}$$

and write down the equations $\frac{\partial \Psi}{\partial a_j} = 0$ and $\frac{\partial \Psi}{\partial \mu_l} = 0$:

$$\left.\begin{aligned} \sum_{j_1=1}^{k_a} \Big(\sum_i w_i\, u_{ij}\, u_{ij_1} \Big)\, a_{j_1} + \sum_{l=1}^{m} k_{lj}\, \mu_l &= \sum_i w_i\, y_i\, u_{ij} \\ \sum_{j=1}^{k_a} k_{lj}\, a_j &= \delta_l \end{aligned}\right\} \qquad (38)$$

where u_{ij} stands for $u_j(x_i; \beta)$ (here and in the following it is understood that summations over i run from 1 to n). (38) is a linear system of the order $k_a + m$:

$$\begin{array}{c} \\ k_a \\ m \end{array} \begin{array}{c} \begin{array}{cc} k_a & m \end{array} \\ \left[\begin{array}{c|c} C & K^T \\ \hline K & \theta \end{array}\right] \end{array} \begin{bmatrix} a \\ \hline \mu \end{bmatrix} = \begin{bmatrix} \gamma \\ \hline \delta \end{bmatrix} \qquad (39)$$

where $C_{jj_1} = \sum_i w_i\, u_{ij}\, u_{ij_1}$ and $\gamma_j = \sum_i w_i\, y_i\, u_{ij}$ (40)

In the nonlinear β-iterations we shall need the quantities $\frac{\partial f_i}{\partial \beta_{j'}}$ ($f_i \equiv f(x_i; a, \beta)$); according to the method applied, a is a function of β, $a = a(\beta)$, and we have

$$\frac{\partial f_i}{\partial \beta_{j'}} = \sum_{j_1=1}^{k_a} \left[\frac{\partial a_{j_1}}{\partial \beta_{j'}}\, u_{ij_1} + a_{j_1}\, \frac{\partial u_{ij_1}}{\partial \beta_{j'}} \right] \quad (j' = 1, \ldots, k_\beta) \qquad (41)$$

Hence, to evaluate $\frac{\partial f_i}{\partial \beta_{j'}}$, $\frac{\partial a_j}{\partial \beta_{j'}}$ has to be evaluated, and this can be done from (38) by taking the derivative of both members with respect to $\beta_{j'}$. The result of this procedure is

$$\sum_{j_1=1}^{k_a} \sum_i w_i u_{ij} u_{ij_1} \frac{\partial a_{j_1}}{\partial \beta_{j'}} + \sum_{j_1=1}^{k_a} \sum_i w_i \left[u_{ij} \frac{\partial u_{ij_1}}{\partial \beta_{j'}} + \frac{\partial u_{ij}}{\partial \beta_{j'}} u_{ij_1} \right] a_{j_1}$$

$$+ \sum_{l=1}^{m} k_{lj} \frac{\partial \mu_l}{\partial \beta_{j'}} = \sum_i w_i y_i \frac{\partial u_{ij}}{\partial \beta_{j'}} \qquad (42)$$

$$\sum_{j=1}^{k_a} k_{lj} \frac{\partial a_j}{\partial \beta_{j'}} = 0$$

or, in matrix notation:

$$\begin{array}{c} \\ k_a \\ m \end{array} \begin{array}{c} \begin{array}{cc} k_a & m \end{array} \\ \left[\begin{array}{c|c} C & K^T \\ \hline K & \theta \end{array}\right] \end{array} \begin{array}{c} \begin{array}{c} k_\beta \end{array} \\ \left[\begin{array}{c} A' \\ \hline M' \end{array}\right] \end{array} = \begin{array}{c} \begin{array}{c} k_\beta \end{array} \\ \left[\begin{array}{c} E \\ \hline \theta \end{array}\right] \end{array} \qquad (43)$$

where

$$a'_{jj'} = \frac{\partial a_j}{\partial \beta_{j'}} \quad , \qquad (44)$$

$$m'_{lj'} = \frac{\partial \mu_l}{\partial \beta_{j'}} \qquad (45)$$

and

$$e_{jj'} = \sum_i w_i \left[\frac{\partial u_{ij}}{\partial \beta_{j'}} (y_i - f_i) - u_{ij} \sum_{j_1=1}^{k_a} a_{j_1} \frac{\partial u_{ij_1}}{\partial \beta_{j'}} \right] \qquad (46)$$

The two systems (39) and (43) have the same matrix.

5. Gauss - Newton - Marquardt Iterative Technique

As stated earlier, iterations take place in the β-space only, where $b = (a, \beta)$ is the parameter vector. By the semi-linear technique we could express a as a function of β, $a = a(\beta)$, through eq. (39). In this section we shall focus on β and consider the following problem: Minimize

$$\Phi = \sum_i w_i (y_i - f(x_i; \beta))^2 \tag{47}$$

by varying β without any constraints (notice that $f(x_i; \beta)$ has been written for $f(x_i; a(\beta), \beta)$).

Basically, we use the Gauss - Newton iteration technique [1] (also called Taylor-series method). We expand the model $f(x; \beta)$ from a guessed or previously iterated value β_o through the linear terms. Then Φ is replaced by its linearized ($\langle\ \rangle$) form

$$\langle \Phi \rangle = \sum_i w_i (y_i - f_i - \sum_{j=1}^{k_\beta} \frac{\partial f_i}{\partial \beta_j} \delta\beta_j)^2 \tag{48}$$

where $\delta\beta_j = \beta_j - \beta_j^o$ are the components of the Gauss - Newton method correction vector d, $f_i = f(x_i; \beta_o)$, and $\partial f_i / \partial \beta_j$ are calculated at β_o. $\langle \Phi \rangle$ is minimized by

$$A\,d = g \tag{49}$$

where $A = P^T W P$, $p_{ij} = \frac{\partial f_i}{\partial \beta_j}$, $w_{ij} = \delta_{ij} w_i$,

$$g_j = \sum_i w_i (y_i - f_i) \frac{\partial f_i}{\partial \beta_j} \tag{50}$$

We cannot guarantee that the new Φ is smaller than the old one with the pure Gauss - Newton iteration technique. To achieve this, we introduce the Marquardt [2] modification of eq. (49):

$$(A + \lambda D^2)\, d = g \tag{51}$$

where D is a diagonal matrix with its elements scaled according to A, $d_{ij} = \delta_{ij}\sqrt{a_{ii}}$. λ is a parameter that is at our disposal, and as we shall see, λ provides for interpolation between the Gauss - Newton method and a gradient-like method. The former is obtained by taking $\lambda = 0$. On the other hand, for $\lambda \to \infty$ we obtain a solution vector proportional to $D^{-2} g$. It is easily seen that g is proportional to the gradient vector

$$dg = -\left(\frac{\partial \Phi}{\partial \beta_1}, \ldots, \frac{\partial \Phi}{\partial \beta_{k\beta}} \right)^T \tag{52}$$

so $D^{-2} g$ becomes a scaled form of dg and shares with dg the property that $\Phi(\rangle\Phi_{min})$ certainly does decrease initially along the correction vector, although it need not have the steepest-descent direction. Three theorems concerning the solution $d(\lambda)$ of eq. (51) exist which provide the background for our algorithm. They are scaled versions* of those given by Marquardt [2] and are proved in the same way.

Theorem 1: Let $\lambda \geq 0$ be arbitrary and let d' satisfy (51). Then d' minimizes $\langle\Phi\rangle$ (cf. (48)) on the ellipsoid $||D\,d|| = ||D\,d'||$.

Theorem 2: Let $d(\lambda)$ be the solution of (51). Then the norm $||D\,d(\lambda)||$ is a continuously decreasing function of λ tending to zero when $\lambda \to \infty$.

Theorem 3: The angle between $D\,d(\lambda)$ and $D\,d(\infty)$ is a continuously decreasing function of λ tending to zero when $\lambda \to \infty$.

These theorems lead directly to the algorithm. The equation to be solved at iteration no r reads

$$(A^{(r)} + \lambda^{(r)} D^{2(r)})\, d^{(r)} = g^{(r)} \tag{53}$$

From its solution $d^{(r)}$ we calculate

$$\beta^{(r+1)} = \beta^{(r)} + d^{(r)} \tag{54}$$

and a new Φ-value, $\Phi^{(r+1)}$. Now it is essential that $\lambda^{(r)}$ is so chosen that

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*Marquardt has in his exposition the unit matrix I instead of D. At a later stage, however, he introduces a scaling of the method, and his scaled algorithm is in fact equivalent to (51).

$$\Phi^{(r+1)} \leq \Phi^{(r)} \tag{55}$$

If $\Phi^{(r)} > \Phi_{min}$, it is always possible to satisfy (55) by selecting a sufficiently large $\lambda^{(r)}$, and so we avoid the divergence problems encountered in the Gauss - Newton method. However, $\lambda^{(r)}$ should not be chosen unnecessarily large, because we then get a small correction vector of a gradient-like type (theorem 3) involving slow convergence. In the later iterations, when convergence is approached, λ should be small. Then we approach the Gauss - Newton method which shows a very fast (quadratic) rate of convergence. The following Marquardt strategy is used:

Let ν be a fixed number >1 (Marquardt recommends $\nu = 10$). Let $\lambda^{(r)}$ be the λ-value from the previous iteration; we choose as $\lambda^{(o)}$ a suitable value, e. g. 0. 01. $\lambda^{(r+1)}$ will be determined by the following procedure:

$$\text{If } \Phi\left(\frac{\lambda^{(r)}}{\nu}\right) \leq \Phi^{(r)}, \text{ let } \lambda^{(r+1)} = \frac{\lambda^{(r)}}{\nu} \tag{56}$$

(the iteration is of "type A").

Otherwise, choose as $\lambda^{(r+1)}$ that value of $\lambda^{(r)} \cdot \nu^m$ $(m = 0, 1, 2, \ldots)$ which for the smallest value of m satisfies the inequality

$$\Phi(\lambda^{(r)} \nu^m) \leq \Phi^{(r)} \tag{57}$$

(the iteration is of "type B").

The iteration procedure has converged when $\Phi^{(r)}$ and $\beta^{(r)}$ are stationary for increasing r.

6. Summary and Conclusions

The present report has presented a discussion of the statistical and computational aspects of the general least-squares problem.

Special attention was devoted to the case where the model was only partially nonlinear.

Apart from the trivial constraints with fixed parameters, the formalism included linear constraints between the linear parameters.

Based on the theoretical background in this report, several computer

programmes have been worked out related to specific models. Examples are the sum-of-exponential problem [6] and the similar POSITRONFIT-programme [7, 8, 9] where the exponentials are folded with a Gaussian resolution function. These programmes have worked very satisfactorily and have yielded practical evidence of the soundness of the underlying principles.

7. References

1) R. H. Moore and R. K. Zeigler, The Solution of the General Least Squares Problem with Special Reference to High-Speed Computers. Los Alamos Scientific Laboratory, LA-2367 (1960) 94. pp.

2) D. W. Marquardt, An Algorithm for Least-Squares Estimation of Nonlinear Parameters, J. Soc. Ind. Appl. Math. 11 (1963) 431-441.

3) H. Cramer, Mathematical Methods of Statistics (Princeton University Press, Princeton, 1946) 575. pp.

4) G. E. Forsythe and C. B. Moler, Computer Solutions of Linear Algebraic Systems (Prentice-Hall, Englewood Cliffs, 1967) 148 pp.

5) G. H. Golub, Matrix Decompositions and Statistical Calculations. In: Statistical Computation. Edited by Roy C. Milton and John A. Nelder. Proceedings of a Conference held at The University of Wisconsin, Madison, Wisconsin, April 28-30, 1969 (Academic Press, New York, 1969) 365-397.

6) P. Kirkegaard, A Fortran IV Version of the Sum-of-Exponential Least Squares Code EXPOSUM, Risø-M-1279 (1970) 57 pp.

7) P. Kirkegaard and M. Eldrup, The Least Squares Fitting Program POSITRONFIT: Principles and Formulas, Risø-M-1400 (1971).

8) P. Kirkegaard and M. Eldrup, POSITRONFIT: A Versatile Least-Squares Fitting Computer Program for Analysing Positron Annihilation Lifetime Spectra. Submitted to the International Position Annihilation Conference 1971, Kingston, Ontario, Canada, 31 August - 2 September 1971.

9) P. Kirkegaard and M. Eldrup, POSITRONFIT: A Versatile Program for Analysing Positron Lifetime Spectra. Submitted to "Computer Physics Communications" 1971.

10) J. H. Wilkinson, Error Analysis of Direct Methods of Matrix Inversion, J. Ass. Comput. Mach. 8 (1961) 281-330.

APPENDIX

Solution of Linear Equations

According to (39), (43) and (51), an essential part of the least-squares problem is the solution of a symmetric linear system

$$A x = b \tag{58}$$

We first observe that the matrix $P^T W P$ (cf. (50)) is symmetric and positive-definite. By addition of positive terms in the diagonal we obtain the matrix of (51), and so this is also positive-definite.

The same is obviously true for the matrix of (39) and (43) as long as we disregard constraints.

This property permits a solution method of (58) which, in spite of the usual ill-conditioned behaviour of A, guarantees a solution that is stable in the sense of Wilkinson [10], i. e. it satisfies exactly an equation close to (58). One such method is that of Cholesky, where A is factorized as

$$A = GG^T \tag{59}$$

where G is a lower triangular matrix with positive diagonal elements. The merits of the Cholesky decomposition method applied to statistical problems have been discussed intensively by Golub [5].

The situation is less satisfactory when constraints are included. In that case, the matrix of (39) and (43) fails to be positive-definite, and the pure Cholesky decomposition (59) breaks down. One way to handle this case is to extend Cholesky's method to a decomposition of the type

$$A = G J G^T \tag{60}$$

where G has the same properties as in (59), and the diagonal matrix J has only ± 1 in the diagonal. Unfortunately, the solution obtained in this way is not necessarily stable. Another possibility is to ignore the symmetry of A and use standard Gaussian elimination with partial pivoting or Crout's method, which are both stable.

Depending on the nature of the problem and the precision of the available computer, it may be necessary to use iterative improvement [4] when solving (58).