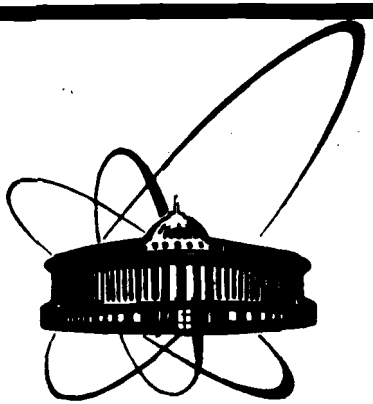

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V.I.Ilyushchenko, P.Kozma

# THE SOLUTION OF LEAST SQUARES PROBLEMS BY STANDARD AND SVD CODES

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1. Introduction

The general user's approach to the fitting of experimental data by means of analytical formulas consists in applying some more or less sophisticated standard minimization method enabling one to solve the given least squares (LSQ) problem, $Ax=b$, where A is a real mxn-matrix (design matrix) of rank $k \leq \min(m,n)$ to represent computed points, b is a real m-vector of the experimental data, and x is a real n-vector of the parameters to be found[1]. However, the most popular standard programs, e.g. MINUIT[2], generally produce only a partial subset of the parameters in question. Additionally, such programs require an input seed of the parameters being within strictly limited boundaries. As a result, these codes produce a single subset of the parameters to match a certain local minimum of the problem $Ax = b$.

2. Single value decomposition (SVD)

One of the most efficient tools to produce the full set of the searched parameters, x, is the SVD method[1,3] which consists in applying a factorisation of the type $A = U\Sigma V^T$, where U is an orthogonal unitary mxn-matrix, V is an orthogonal unitary nxn-matrix and $\Sigma$ is a diagonal mxn-matrix which elements $\sigma_{ij} = 0$ at $i \neq j$ and $\sigma_{ii} = \sigma_i \geq 0$. These latter are called singular values of the matrix A while the corresponding columns of the matrices U and V are left and right singular vectors.

One of the useful properties of the singular values is expressed as

$$\det(A) = \det(U) \cdot \det(\Sigma) \cdot \det(V^T) = \sigma_1 \cdot \sigma_2 \cdot \ldots \sigma_n \quad (1)$$

since $\det(U) = \det(V^T) = \pm 1$.

Furthermore, the matrix conditionality

$$\mathrm{COND}(A) = \sigma_{max}/\sigma_{min} \quad (2)$$

allows to compute the relative parameter errors as

$$\frac{\Delta x}{x} = \mathrm{COND}(A) \cdot \frac{\Delta b}{b} \quad (3)$$

and to evaluate both degeneracy and orthogonality of the matrix A. It is well known that the matrix A is more degenerate than the matrix B, if

$$COND(A) > COND(B) \qquad (4)$$

while for the orthogonal matrix A we have

$$COND(A) = 1 . \qquad (5)$$

This corresponds to the case of the totally independent parameters, x.

A subsequent analysis of the found singular values (SVA) provides not only the full set of the fitted parameters, but also some additional information to choose an optimum subset. Such an approach is exemplified by the program system SALS[4].

## 3. Available SVD codes

The well-known program library LIBCERN, incorporated as LIB1.LIBRARIES on the computer EC-1055M, contains, as its member F600, the single precision subroutine SVD being a real version of the Fortran subroutine developed by Businger and Golub[5].

The same algorithm is realised in another single precision SVD subroutine from[3]. We have also produced its double precision version.

Finally, we have implemented the program PROG4 with the SVD subroutine, SVA[1], as an original single/double precision version and a new double precision version, SVAD. To provide crosscheck possibilities, we have also used the program PROG2 with HFTI and COV algorithms incorporated in it.

## 4. An illustrative example

To compare adequately the computational results, we have used the parametrization Gaussian from[6]

$$\sigma(A,Z) = \sigma(A)\left[2\pi C_z^2(A)\right]^{-1/2} \exp\left[-\frac{(Z - Z_p(A))^2}{2C_z^2(A)}\right], \qquad (6)$$

where $\sigma(A)$ are isobaric yields, $C_z(A)$ is the charge dispersion width parameter for the mass number A, and $Z_p(A)$ is the most probable atomic number for that A. The sample input data set[7] for the reaction $^{12}C + ^{238}U$ at an energy of 3.65 AGeV is presented in Table 1.

The main technical difference between the SVD and standard MINUIT codes consists in the presentation method of trial functions. The SVD codes require a special design matrix A to be consistent with the linear LSQ problem in question, while the standard codes allow the analytical fitting formulas including nonlinear ones to be used in their original form.



The MINUIT double precision version has been used as a mass production fitting code, while the SVD and complementary HFTI codes served as checking tools, e.g. in some ambiguous cases with abnormally low or high values of $\chi^2$/NDF.

The analytical expression for presenting Formula 6 as an input design matrix is:

$$A_{I1}.X1 + A_{I2}.X2 + A_{I3}.X3 + A_{I4}.X4 + A_{I5}.X5 = B , \qquad (7)$$

where

$$X1 + X2.A = Z_p(A) ,$$

$$X3 = \ln(\sigma(A)) - \frac{X1^2}{2C_z^2(A)},$$

$$X4 = X1.X2 ,$$

$$X5 = X2^2,$$

$$A_{I1} = 2C_z^2(A) ,$$

$$A_{I2} = 2Z ,$$

$$A_{I3} = 2ZA ,$$

$$A_{I4} = -2A,$$

$$A_{I5} = -A^2 .$$

The results obtained by means of the MINUIT, SVD and HFTI codes are presented in Table 2. It can be easily shown that the best SVD solution corresponds to the 4-th subset of the searched parameters.

## 5. Conclusion

The available SVD codes produce the full set of the searched parameters with some additional information to choose an optimum subset. The latter can be used, e.g., as an initial seed for the conventional codes of the MINUIT type to yield a final high precision result with accompanying error analysis, contour diagrams and other servicing tools.

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Table 1. Input data set[7]

| | Z | A | $\sigma(A,Z)$ [mb] | $\sigma(A,Z)$ [mb] |
|---|---|---|---|---|
| 1 | 21 | 44 | 4.7 | 0.6 |
| 2 | 21 | 46 | 10.9 | 1.3 |
| 3 | 21 | 48 | 6.0 | 0.6 |
| 4 | 23 | 48 | 3.6 | 0.4 |
| 5 | 25 | 52 | 1.7 | 0.5 |
| 6 | 25 | 56 | 12.0 | 3.5 |
| 7 | 26 | 59 | 14.6 | 2.1 |

Table 2. Computational results

| Code | X1 | X2 | X3 | X4 | X5 | $\sigma_i$ |
|---|---|---|---|---|---|---|
| MINUIT | 1.63 | 0.42 | 21.0 | ---- | ---- | ---- |
| HFTI | 1.98 | 0.41 | 17.1 | 0.83 | 0.16 | ---- |
| SVD-1 | 0.002 | 0.1 | 20.0 | -0.4E-2 | -0.11 | 0.9E4 |
| SVD-2 | 0.027 | 0.45 | 20.0 | -0.03 | 0.2 | 0.2E3 |
| SVD-3 | 0.033 | 0.45 | 19.9 | -0.04 | 0.2 | 24.9 |
| SVD-4 | 1.97 | 0.41 | 22.8 | 0.83 | 0.17 | 0.31 |
| SVD-5 | 2.01 | 0.41 | 11.8 | 0.83 | 0.17 | 0.01 |

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Илющенко В.И. Козма П.


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Решение задач МНК с применением стандартных и SVD программ


Метод сингулярного разложения (SVD)позволяет решать задачи МНК (Ax = b) в общем виде, обеспечивая полный набор искомых параметров. Единственной технической особенностью этого метода является преобразование исходной фитирующей формулы в адекватную матрицу плана A. Комбинация из SVD и стандартных программ типа MINUIT обеспечивает возможности для взаимного контроля полученных результатов.



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Ilyushchenko V.I., Kozma P.


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The Solution of Least Squares Problems by Standard and SVD Codes


The method of singular value decomposition (SVD) enables one to solve the least squares problem (Ax = b) in a most general manner producing the full set of searched for parameters, x. The only technical peculiarity of this method consists in transforming an initial analytical fitting formula into the appropriate design matrix, A. A combination of any SVD code with a standard one, e.g. MINUIT, provides a reliable tool to crosscheck the obtained results.



The investigation has been performed at the Laboratory of High Energies, JINR.

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