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Solution of Large Systems of Linear Equations with Quadratic or Non-Quadratic Matrices and Deconvolution of Spectra

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SOLUTION OF LARGE SYSTEMS OF LINEAR EQUATIONS WITH QUADRATIC OR NON-QUADRATIC MATRICES AND DECONVOLUTION OF SPECTRA

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ABSTRACT

The numerical deconvolution of spectra is equivalent to the solution of a (large) system of linear equations with a matrix which is not necessarily a square matrix. The demand that the square sum of the residual errors shall be minimum is not in general sufficient to ensure a unique or "sound" solution. Therefore other demands which may include the demand for minimum square errors are introduced which lead to "sound" and "non-oscillatory" solutions irrespective of the shape of the original matrix and of the determinant of the matrix of the normal equations.

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INTRODUCTION

The classical measuring theories deal mainly with a statistical treatment of data obtained by measurements on identified objects. However, in modern physics one often collects a series of data and the task is then to identify some objects by means of a statistical treatment of the collected data. Hereby the conditions for using the classical theories on modern measurements are altered, a fact which is often overlooked and which might give rise to completely misleading results. For instance, there is a great difference in evaluating data from a spectrum consisting of known spectral lines and in evaluating which lines are present in a measured spectrum. Naturally one ought to use different statistical methods in the two cases, but the classical theories which are applicable to the former problem have such an authority that they are often applied without reservation to the latter despite the fact that one of the conditions (identified objects) is missing. It is the aim of this paper to present a new method for deconvolution of spectra. This is done numerically and is equivalent to the solving of a system of linear equations with square or non-square matrices.

I. DESCRIPTION OF THE PROBLEM

Let

$$y(t) = \int_{u_1}^{u_2} x(u)g(t,u)du \tag{1}$$

represent a known (measured) spectrum $t_1 \le t \le t_2$, $g(t,u)$ the generating function and $x(u)$, $u_1 \le u \le u_2$, the wanted spectrum. In order to treat the problem numerically it is common to write the numerical values of y and g in a, naturally finite number of points or

$$\begin{aligned} y(t_1) &= \Delta u[\, g(t_1,u_1)x(u_1) + g(t_1,u_1+\Delta u)x(u_1+\Delta u) + \ldots \,] \\ y(t_1+\Delta t) &= \Delta u[\, g(t_1+\Delta t,u_1)x(u_1) + g(t_1+\Delta t,u_1+\Delta u)x(u_1+\Delta u) + \ldots \,] \end{aligned} \tag{2}$$

With the abbreviations

$$y_r = y(t_1 + (r-1)\Delta t) \tag{3}$$

$$\underline{y} = \begin{Bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ y_N \end{Bmatrix} \tag{4}$$

$$x_s = [\, x(u_1 + (s-1)\Delta u)]\Delta u \tag{5}$$

$$\underline{x} = \begin{Bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_M \end{Bmatrix} \tag{6}$$

$$a_{rs} = g(t_1 + (r-1)\Delta t,\ u_1 + (s-1)\Delta u) \tag{7}$$

$$\underline{a}_s = \begin{Bmatrix} a_{1s} \\ a_{2s} \\ \cdot \\ \cdot \\ a_{Ns} \end{Bmatrix} \tag{8}$$

$$\underline{A} = \left\{ \begin{array}{cccc} a_{11} & a_{12} & \cdots & a_{1M} \\ a_{21} & & & \\ \vdots & & & \\ a_{N1} & & & a_{NM} \end{array} \right\} \tag{9}$$

the equations (2) are written

$$\underline{y} = \underline{A}\,\underline{x} \tag{10}$$

In (10) $\underline{y}$ and $\underline{A}$ are known quantities and $\underline{x}$ is to be found. Seemingly (10) can be solved by assuming that N = M and that $|\,\underline{A}_{NM}\,|$, the determinant of $\underline{A}$, is different from zero. In that specific case

$$\underline{x} = \underline{A}^{-1}_{NN}\,\underline{y} \tag{11}$$

If $\underline{x}$ found from (11) is to be regarded as a sound solution to (1) it must be only marginally dependent on the chosen number N = M. In practice N, the dimension of $\underline{y}$, has an upper limit. If $\underline{y}$ is a spectrum recorded by means of a multichannel analyzer, N_{max} is equal to the number of channels and, if $\underline{y}$ is logged from a continuously recorded spectrum, it is of no use to go beyond the point at which any value of y(t) can be found - within the experimental error limits - by means of linear interpolation between two chosen neighbour points y_2 and y_{r+1}. Now suppose that $M = N_{max}$ and $|\,A_{NN}\,| \neq 0$. Then (11) represents a solution which can be found with a computer in the well known way. Let the solution be denoted $\underline{x}_o$. The solution $\underline{x}_o$ inserted in (10) yields

$$\underline{y} = \underline{A}_{NN}\,\underline{x}_o + \underline{\varepsilon}$$

where $\underline{\varepsilon}$ represents the unavoidable computational errors which ought to be well within the limit of the experimental errors. To judge the "quality" of $\underline{x}_o$ a new subdivision $\Delta_1 u = \frac{1}{2}\,\Delta u$ is made.

By defining

$$\underline{x}_d = \begin{Bmatrix} x_1 \\ x_3 \\ x_5 \\ \cdot \\ \cdot \\ x_{2N-1} \end{Bmatrix} \tag{13}$$

and

$$\underline{x}_f = \begin{Bmatrix} x_2 \\ x_4 \\ \cdot \\ \cdot \\ x_{2N-2} \end{Bmatrix} \tag{14}$$

we get

$$\underline{A}_{NN}\,\underline{x}_d + \underline{B}\,\underline{x}_f = \underline{y}_N \tag{15}$$

where B is an $(N-1)\cdot N$ dimensional matrix. As it is assumed that $|A_{NN}| \neq 0$, (15) can be solved for $\underline{x}_d$ by assuming an arbitrarily chosen vector $\underline{x}_f$. This simply means means that we can choose half of the x coordinates arbitrarily and calculate the other half or, in other words, there are infinitely many functions x(u) which satisfy (1) for given y(t) and given g(t,u) in a finite interval t_1 through t_2 and u_1 through u_2. A unique solution does not exist unless further conditions are forced on x(u). One might, for instance, demand that x(u) shall be a, in some sense, smooth function of u, but first it is valuable to study (10) a little further. It is evident that the better this equation represents (1), the greater the probability of finding a representative solution. That means that a very small Δu is desirable. On the other hand it is desirable to have as few numbers as possible in $\underline{A}$ to save computational work. A suitable compromise is to make the interval Δu so small that any three succeeding $\underline{a}_s$, $\underline{a}_{s+1}$ and $\underline{a}_{s+2}$ (see (8)) are mutually linearly dependent (within the error limits). In that case the equation (10)

contains all information available from (1) because any g(t,u) value can be obtained by linear interpolation if necessary. We might say that any $\underline{x}$ vector which satisfies (10) is a solution to the deconvolution of the y(t) spectrum, but the fact that the physicist who poses the problem will not accept such an answer means that he has certain expectations on the solution which are not contained in (10). Such expectations are very hard to express in a way that is understandable to a computer, especially because they may be contradictiory to the demand that (10) must also be satisfied. Thus the expectations must be expressed in such a way that they are satisfied as far as possible - i.e. without violating (10). A very fruitful way to express the expectations is to deliver an expected solution $\underline{x}_e$ and to demand $(\underline{x}_e - \underline{x})^T (\underline{x}_e - \underline{x})$ = minimum on condition that (10) is satisfied. Then the problem has a unique solution and a series of computations has shown that the solution does not depend much on $\underline{x}_e$, which therefore might be put equal to the zero vector. Even if the solution found in this way is not quite satisfactory, it is nevertheless much better than the assumed $\underline{x}_e$. It can therefore be used as basis for an estimation of a new $\underline{x}_e$ provided that one can present a more explicit formulation of one's demands. At least one should be able to tell why the solution found was not satisfactory.

II. TRANSFORMING A RECTANGULAR MATRIX INTO AN EQUIVALENT TRIANGULAR MATRIX

The problem of deconvolution of spectra has now turned into the problem of solving the equation

$$\underline{y} = \underline{A}\,\underline{x} \tag{16}$$

for given $\underline{y}$ and $\underline{A}$ which is not necessarily a square matrix. If there is more than one solution, the one which gives

$$(\underline{x} - \underline{x}_e)^T(\underline{x} - \underline{x}_e) = \text{minimum} \tag{17}$$

is chosen. $\underline{x}_e$ represents an "expected" solution which is considered to be given. The system of equations (16) might be overdetermined (N > M) and in that case we may write

$$\underline{y} = \underline{A}\,\underline{x} + \underline{\varepsilon} \tag{18}$$

and determine the solution which yields $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum. The vector $\underline{\varepsilon}$ may be considered to consist of experimental errors and for a "sound" problem we shall have $\underline{y}^T\underline{y} >> \underline{\varepsilon}^T\underline{\varepsilon}$. In practice, especially when larger systems are considered, $\underline{\varepsilon}$ also depends on computational errors which cannot be disregarded, in fact the computation itself is often the main source of errors. It is therefore necessary to choose a suitable method for the computation. First (18) is considered for N > M (the number of equations is larger than the number of unknowns) with the condition that $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum. A traditional method of solving (18) is to multiply both sides by $\underline{A}^T$ and solve

$$\underline{A}^T\underline{y} = \underline{A}^T\underline{A}\,\underline{x} \tag{19}$$

as it can be proved that $\underline{A}^T\underline{\varepsilon} = 0$ for $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum. This method has the drawbacks that it only works for N ≥ M and when the determinant of $|A^TA| \neq 0$, and that it is very sensitive to small errors. A much more direct method which demands less computational work and is less sensitive to errors is shown next.

Consider $\underline{y}$ to be a linear combination of the $\underline{a}$ vectors

$$\underline{y} = \underline{a}_1 x_1 + \underline{a}_2 x_2 + \cdots \underline{a}_M \tag{20}$$

Now each vector in (20) is split into a sum of two vectors, the one being proportional to $\underline{a}_1$, the other orthogonal to $\underline{a}_1$. Thus

$$\underline{a}_s = k_s\underline{a}_1 + \underline{b}_s$$

and

$$\underline{y} = k_y\underline{y} + \underline{b}_y \tag{21}$$

As $\underline{b}_s$ is orthogonal to $\underline{a}_1$, ($\underline{a}_1^T\,\underline{b}_s = 0$), k_s is found by multiplying the equations (21) by $\underline{a}_1^T$ or

$$k_s = \frac{\underline{a}_1^T \underline{a}_s}{\underline{a}_1^T \underline{a}_1} \tag{22}$$

and

$$\underline{b}_s = \underline{a}_s - \frac{\underline{a}_1^T \underline{a}_s}{\underline{a}_1^T \underline{a}_1} \cdot \underline{a}_1 \tag{23}$$

Hence (20) can be written

$$k_y \underline{a}_1 + \underline{b}_y = \underline{a}_1 \{x_1 + k_2 x_2 + \cdots k_M x_M\} + \underline{b}_2 x_2 + \underline{b}_3 x_3 + \cdots \underline{b}_M x_M \tag{24}$$

Equations (24) consist of two systems which are orthogonal to each other and can therefore be split into two independent systems, namely

$$k_y \underline{a}_1 = (x_1 + k_2 x_2 + \cdots k_M x_M) \underline{a}_1 \tag{25}$$

and

$$\underline{b}_y = \underline{b}_2 x_2 + \underline{b}_3 x_3 + \cdots \underline{b}_M x_M \tag{26}$$

Equations (25) are mutually proportional and are transformed into a single equation by multiplying by $\underline{a}_1^T$. Using the abbreviations

$$z_1 = k_y (\underline{a}_1^T \underline{a}_1) = a_1^T y \tag{27}$$

$$c_{1s} = k_s (\underline{a}_1^T \underline{a}_1) = \underline{a}_1^T \underline{a}_s \tag{28}$$

Equations (25) become

$$z_1 = c_{11} x_1 + c_{12} x_2 + c_{13} x_3 + \cdots c_{1M} x_M \tag{29}$$

Equations (26) do not contain x_1. They are now treated as the original system, namely each vector in (26) is split into two vectors, one proportional to $\underline{b}_2$ and one orthogonal to $\underline{b}_2$, and so the result becomes a new equation

$$z_2 = c_{22}x_2 + c_{23}x_3 + \cdots c_{2M}x_M \tag{30}$$

and a new set of equations which do not contain x_2 and the process can proceed. The final result becomes

$$\begin{aligned} z_1 &= c_{11}x_1 + c_{12}x_2 + \cdots \quad c_{1M}x_M \\ z_2 &= \quad c_{22}x_2 + c_{23}x_3 + \cdots c_{2M}x_M \\ &\cdot \\ &\cdot \\ z_M &= \quad c_{MM}x_M \end{aligned} \tag{31}$$

or in shorthand $\underline{z} = \underline{C}\ \underline{x}$ (31a)

Equations (31) form a very interesting system containing M equations with M unknowns. It can be computed for any N irrespective of the rank of $\underline{A}$, and any solution $\underline{x}$ which satisfies the system also satisfies (18) with $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum (the easy proof will be omitted here). The system might be well fitted for determining $\underline{x}$ by starting with the last equation; c_{MM}, however, is often small, so that x_M is poorly defined. Whenever there is a small value of c_{ss} in the main diagonal, the corresponding x_s will be poorly defined and a possible error will be transmitted to the x_p's with $p < s$. (When the calculations are carried out with a computer, the probability that any c_{ss} will be exactly zero is almost null owing to residual errors). Even a poorly defined solution to (31), however, satisfies all conditions presented so far. It satisfies (18) with $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum. If the solution is not satisfactory, it must be because further expectations are placed on the solution which are not expressed by means of the original system of equations. The only way to get out of the dilemma is to express the expectations in a logical way and find the $\underline{x}$ vector which satisfies (18) within the error limits and which is as close to the expectations as possible. This can be done, for instance, by introducing an "expected" vector $\underline{x}_e$ and demanding that $(\underline{x} - \underline{x}_e)^T(\underline{x} - \underline{x}_e)$ = minimum with the condition that (18) is satis-

fied within the error limits. In general the assumption that $\underline{x}_e$ is equal to the zero vector suffices to deliver an acceptable "non-oscillatory" solution. So we are again at the starting point: solve (16) and (17). However, on the way we have got a method for transforming a matrix, square or non-square, into an equivalent triangular matrix which can be used to solve the complete problem as shown below.

III. THE COMPUTER SOLUTION

The problem: find $\underline{x}$ such that

$$(\underline{x} - \underline{x}_e)^T(\underline{x} - \underline{x}_e) = \text{minimum} \qquad (17) \qquad (32)$$

on the condition that

$$\underline{y} = \underline{A}\,\underline{x} \qquad (16) \qquad (33)$$

within the experimental errors. $\underline{x}_e$, $\underline{y}$ and $\underline{A}$ are given. Further $\underline{y}$ is subject to experimental errors, the mean square of which is approximately known. Naturally the elements of $\underline{A}$ are also subject to errors. This might play a certain role when large systems are considered and will be discussed in the last chapter. We start by assuming that $\underline{\varepsilon}^T\underline{\varepsilon} \ll \underline{y}^T\underline{y}$ such that (33) is essentially correct. Differentiating (32) yields

$$(\underline{x} - \underline{x}_e)^T\, d\underline{x} = 0 \qquad (34)$$

and from (33)

$$\underline{A}\, d\,\underline{x} = 0 \qquad (35)$$

For any vector

$$\underline{q} = \begin{Bmatrix} q_1 \\ q_2 \\ \cdot \\ \cdot \\ \cdot \\ q_N \end{Bmatrix} \qquad (36)$$

we then have

$$(\underline{x} - \underline{x}_e)^T \, d\underline{x} = - \underline{q}^T \underline{A} \, d\underline{x} \; (= 0) \tag{37}$$

On the other hand, if we can find a vector $\underline{q}$ (Lagrangeian factors) such that

$$(\underline{x} - \underline{x}_e)^T = - \underline{q}^T \underline{A} \tag{38}$$

then (34) is satisfied when (35) is satisfied. Thus (32) and (33) are equivalent to (33) and (38), which can be symbolized together in one system of equations

$$\begin{Bmatrix} \underline{O} & \underline{A} \\ \underline{A}^T & \underline{E} \end{Bmatrix} \begin{Bmatrix} \underline{q} \\ \underline{x} \end{Bmatrix} = \begin{Bmatrix} \underline{y} \\ \underline{x}_e \end{Bmatrix} \tag{39}$$

where $\underline{O}$ is the N·N dimensional zero matrix and $\underline{E}$ the M·M dimensional unit matrix. The matrix of (39) is an (N+M)(N+M) square matrix which can be transformed into a triangular matrix according to the procedure described in the previous chapter. We get

$$\begin{Bmatrix} c'_{11} & c'_{12} & c'_{13} & \cdots & c'_{1,M+N} \\ 0 & c'_{22} & \cdots & & \\ 0 & 0 & c'_{33} & \cdots & \\ & & & c'_{NN} & \cdots \\ 0 & & & 0 & c'_{N+1,N+1} \\ 0 & 0 & 0 & & c'_{M+N,M+N} \end{Bmatrix} \begin{Bmatrix} \\ \underline{q} \\ \\ \\ \underline{x} \\ \end{Bmatrix} = \underline{z}' \tag{40}$$

From (40) $\underline{x}$ can be found immediately from the lower part of the matrix (the upper part and $\underline{q}$ are without interest) and so the problem is solved apart from a discussion of errors.

IV. DISCUSSION OF ERRORS

First we consider the equations

$$\underline{y} = \underline{A}\,\underline{x} + \underline{\varepsilon} \tag{41}$$

where $\underline{\varepsilon}$ represents unknown errors in the $\underline{y}$ elements. The complete solution of (41) implies that the errors have been found. As this is impossible, it is common to demand that $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum. In general one knows the expected mean value of $\underline{\varepsilon}^T\underline{\varepsilon}$ and, if N (the dimension of $\underline{y}$) is large, $(\underline{\varepsilon}^T\underline{\varepsilon})_{mean}$ is known with a high degree of accuracy. From a logical point of view an $\underline{x}$ vector which leads to a probable error vector $\underline{\varepsilon}$ with $\underline{\varepsilon}^T\underline{\varepsilon} = (\varepsilon^T\varepsilon)_{mean}$ should be a more probable solution than the $\underline{x}$ vector which leads to $\underline{\varepsilon}^T\underline{\varepsilon} = (\underline{\varepsilon}^T\underline{\varepsilon})_{minimum}$ unless $(\underline{\varepsilon}^T\underline{\varepsilon})_{mean} \approx (\underline{\varepsilon}^T\underline{\varepsilon})_{min}$. The use of $(\underline{\varepsilon}^T\underline{\varepsilon})_{min}$, however, has the advantage that $\underline{x}$ becomes uniquely defined if $N \geq M$ and the rank of $\underline{A}$ is equal to M (the dimension of $\underline{x}$). On the other hand it has the drawback that one tries to compensate the errors (which are known to exist) in the $\underline{y}$ vector by means of errors in the $\underline{x}$ vector. If the $\underline{a}$ vectors are not almost mutually orthogonal, there is a large risk that small errors in $\underline{y}$ are exchanged for large errors in $\underline{x}$ and we get the so-called "oscillatory" solutions. But only if one has some expectations as regards the proper solution is one able to judge whether a solution is "oscillatory" or "sound". We cannot disregard the fact that a system like (41) is uncertain to some degree and, pushing the matter to extremes, one may say that if one has no expectations on the solution whatsoever one has no reason to solve the system. As shown in the previous chapter the expectations can be used to remove uncertainties if they are logically expressed and fit into the system. The expectation that $\underline{\varepsilon}^T\underline{\varepsilon}$ shall be minimum is, under certain conditions, sufficient to ensure a proper solution, but not in general.

Equations (39) contain the original system $\underline{y} = \underline{A}\,\underline{x}$ and, theoretically that means - without paying attention to computational errors - that the solution of (39) by means of the method shown will be a "minimum square" solution. However, in the calculations the number of digits is limited and computational errors are unavoidable. Such errors depend both on the method of computation and on the relative size of the elements in the matrix. If, for instance, all elements of $\underline{A}$ are very small compared to

1, the elements in the main diagonal of $\underline{E}$, then the system (39) in practice becomes nearly $\underline{x} = \underline{x}_e$, or, if all elements in $\underline{A}$ are very large compared to 1, the lower part of the system loses in importance and $\underline{y} = \underline{A}\,\underline{x}$ becomes the essential part. That means that the solution obtained in practice might depend to some extent on the weight of the original system, which therefore must be given some thought. In parctice the following method is recommended. Multiply each equation in $\underline{y} = \underline{A}\,\underline{x}$ by a constant divided by the expected mean error (not mean square error). Thereby we get a new system $\underline{y}' = \underline{A}'\underline{x}$ with equal mean error for each equation. Choose the constant such that the expected mean error per equation becomes $1 \cdot 10^{-v}$, where v is the number of digits used per element in the computation. Make the substitution

$$\underline{W}\,\underline{x}' = \underline{x} \tag{42}$$

with

$$\underline{W} = \begin{pmatrix} w_1 & & & \\ & w_2 & & O \\ & & \ddots & \\ & O & & w_M \end{pmatrix} \tag{43}$$

and choose the w's such that the largest mean error in one element of $\underline{a}_s \cdot w_s$ is equal to $1 \cdot 10^{-v}$. Insert the new system

$$\underline{y}' = \underline{A}'\,\underline{W}\underline{x}' = \underline{A}''\underline{x}' \tag{44}$$

in (39) (instead of $\underline{y} = \underline{A}\,\underline{x}$). Solve it according to (40) and the solution will be the very solution which satisfies $\underline{y} = \underline{A}\,\underline{x}$ within the error limits and is "closest" to the expected solution.

The use of the "expected" $\underline{x}_e$ in (39) has an influence on the solution only if the rank of $\underline{A}$ is small (compared to M, the number of unknowns). If not, the solution might still depend too much on experimental errors (in $\underline{y}$) to be acceptable, because the errors in $\underline{y}$ are in general <u>not</u> due

to errors in $\underline{x}$. In such case the best way is to look for a more probable square error sum (which is in general known) and relax the demand that $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum, for instance by demanding that $\underline{\varepsilon}^T\underline{\varepsilon}$ = minimum on condition that x(u) = P(u), where P(u) is a polynomial of maximum pth order. This leads to an expression similar to (39). Rather than the matrix inversion, the main problem is often to express one's demands in a rational way.

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