MATRIX-ORTHONORMALIZATION METHOD IN ADJUSTMENT

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> (Received October 28th, 1974) Presented by Dr. Péter Biró

Several factors may have a decisive influence on the precise solution of adjusting problems with many unknowns. Accuracy may significantly be reduced by four basic sources of error [1], such as:

i. Inherent errors of the theory

To solve any problem, first a mathematic model has to be chosen which, however, only approximates the basic problem with certain simplifications and neglects.

ii. Inherent errors of measurement

Errors bear often on the observation results in the computation, because of the finite accuracy proper to the measuring instruments. If the matrix formed of the coefficients of some equation system and the vector of absolute terms are quantities obtained by measurement and calculation — i. e. known only approximately — then a single approximation of the "theoretical" equation system is known.

iii. Approximation errors

To solve the mathematical model chosen according to i., often numerical approximation methods have to be applied. Linearization of the observation or condition equations, the use of iteration methods etc... may act as sources of error.

iv. Rounding-off errors

The limited number representation of computers and the primary operations — especially calculation of product sums type $\sum_{i=1}^n a_i \, b_i$ — imply important sources of error by rounding-off. If the accuracy of operations in a calculation set is limited, the rounding-off errors in each operation add up to decisively affect the accuracy of the final result.

Let us consider particulars of the enumerated error types.

In the majority of the problems, adjustment is based on Gauss' theory of errors using the least squares adjustment through writing and solving the so-called normal equations. This implies a possible mathematical formulation according to i. Of course this is not the only existing model, even as will be pointed out later, in some cases it is unworkable.

After the best fitting mathematical model is chosen, knowing the laws of error propagation and the desired accuracy, the necessary observation accuracy can be determined, in view of ii. (Since, however, the two are related, it is imperative to choose the model according to i, and to determine the adequate observation accuracy simultaneously.)

Numerical solution of a problem is connected with approximations according to iii. Also the choice of the mathematical model and item iii may be interrelated, because in general the different mathematical models may involve different numerical approximative methods.

Among the sources of error referred to in iv, the rounding-off errors may greatly influence the accuracy of the final result. There are two possibilities to eliminate, or better to diminish them, viz.: use of double-accuracy number representation when collecting inner products (product sums); and choice of a suitable mathematical model. Obviously, algorithms requiring to form as few product sums type $\sum_{i=1}^{n} a_i b_i$ during the calculations as possible are preferred.

Analyzing the adjustment problems, great many problems are found where the most common method (solution by writing and solving normal equations) fails in accuracy, — in some cases the error of the solution may exceed the expected error limits by orders of magnitude.

To mention but a few examples, recently we were faced by this problem in adjusting certain gravimetric nets, orbit elements of satellites, or deflections of the vertical calculated e. g. from Eötvös torsion balance measurements.

Now, some statements concerning the solution of normal equation systems will be made to confirm the insufficient accuracy and even uselessness or falseness of the adjustment method by setting up and solving normal equations in the case of so-called poorly conditioned adjustment problems.

Be the matrix equation (n > r)

$$\mathbf{v} = \mathbf{A} \quad \mathbf{x} + \mathbf{l} \\ (n,1) \quad (n,r) \quad (r,1) \quad (n,1)$$

the form expressed for correction of the linearized observation equations of some adjustment problem — where v is the vector of residuals, x the vector of unknowns, A the coefficient matrix of the observation equations and I the vector of absolute terms.

The condition

$$\mathbf{v}^* \mathbf{v} = \min_{(1,n)} \min_{(n,1)}$$

is likely to be satisfied by the normal equation system

using symbols

$$\begin{array}{ccc}
\mathbf{A}^{\star} & \mathbf{l} = \mathbf{n} \\
\mathbf{r},\mathbf{n}) & (\mathbf{r},\mathbf{l}) & (\mathbf{r},\mathbf{l})
\end{array} \tag{2}$$

and

$$\mathbf{A}^* \quad \mathbf{A} = \mathbf{N}$$

$$\mathbf{N} \quad (r,n) \quad (r,r) \quad (r,r)$$

hence

$$\mathbf{x} = -\mathbb{N}^{-1} \mathbf{n}$$
.

Matrix N formed according to (3) is the so-called coefficient matrix of the normal equation system (1). (The transpose of matrix (vector) A will be denoted by A^* , its inverted by A^{-1} , the transpose of the inverted or the inverted of its transpose by A^{-*} .)

Thus, the coefficient matrix N of the normal equation system and its vector n are seen to be functions of the coefficient matrix A of the observation equation system and of its absolute term I. The coefficients of the observation equation system being measured and calculated quantities therefore according to ii, only an approximation of the "theoretically accurate" equation system is known and can be solved. If the theoretically exact equation system has an unambiguous solution, it is not sure at all that the approximation has one single solution and even if it has, the two solutions might greatly differ. One may wonder how much the coefficients of a linear equation system of unambiguous solution can be changed to produce a new approximative system with a necessarily unambiguous solution so that the solutions of the two systems are rather similar in some respect. And also, what are conditions for matrix N obtained by slightly changing the invertible matrix $\widetilde{\bf N}$ to have an inverted for the difference of matrices ${\bf N}^{-1}$ and $\widetilde{\bf N}^{-1}$ to be small in some respect.

Let us introduce now the concept of stable and unstable inverted matrices. An inverted matrix is stable if a small variation of the original matrix elements results in a proportionally small change in the elements of the inverted matrix, in the opposite case it is unstable.

The original matrix of the stable inverted matrix is termed a wellconditioned matrix, and that of the unstable inverted matrix is termed a poorly conditioned one.

(To be noted that the conditioning of matrices is well characterized by the condition number. Among the common definitions, condition number of a matrix N is the numerical value

$$\operatorname{cond}\left(\mathbb{N}\right) = \frac{\max\left|\lambda_{i}\right|}{\min\left|\lambda_{i}\right|} \tag{4}$$

where λ_i $(i=1, 2, \ldots, k)$ are the eigenvalues of matrix N.)

If the elements of a poorly conditioned matrix are but approximately known, this matrix may prove practically singular. Namely the determinant of the "theoretical" matrix may happen to be non-zero, but changing a single element of the matrix within the observation of computation accuracy a matrix with zero determinant may be obtained. For instance in case of $\delta=0$, matrix

$$\mathbf{N} = \begin{bmatrix} 4+\delta & 6 & 5 & 4 \\ 6 & 9 & 7 & 6 \\ 5 & 7 & 9 & 8 \\ 4 & 6 & 8 & 3 \end{bmatrix}$$

has a determinant det (N) = 1, but for $\delta = \frac{1}{156}$ ($\approx 6 \cdot 10^{-3}$), det (N) = 0, the matrix can be considered as practically singular.

In case of an equation system with a poorly conditioned matrix, a minute change of the coefficients may result in a change of the solution vector by orders of magnitude. The equation system

$$x_1 + 100,0$$
 $x_2 = 101,0$
 $x_1 + 100,1$ $x_2 = 101,1$

is considered as an example. The condition number of the coefficient matrix is very high, thus it is poorly conditioned. The solution of the equation system is $x_1=x_2=1$. Changing the first coefficient of the first row of the system by as little as $\approx 10^{-3}$, we obtain $x_1=100$, $x_2=0$.

It has still to be shown that certain adjusting problems lead to normal equation systems with an a priori poorly conditioned matrix. (These are the so-called problems of poorly conditioned adjustment.)

Let us consider the following problem [2]. Be the matrix of the observation equations

$$\mathbf{A} = \left[\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ \delta & 0 & 0 & 0 & 0 \\ 0 & \delta & 0 & 0 & 0 \\ 0 & 0 & \delta & 0 & 0 \\ 0 & 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & 0 & \delta \end{array} \right]$$

where δ is a random variable. According to (3)

with a condition number according to (4) in case of $\delta \to 0$:

$$\lim_{\delta \to 0} \ \mathrm{cond} \ (\mathbb{N}) = \lim_{\delta \to 0} \ (5 + \delta^2) \delta^{-2} = \infty \,.$$

There are great many similar problems, not to be discussed here.

Above, adjustment problems were shown to exist, leading to a normal equation system of a priori poorly conditioned matrix. It was also demonstrated that in case of a poorly conditioned coefficient matrix, changing coefficients within the observation or computation accuracy may change the solution vector by orders of magnitude. In such cases the adjusting method involving setting up and solving normal equations is little more than a guarantee of the existence of a solution.

According to item i of the introduction, use of the above adjustment model for poorly conditioned adjustment problems is inexpedient, therefore a method likely to offer an adequate solution also for normal equations with poorly conditioned coefficient matrix is required.

In the following a more or less known mathematical model to bypass the normal equations is outlined, likely to give a direct solution applying matrix transformation on the observation (or condition) equation system. This model — the so-called orthonormalization method — is also efficient in solving poorly conditioned problems.

The general orthonormalization method and its application

Matrix A is partitioned in the form:

$$\hat{\mathbf{A}} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 \\ \mathbf{A}_3 & \mathbf{A}_4 \\ \vdots \\ \mathbf{A}_{2t-1} & \mathbf{A}_{2t} \end{bmatrix} \right\}_m^n$$

where thus the hypermatrix A will have submatrices $A_1, A_2, \ldots, A_{2t-1}$, A_{2t} as blocks. The joint matrix blocks of odd and of even subscripts are named left-side and right-side submatrices, respectively, and block A_1 the fundamental submatrix. According to the orthonormalization algorithm, each matrix block will be treated differently.

The orthonormalization method is aimed at transforming hypermatrix $\hat{\mathbf{A}}$ into a hypermatrix

$$\hat{\mathbf{W}} = \begin{bmatrix} & & & & p & \\ & \mathbf{W}_1 & \mathbf{W}_2 & \\ & \mathbf{W}_3 & \mathbf{W}_4 & \\ & & \ddots & \ddots & \ddots & \\ & & \mathbf{W}_{2i-1} & \mathbf{W}_{2i} & \end{bmatrix} n$$

of identical structure.

The transformation is done in two steps, according to the following algorithm.

Columns of matrices A and W are denoted by vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_r$ and $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_r$, respectively:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1r} \\ a_{21} & a_{22} & \dots & a_{2r} \\ \dots & \dots & \dots & \dots \\ a_{r1} & a_{r2} & \dots & a_{rr} \end{bmatrix} = [\mathbf{a}_1 \mathbf{a}_2 \dots \mathbf{a}_r]$$

and

$$\mathbf{W} = \begin{bmatrix} w_{11} & w_{12} & \dots & w_{1r} \\ w_{21} & w_{22} & \dots & w_{2r} \\ \dots & \dots & \dots & \dots \\ w_{n1} & w_{n2} & \dots & w_{nr} \end{bmatrix} = [\mathbf{w}_1 \, \mathbf{w}_2 \, \dots \, \mathbf{w}_r].$$

Denote the inner products of two arbitrary vectors by

$$\mathbf{b}^* = \begin{bmatrix} b_1 & b_2 & \dots & b_n \end{bmatrix}$$

and

$$\mathbf{c}^* = \begin{bmatrix} c_1 & c_2 & \dots & c_n \end{bmatrix}$$

as (\mathbf{b}, \mathbf{c}) and the Euclidean norm of a vector in form of $\|\mathbf{b}\|_{E}$. As known:

$$(\mathbf{b}, \mathbf{c}) = \sum_{i=1}^{n} b_i c_i = \mathbf{b}^* \mathbf{c} = \mathbf{c}^* \mathbf{b}$$

and

$$||\mathbf{b}||_F = (\mathbf{b}, \mathbf{b})^{1/2}$$
.

The orthonormalization of matrix A can be considered as decomposition into the product of a matrix W with orthonormal columns by an upper triangular matrix G [3], thus

$$\mathbf{A} = \mathbf{W} \quad \mathbf{G} \tag{5}$$

With a modification of the Schmidt's procedure [4], [5] orthonormalization can be performed as follows:

$$\mathbf{w}_{1} = \frac{\mathbf{a}_{1}}{\|\mathbf{a}_{1}\|_{E}}$$

$$\mathbf{w}_{i} = \frac{\overline{\mathbf{w}}_{i}}{\|\overline{\mathbf{w}}_{i}\|_{E}}, (i = 2, 3, \dots, r)$$

$$(6)$$

where

$$\mathbf{a}_{i}^{(j+1)} = \mathbf{a}_{i}^{(j)} - (\mathbf{a}_{i}^{(j)}, \mathbf{w}_{j}) \mathbf{w}_{j}$$

$$(j = 1, 2, \dots, i-1)$$

$$\overline{\mathbf{w}}_{i} = \mathbf{a}_{i}^{(j)}.$$

$$(7)$$

Now the transformation $\hat{\mathbf{A}} \to \hat{\mathbf{W}}$ is carried out. First the left-side submatrix of $\hat{\mathbf{A}}$ is transformed into the corresponding left-side submatrix of matrix $\hat{\mathbf{W}}$ by algorithms (6) and (7) in a way that the inner products $(\mathbf{a}_i^{(j)}, \mathbf{w}_j)$ in (7) and the vector norms $||\mathbf{a}_1||_E$ and $||\mathbf{w}_i||_E$ in (6) are formed by using only fundamental submatrix elements.

Then the right-side submatrix of $\hat{\mathbf{A}}$ will be transformed into the corresponding right-side submatrix of matrix $\hat{\mathbf{W}}$ such as:

$$\begin{bmatrix} \mathbf{w}_{2}^{(i)} \\ \mathbf{w}_{4}^{(i)} \\ \vdots \\ \mathbf{w}_{2t}^{(i)} \end{bmatrix} = \begin{bmatrix} \mathbf{a}_{2}^{(i)} \\ \mathbf{a}_{4}^{(i)} \\ \vdots \\ \mathbf{a}_{2t}^{(i)} \end{bmatrix} - \sum_{j=1}^{r} (\mathbf{a}_{2}^{(i)}, \mathbf{w}_{1}^{(j)}) \begin{bmatrix} \mathbf{w}_{1}^{(j)} \\ \mathbf{w}_{2}^{(j)} \\ \vdots \\ \mathbf{w}_{2t-1}^{(j)} \end{bmatrix}$$
$$(i = 1, 2, \dots, p)$$

where $\mathbf{a}_k^{(l)}$ and $\mathbf{w}_k^{(l)}$ are *l*-th columns of submatrices \mathbf{A}_k and \mathbf{W}_k , respectively, for $k=1,2,\ldots,2t$. Also here the necessary inner products can only be computed from the fundamental submatrix elements.

In accordance with (5) thus:

It must be noted that transformation $\widehat{A} \to \widehat{W}$ can also be performed by omitting an arbitrary number s of rows, corresponding of course to the omission of an arbitrary even number of submatrices A_k and W_k of higher subscripts.

By way of illustration, the above orthonormalization method is applied for the adjustment of intermediate observations in case of mutually independent unknowns [6]. For the sake of simplicity, observed values with unit weights are supposed. Now, with suitable substitutions the transformation $\widehat{A} \to \widehat{W}$ takes the form

where

$$\mathbf{h} = \mathbf{F} \quad \mathbf{x} + \mathbf{f}$$
(s,1) (s,r) (r,1) (s,1)

are functions of the adjusted quantities (s is the number of functions), 0 is a zero vector, and \mathbf{E} a unit matrix. — Other symbols are already known from the foregoing.

From relationships (8) it is evident that in fact, transformation (9) yields the wanted quantities directly at the indicated places, namely:

$$\begin{aligned} \mathbf{v} &= \mathbf{l} - \mathbf{W} \quad \mathbf{W}^{*} \quad \mathbf{l} \\ {\scriptstyle (n,1)} &\; {\scriptstyle (n,1)} \quad {\scriptstyle (n,r)} \quad {\scriptstyle (r,n)} \quad {\scriptstyle (n,1)} \\ \mathbf{x} &= -\mathbf{G}^{-1} \quad \mathbf{W}^{*} \quad \mathbf{l} \\ {\scriptstyle (r,1)} &\; {\scriptstyle (r,r)} \quad {\scriptstyle (r,n)} \quad {\scriptstyle (n,1)} \\ \mathbf{h} &= \mathbf{f} - \mathbf{F}\mathbf{G}^{-1} \quad \mathbf{W}^{*} \quad \mathbf{l} \\ {\scriptstyle (s,1)} &\; {\scriptstyle (s,1)} \quad {\scriptstyle (s,r)} \quad {\scriptstyle (r,n)} \quad {\scriptstyle (n,1)} \\ \end{aligned}$$

It is easy to prove that

$$\mathbf{N} = \mathbf{G}^{\star} \mathbf{G}$$

there is, however, no direct need of it, as the different matrices of reciprocal weight are obtained simply from the left-side submatrix of \hat{W} . The matrices of reciprocal weight of the unknowns $Q_{(x)}$ and of the adjusted quantities are, respectively:

$$\underset{(r,r)}{\mathbb{Q}_{(\mathtt{x})}} = \mathbb{N}^{-1} \underset{(r,r)}{\mathbb{G}^{-1}} \underset{(r,r)}{\mathbb{G}^{-\frac{1}{2}}}$$

and

$$\mathbf{Q}_{(\mathbf{F})} = \mathbf{F} \mathbf{N}^{-1} \ \mathbf{F}^* = \mathbf{F} \mathbf{G}^{-1} \ (\mathbf{F} \mathbf{G}^{-1})^* \ .$$

Also the case should be shortly mentioned where, rather than a unit matrix, weight matrix P is a diagonal matrix with only positive elements in the principal diagonal. Matrices A and I in transformation (9) are substituted by the following:

$$\widetilde{\mathbf{A}} = \mathbf{P}^{1/2} \mathbf{A}_{(n,r) (n,r) (n,r)}$$

$$\widetilde{\mathbf{l}} = \mathbf{P}^{1/2} \mathbf{l}_{(n,1) (n,n) (n,1)}.$$

Now the transformation becomes, similarly to (9):

$$\begin{bmatrix} \widetilde{\mathbf{A}} & | \ \widetilde{\mathbf{I}} \\ \hline \mathbf{E} & \mathbf{0} \\ \hline \mathbf{F} & | \mathbf{f} \end{bmatrix} \longrightarrow \begin{bmatrix} \widetilde{\mathbf{W}} & \widetilde{\mathbf{v}} \\ \hline \widetilde{\mathbf{G}}^{-1} & \widetilde{\mathbf{x}} \\ \hline \widetilde{\mathbf{F}}\widetilde{\mathbf{G}}^{-1} & \widetilde{\mathbf{h}} \end{bmatrix}.$$

It can be proved that in this case

$$\begin{array}{ll} v &= P^{-1/2}\,\widetilde{v} \\ x &= \widetilde{x} \\ h &= \widetilde{h} \\ Q_{(x)} = \,\widetilde{Q}_{(x)} \\ Q_{(F)} = \,\widetilde{Q}_{(F)} \;. \end{array}$$

For the sake of completeness it is noted that the above transformation $\hat{\mathbf{A}} \to \hat{\mathbf{W}}$ is a highly accurate method for solving linear equation systems for n = r if the last s rows are omitted.

In the above problem, application of the orthonormalization adjusting method was shown only for the adjustment of intermediate observations. Discussion of the adjustment of conditioned observations would mean to repeat the above derivation, and therefore it is omitted here. Adjustment of intermediate observations with conditions and of conditioned observations with unknowns [6] would proceed similarly. Adjustment of the latter two problems by orthonormalization is, however, somewhat more complicated.

Finally, it will be shown that adjusting calculations by setting and solving normal equations are always poorer in numerical stability than are those by the orthonormalization method.

According to item iv, among two mathematical models, that one is more stable where less product sums type $\sum_{i=1}^{n} a_i b_i$ are to be formed in computation.

It is easy to calculate that in using the orthonormalization method represented by (9), altogether $\frac{n\,(r^2+3\,r-2)}{2}$ product sums type $\sum_{i=1}^n a_i\,b_i$ are necessary to obtain the value of the solution vector x. Using the other method, to produce the normal equation system (3), according to (1) and (2), $n\,(r^2+r)$ product sums type $\sum_{i=1}^n a_i\,b_i$ have to be formed.

Since for $n \ge r$

$$n(r^2+r) > \frac{n(r^2+3r-2)}{2}$$

the orthonormalization method has the greater numerical stability (although at this point the classic method would only establish the normal equation system as yet to be solved, — whereas the orthonormalization method produced already the complete solution).

As a matter of fact, however, the orthonormalization model has also its limits of validity. Where the vector columns of matrix A include linearily related (or nearly related) vectors, the use of the orthonormalization method must be avoided, despite the higher numerical stability.

Summary

First, possible sources of unexpected errors in up-to-date computerized adjustment are outlined. Attention is called to the importance of selecting the best fitting mathematic models. In certain cases the adjusting calculation by establishment and solution of normal equations is inefficient, use of the orthonormalization method is suggested instead. Finally a model directly applicable in the orthonormalization method for adjustment calculations is presented and illustrated on a well-known problem.

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