

On Generalization of Conjugate Directions Methods *

Report [1] researched generalized conjugate directions methods for systems of linear equations with nonsymmetric matrices and indicated simple conditions sufficient for application of the methods. We now prove necessary conditions for the case when the solution of an n th order system is accurately obtained within n steps of the process, though not earlier for one first approximation x_0 . We deduce necessary and sufficient conditions for a k -term relation involving the residual and the vectors that make up the pseudoorthogonal system. When possible, we will use the same notation and terminology as [1].

We move now to a more exact formulation. To solve the system $Ax = b$, we obtain a sequence of approximations x_i , corresponding residuals r_i , and auxiliary vectors s_i , and generate R -pseudoorthogonal systems, where $R = CAB$, for given matrices C and B . Recall that an ordered system of vectors s_1, \dots, s_m is called R -pseudoorthogonal if, for $i < j \leq m$,

$$(Rs_j, s_i) = 0 \quad \text{and} \quad (Rs_j, s_j) \neq 0.$$

The zeroth step is composed of choosing a first approximation x_0 , calculating the residual $r_0 = b - Ax_0$, and setting $s_1 = r_0$. At the i th step ($i = 1, \dots$), we carry out the following operations:

$$\begin{aligned} a_i &= (Cr_{i-1}, r_{i-1}) / (CABs_i, s_i), \\ r_i &= r_{i-1} - a_i ABs_i, \\ x_i &= x_{i-1} + a_i Bs_i, \\ s_{i+1} &= r_i + \sum_{j=1}^i \beta_{i+1,j} s_j. \end{aligned} \tag{1}$$

Coefficients $\beta_{i+1,j}$ in (1) are found from the R -pseudoorthogonality condition of vector s_{i+1} to vectors s_1, \dots, s_i :

$$\begin{pmatrix} (Rs_1, s_1) & & 0 \\ \vdots & \ddots & \\ (Rs_1, s_i) & \dots & (Rs_i, s_i) \end{pmatrix} \begin{pmatrix} \beta_{i+1,1} \\ \vdots \\ \beta_{i+1,i} \end{pmatrix} = - \begin{pmatrix} (Rr_i, s_1) \\ \vdots \\ (Rr_i, s_i) \end{pmatrix}. \tag{2}$$

If $r_i = 0$, then we will say that the process terminates at the i th step. If $r_{i-1} \neq 0$, but $a_i = 0$ or $(Rs_i, s_i) = 0$, we will say that the process breaks down at the i th step. Indeed, if the process does not break down at the i th step, it does not break down at the j th step, for $j \leq i$.

If the process does not break down at the i th step, then

$$(Cr_i, s_j) = 0, \quad 1 \leq j \leq i, \tag{3}$$

and residuals r_0, \dots, r_{i-1} generate a C -pseudoorthogonal system. It is possible to find a proof of this assertion in [1].

If the process does not break down at the n th step, then it is necessarily complete, i.e., $r_n = 0$. For, in this case residuals r_0, \dots, r_{n-1} compose a C -pseudoorthogonal system which is linearly independent. We determine the coefficients of the expansion $r_n = \alpha_1 r_0 + \dots + \alpha_n r_{n-1}$ from the resulting system of equations:

$$\begin{pmatrix} (Cr_0, r_0) & & 0 \\ \vdots & \ddots & \\ (Cr_0, r_{n-1}) & \dots & (Cr_{n-1}, r_{n-1}) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} (Cr_n, r_0) \\ \vdots \\ (Cr_n, r_{n-1}) \end{pmatrix},$$

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with nonsingular matrix and null right hand side. This latter point is established in the following way. Obviously,

$$(Cr_n, r_j) = (Cr_{n-1}, r_j) - a_n(CABs_n, r_j). \quad (4)$$

Let $j \leq n-2$. Then the first summand of (4) equals zero, by virtue of the C -pseudoorthogonality of vectors r_0, \dots, r_{n-1} ; but the second equals zero, by virtue of the CAB -pseudoorthogonality of vectors s_1, \dots, s_n and the fact that r_j is a linear combination of vectors s_1, \dots, s_{j+1} . Now, let $j = n-1$. Then equality $(Cr_n, r_{n-1}) = 0$ is guaranteed by the choice of quantity a_n . And so, $\alpha_1 = \dots = \alpha_n = 0$, i.e., $r_n = 0$.

It is easy to see that if the process does not break down for a certain first approximation x_0 , then it does not break down for any first approximation x_0 , except for the union of a finite number of smooth manifolds of dimension not greater than $n-1$. This apparently means that in the general case the calculation corresponding to (1) almost always permits the result of the sought solution x , insofar as, for almost all such first approximations, the process does not break down before it terminates. Nonetheless, in the general case all coefficients $\beta_{i+1,j}$ are distinct from zero, and consequently we must save all vectors s_j ; in other words, we lose the attractive characteristics of the classical conjugate directions method.

From [1], it is clear that condition

$$(CABC^{-1})^* = \alpha I + \beta AB \quad (5)$$

(I identity matrix, α, β numbers) is sufficient in order that $\beta_{i+1,j} = 0$ for $j \leq i-1$. Naturally, we could ask the question whether there exists a matrix possessing an analogous characteristic and not satisfying condition (5). This is clearly the question and the direction of our research.

In what follows, we will study the condition

$$(CABC^{-1})^* = \sum_{j=0}^k \alpha_j (AB)^j. \quad (6)$$

Obviously, (5) is a particular case of (6).

Theorem 1. Suppose (6) holds. Then,

$$\beta_{i+1,j} = 0, \quad j \leq i-k. \quad (7)$$

Theorem 2. Suppose that, for all first approximations x_0 , the process does not break down and satisfies (7), and for one first approximation x_0 it terminates at exactly the n th step. Assume $n \geq 2k+3$ and matrices A, B and C are nonsingular. Then, we have (6).

Proof of Theorem 1: Generating the system of equations (2), it appears that $(Rr_i, s_j) = 0$ for $j \leq i-k$. We have:

$$\begin{aligned} (Rr_i, s_j) &= ((CABC^{-1})Cr_i, s_j) = (Cr_i, (CABC^{-1})^*s_j) \\ &= \sum_{l=0}^k \bar{\alpha}_l (Cr_i, (AB)^l s_j). \end{aligned}$$

From relation (1), it is not difficult to obtain that vector $(AB)^l s_j$ is a linear combination of vectors s_1, \dots, s_{j+l} . Insofar as $j+l \leq i$, from (3),

$$(Cr_i, (AB)^l s_j) = 0.$$

Theorem proven.

Proof of Theorem 2: Suppose residual r_0 results from a first approximation x_0 such that the process terminates at exactly the n th step. Then vectors r_0, \dots, r_{n-1} are clearly C -pseudoorthogonal and, consequently, linearly independent. We can find numbers γ_j such that:

$$(CABC^{-1})^* r_0 = \gamma_0 r_0 + \dots + \gamma_{n-1} r_{n-1}. \quad (8)$$

Taking scalar products from the left by vectors Cr_0, \dots, Cr_{n-1} results in the following relation:

$$\begin{pmatrix} (Cr_0, r_0) & \dots & (Cr_0, r_{n-1}) \\ & \ddots & \vdots \\ 0 & & (Cr_{n-1}, r_{n-1}) \end{pmatrix} \begin{pmatrix} \gamma_0 \\ \vdots \\ \gamma_{n-1} \end{pmatrix} = \begin{pmatrix} (Rr_0, r_0) \\ \vdots \\ (Rr_{n-1}, r_0) \end{pmatrix}. \quad (9)$$

It appears that

$$(Rr_i, r_0) = 0, \quad i \geq k+1. \quad (10)$$

From (1), (7), we have

$$\begin{aligned} r_{i+1} &= r_i - a_{i+1}ABs_{i+1} \\ &= r_i - a_{i+1}(ABr_i + \sum_{j=i-k+1}^i \beta_{i+1,j}ABs_j) \\ &= r_i - a_{i+1}ABr_i - a_{i+1} \sum_{j=i-k+1}^i \frac{\beta_{i+1,j}}{a_j}(r_{j-1} - r_j) \\ &= (1 + \frac{a_{i+1}}{a_i} \beta_{i+1,i})r_i - a_{i+1}ABr_i \\ &\quad - a_{i+1} \sum_{j=i-k+1}^{i-1} (\frac{\beta_{i+1,j+1}}{a_{j+1}} - \frac{\beta_{i+1,j}}{a_j})r_j \\ &\quad - a_{i+1} \frac{\beta_{i+1,i-k+1}}{a_{i-k+1}}r_{i-k} \end{aligned}$$

This having been formed, vector ABr_i is clearly a linear combination of vectors r_{i-k}, \dots, r_{i+1} . Consequently,

$$(CABr_i, r_j) = 0, \quad j \leq i-k-1. \quad (11)$$

Obviously, (10) is a special case of (11). From basic relation (10), and taking into account matrix system (9), we have the result $\gamma_j = 0, j \geq k+1$, so

$$(CABC^{-1})^*r_0 = \gamma_0r_0 + \dots + \gamma_kr_k.$$

It is easily seen that vector r_l is a linear combination of vectors $r_0, (AB)r_0, \dots, (AB)^l r_0$. Letting $r = r_0$ for simplicity, as a result, there exist numbers $\delta_0(r), \dots, \delta_k(r)$, such that

$$(CABC^{-1})^*r = \sum_{j=0}^k \delta_j(r)(AB)^j r. \quad (12)$$

We will consider the $\delta_j(r)$ as functions, defined on set M of vectors $r = r_0$ that result from first approximations x_0 such that the process terminates at the n th step. Clearly, M contains all vectors excluding a finite number of smooth manifolds $N_q, q = 1, \dots$, of dimension not higher than $n-1$. A finite sum from the manifolds $(AB)^{-1}N_q$ cannot give M . We know there exists a vector $r_0 \in M$ such that

$$r_0, (AB)r_0, \dots, (AB)^{n-1}r_0 \in M. \quad (13)$$

If r is one of the vectors from (13), then (12) is satisfied. Clearly, vectors (13) are linearly independent, since otherwise the process with first residual r_0 could not terminate at the n th step.

Pick integers $l, m \geq 0$ such that

$$k+1 \leq m-l \leq n-k-1, \quad (14)$$

and consider vectors

$$u = (AB)^l r_0, \quad v = (AB)^m r_0.$$

From (14), the vectors are linearly independent, and there exist numbers $\phi, \psi \neq 0$ such that M contains vector

$$z = \phi u + \psi v.$$

We have

$$\begin{aligned} (CABC^{-1})^* z &= \sum_{j=0}^k \delta_j(z) (AB)^j (\phi u + \psi v) \\ &= \phi \sum_{j=0}^k \delta_j(z) (AB)^{l+j} r_0 + \psi \sum_{j=0}^k \delta_j(z) (AB)^{m+j} r_0. \end{aligned}$$

On the other hand,

$$(CABC^{-1})^* z = \phi \sum_{j=0}^k \delta_j(u) (AB)^{l+j} r_0 + \psi \sum_{j=0}^k \delta_j(v) (AB)^{m+j} r_0.$$

From (14), vectors

$$(AB)^l r_0, \dots, (AB)^{l+k} r_0, (AB)^m r_0, \dots, (AB)^{m+k} r_0$$

are clearly part of the basis

$$(AB)^l r_0, \dots, (AB)^{l+n-1} r_0$$

which we know is linearly independent. Consequently,

$$\delta_j(u) = \delta_j(v) = \delta_j(z). \quad (15)$$

For every $q \geq 0$, and considering vectors

$$(AB)^q r_0, \dots, (AB)^{q+2k+2} r_0$$

and values of l and m satisfying (14), we choose consecutive pairs from the sequence of indices

$$\begin{array}{cccc} q, & q + (k + 1), & q + 2(k + 1), & \\ (q + 1), & (q + 1) + (k + 1), & (q + 1) + 2(k + 1), & \\ (q + 2), & (q + 2) + (k + 1), & (q + 2) + 2(k + 1), & \dots \end{array}$$

Repeating the calculations for these l and m reduces to (15), and we obtain that, if r is one of the vectors (13), then the coefficient $\delta_j(r)$ does not depend on r . This means relation (6) holds, where $\alpha_j = \delta_j(r)$. Theorem proven.

Bibliography

- [1] Voevodin, V. V. "On Methods of Conjugate Directions," *USSR Journal of Computational Mathematics and Mathematical Physics*, Vol. 19, No. 5, 1979, pp. 1313-1317. (translator's note: this reference is available in the English version of the same journal, dated 1981 and on pp. 228-233.)