

A breakdown-free Lanczos type algorithm for solving linear systems

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Summary. Lanczos type algorithms for solving systems of linear equations have their foundations in the theory of formal orthogonal polynomials and the method of moments which leads to a determinantal formula for their iterates. The various Lanczos type algorithms mainly differ by the way of computing the coefficients entering into the recurrence formulae. If the denominator in the formula for one of these coefficients is zero, then a breakdown occurs in the algorithm, and it must be stopped. Such a breakdown is in fact due to the non-existence of some orthogonal polynomial. In this paper we show how to jump over such a singularity by computing the next existing orthogonal polynomial by the block bordering method. The resulting algorithm, called MRZ, is equivalent to the nongeneric BIODIR algorithm (which is a look-ahead Lanczos type algorithm), but our derivation is much simpler.

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1 Introduction

Let us assume that we want to solve in \mathbb{C}^n the system of linear equations

$$Ax = b.$$

An interesting and powerful class of methods, which received much attention, is that of Lanczos type methods. These are projection methods on Krylov subspaces consisting of solving successively the systems

$$A_k(x_k - x_0) = -r_0$$

for $k = 1, \dots, n$ where A_k is an approximation of A such that x_k is uniquely defined. A three-term recurrence relationship between the x_k 's holds. Its coefficients

are computed as the iteration proceeds, and the various Lanczos type algorithms mainly differ in the way of computing these coefficients. However, in all these methods they are ratios of two scalar products. If the scalar product in the denominator of one of them is zero, then a breakdown occurs in the algorithm, and it has to be stopped.

The x_k 's are related by a three-term recurrence relation because the underlying theory involves (formal) orthogonal polynomials, and a breakdown in the algorithm is due to the non-existence of one of these orthogonal polynomials. It is possible to jump over such a singularity by solving the linear system arising in the recursive computation of the orthogonal polynomials by a block bordering method. Bordering the system by a new equation and a new column at each iteration leads to the usual three-term recurrence relation while bordering it by as many new equations and columns as necessary leads to a more general recurrence relation. Thus the purpose of the block bordering method is to avoid possible intermediate singular systems and to jump from one non-singular system to the next one after having determined the length of the jump. Applying such a recurrence relation to our problem gives a Lanczos type algorithm, called the MRZ, with only a possible incurable hard breakdown. Using the connection with orthogonal polynomials, Gutknecht [15] recently derived quite similar algorithms and he gave their complete theory. Our approach here is characterized by the latest possible introduction of linear algebra and the focus on orthogonal polynomials. Such an approach will be useful in interpreting and generalizing other projection and ε -type methods and will be the purpose of a forthcoming paper [6].

The theory of Lanczos type methods will be presented in Sect. 2. Such methods are based on a generalization of the method of moments of Vorobyev [26] and they are oblique projection methods. Thus formal orthogonal polynomials are introduced at an early stage of the theory. They provide a determinantal formula for the iterates produced by the method that will be of primary importance for jumping over singularities and avoiding breakdowns. Section 3 is devoted to the block bordering method which will be our basic tool in deriving the MRZ. Orthogonal polynomials form the subject of Sect. 4 where the block bordering method is used for obtaining their recurrence relationship in the non-regular case (that is when some of them do not exist). Then the MRZ is presented in Sect. 5 together with the computation of the coefficients occurring in its recurrence relations. The method is discussed in Sect. 6. Programming such an algorithm requires to study the minimization of the number of vector operations and the amount of storage. This will be the subject of another paper, which will also contain the treatment of near-breakdown and numerical experiments [10, 11].

2 Theory of Lanczos type methods

Let us consider in \mathbb{C}^n the system of linear equations

$$Ax = b .$$

Let x_0 be any vector that is not a solution, and let $r_0 = Ax_0 - b$ be the corresponding residual.

Let $E_k = \text{span}(r_0, Ar_0, \dots, A^{k-1}r_0)$ and $F_k = \text{span}(y, A^*y, \dots, A^{*k-1}y)$, where y is an arbitrary non-zero vector and where A^* is the conjugate transpose of A .

Let x_k be defined by

$$x_k - x_0 \in E_k$$

$$A_k(x_k - x_0) = -r_0 = -(Ax_0 - b)$$

with $A_k = H_k A H_k$ and with H_k being the oblique projection on E_k with kernel F_k^\perp (that is along F_k^\perp). The matrix A_k is completely defined by

$$A^i r_0 = A_k^i r_0, \quad i = 0, \dots, k-1,$$

$$H_k A^k r_0 = A_k^k r_0.$$

This is a generalization of the method of moments of Vorobyev [26]. Such a generalization was already considered in [2, 4, 17].

Since $x_k - x_0 \in E_k$ we can write it as

$$(1) \quad x_k - x_0 = a_1 r_0 + \dots + a_k A^{k-1} r_0 = a_1 r_0 + \dots + a_k A_k^{k-1} r_0.$$

Thus

$$Ax_k - Ax_0 = a_1 Ar_0 + \dots + a_k A^k r_0 = Ax_k - b - (Ax_0 - b)$$

and it follows that

$$r_k = Ax_k - b = r_0 + a_1 Ar_0 + \dots + a_k A^k r_0 = P_k(A)r_0$$

with $P_k(\xi) = 1 + a_1 \xi + \dots + a_k \xi^k$.

Let us now compute a_1, \dots, a_k . We set

$$\bar{r}_k = P_k(A_k)r_0.$$

We have

$$r_k - \bar{r}_k = a_k(A^k r_0 - A_k^k r_0) \in F_k^\perp.$$

But

$$-r_0 = A_k x_k - A_k x_0 = a_1 A_k r_0 + \dots + a_k A_k^k r_0$$

and thus

$$0 = r_0 + a_1 A_k r_0 + \dots + a_k A_k^k r_0 = P_k(A_k)r_0 = \bar{r}_k.$$

It follows that $r_k \in F_k^\perp$, that is

$$(A^{*i} y, r_k) = 0 \quad \text{for } i = 0, \dots, k-1.$$

If we set $c_i = (y, A^i r_0)$ and if the linear functional c on the space of polynomials is defined by $c(\xi^i) = c_i$, the preceding relations can be written as

$$c(\xi^i P_k(\xi)) = 0 \quad \text{for } i = 0, \dots, k-1,$$

which shows that P_k is the polynomial of degree at most k , normalized by the condition $P_k(0) = 1$, belonging to the family of formal orthogonal polynomials with respect to c [2].

Thus Lanczos type methods consist in determining implicitly the polynomials P_k as defined above (the questions of existence and effective construction of P_k will be discussed below), computing $r_k = P_k(A)r_0$, and finally finding x_k from $r_k = Ax_k - b$ without, of course, inverting A , which is possible as will be explained below.

But now, to complete the theory, let us give some useful formulae connected with x_k . Let us write P_k as

$$P_k(\xi) = a_0^{(k)} + a_1^{(k)}\xi + \dots + a_k^{(k)}\xi^k.$$

The condition $P_k(0) = 1$ implies $a_0^{(k)} = 1$. Writing the orthogonality relations of P_k we obtain it as the solution of the system

$$(2) \quad \begin{pmatrix} 1 & 0 & \dots & 0 \\ c_0 & c_1 & \dots & c_k \\ \vdots & \vdots & & \vdots \\ c_{k-1} & c_k & \dots & c_{2k-1} \end{pmatrix} \begin{pmatrix} a_0^{(k)} \\ a_1^{(k)} \\ \vdots \\ a_k^{(k)} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

Thus it follows that

$$(3) \quad P_k(\xi) = \left| \begin{array}{cccc} 1 & \xi & \dots & \xi^k \\ c_0 & c_1 & \dots & c_k \\ \vdots & \vdots & & \vdots \\ c_{k-1} & c_k & \dots & c_{2k-1} \end{array} \right| \left/ \left| \begin{array}{ccc} c_1 & \dots & c_k \\ \vdots & & \vdots \\ c_k & \dots & c_{2k-1} \end{array} \right| \right|,$$

and we obtain

$$(4) \quad x_k - x_0 = \left| \begin{array}{cccc} 0 & r_0 & \dots & A^{k-1}r_0 \\ c_0 & c_1 & \dots & c_k \\ \vdots & \vdots & & \vdots \\ c_{k-1} & c_k & \dots & c_{2k-1} \end{array} \right| \left/ \left| \begin{array}{ccc} c_1 & \dots & c_k \\ \vdots & & \vdots \\ c_k & \dots & c_{2k-1} \end{array} \right| \right|,$$

where the determinant in the numerator is the vector obtained by expanding it, by the classical rules, with respect to its first row.

Let $(r_0, Ar_0, \dots, A^{k-1}r_0)$ be the matrix whose columns are $r_0, \dots, A^{k-1}r_0$. Then, from (1) and (2), we obtain

$$(5) \quad x_k - x_0 = -(r_0, Ar_0, \dots, A^{k-1}r_0) \begin{pmatrix} c_1 & \dots & c_k \\ \vdots & & \vdots \\ c_k & \dots & c_{2k-1} \end{pmatrix}^{-1} \begin{pmatrix} c_0 \\ \vdots \\ c_{k-1} \end{pmatrix}.$$

This formula, which extends the formula given in [3] when $x_0 = 0$, can also be proved by using the generalization of Schur's formula obtained in [1].

Let us now come back to formula (2). We shall call N_k the matrix of this system, d_k its right hand side and z_k its solution. Obviously P_k exists and is unique if and only if N_k is regular, that is, if and only if its determinant (which is the Hankel determinant usually denoted by $H_k^{(1)}$, see [2]) is different from zero. P_{k+1} is given by solving a system of equations obtained by bordering (2) by a new equation and a new column. Thus, applying the bordering method of Faddeeva [13] seems to be very appropriate. However it needs to be generalized before using it for our problem and this question will be the purpose of the next section.

3 The block bordering method

Let N_k be an $n_k \times n_k$ matrix. We shall consider the $(n_k + m_k) \times (n_k + m_k)$ matrix N_{k+1} given by

$$N_{k+1} = \begin{pmatrix} N_k & U_k \\ V_k & M_k \end{pmatrix}$$

where U_k, V_k and M_k are matrices of the respective dimensions $n_k \times m_k, m_k \times n_k$ and $m_k \times m_k$. N_k is assumed to be regular. We set

$$B_k = M_k - V_k N_k^{-1} U_k.$$

B_k is a $m_k \times m_k$ matrix called the Schur complement of N_k in N_{k+1} . By Schur's formula

$$\det N_{k+1} = \det N_k \cdot \det B_k$$

and, hence, N_{k+1} is singular if and only if B_k is singular.

It is easy to check that, if B_k is regular,

$$N_{k+1}^{-1} = \begin{pmatrix} N_k^{-1} + N_k^{-1} U_k B_k^{-1} V_k N_k^{-1} & - N_k^{-1} U_k B_k^{-1} \\ - B_k^{-1} V_k N_k^{-1} & B_k^{-1} \end{pmatrix}.$$

Let us now consider the systems of linear equations

$$N_k z_k = d_k \quad \text{and} \quad N_{k+1} z_{k+1} = d_{k+1} = \begin{pmatrix} d_k \\ f_k \end{pmatrix}$$

where f_k is a vector of dimension m_k . From the preceding formula for N_{k+1}^{-1} we have

$$z_{k+1} = \begin{pmatrix} z_k \\ 0 \end{pmatrix} + \begin{pmatrix} - N_k^{-1} U_k \\ I \end{pmatrix} B_k^{-1} (f_k - V_k z_k)$$

where I is the $m_k \times m_k$ unit matrix.

These relations generalize the bordering method of Faddeeva [13] which corresponds to the case $m_k = 1$. They are also a recursive application of the formulae given by Keller [18].

We shall now apply this block bordering method to the solution of the system (2), which yields the orthogonal polynomials P_k used in Lanczos type methods.

4 Recursive computation of orthogonal polynomials

Let us now solve the system (2) recursively by the block bordering method. Of course we shall be only interested in those polynomials P_k which exist (they are usually called regular). Changing our notation we let P_k and P_{k+1} be two successive regular polynomials of the respective degrees n_k and $n_{k+1} = n_k + m_k$ at most

$$P_k(\xi) = a_0^{(k)} + a_1^{(k)} \xi + \dots + a_{n_k}^{(k)} \xi^{n_k} \quad \text{with } a_0^{(k)} = 1$$

$$P_{k+1}(\xi) = a_0^{(k+1)} + a_1^{(k+1)} \xi + \dots + a_{n_{k+1}}^{(k+1)} \xi^{n_{k+1}} \quad \text{with } a_0^{(k+1)} = 1$$

and

$$\begin{pmatrix} 1 & 0 & \cdots & 0 \\ c_0 & c_1 & \cdots & c_{n_k} \\ \vdots & \vdots & & \vdots \\ c_{n_k-1} & c_{n_k} & \cdots & c_{2n_k-1} \end{pmatrix} \begin{pmatrix} a_0^{(k)} \\ a_1^{(k)} \\ \vdots \\ a_{n_k}^{(k)} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\left(\begin{array}{cccc|ccc} 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ c_0 & c_1 & \cdots & c_{n_k} & c_{n_k+1} & \cdots & c_{n_k+1} \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ c_{n_k-1} & c_{n_k} & \cdots & c_{2n_k-1} & c_{2n_k} & \cdots & c_{n_k+1+n_k-1} \\ \hline c_{n_k} & c_{n_k+1} & \cdots & c_{2n_k} & c_{2n_k+1} & \cdots & c_{n_k+1+n_k} \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ c_{n_k+1-1} & c_{n_k+1} & \cdots & c_{n_k+1+n_k-1} & c_{n_k+1+n_k} & \cdots & c_{2n_k+1-1} \end{array} \right) \begin{pmatrix} a_0^{(k+1)} \\ a_1^{(k+1)} \\ \vdots \\ a_{n_{k+1}}^{(k+1)} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

Writing these two systems $N_k z_k = d_k$ and $N_{k+1} z_{k+1} = d_{k+1}$ as in the preceding section we have, by the block bordering method,

$$z_{k+1} = \begin{pmatrix} z_k \\ 0 \end{pmatrix} - \begin{pmatrix} -N_k^{-1} U_k \\ I \end{pmatrix} B_k^{-1} V_k z_k \quad \text{with } B_k = M_k - V_k N_k^{-1} U_k,$$

since f_k is the zero vector (I is the $m_k \times m_k$ unit matrix). Taking the scalar product of both sides with $(1, \xi, \dots, \xi^{n_{k+1}})^T$ we obtain

$$P_{k+1}(\xi) = P_k(\xi) - Q_{k+1}(\xi),$$

where

$$Q_{k+1}(\xi) = (1, \xi, \dots, \xi^{n_{k+1}}) \begin{pmatrix} -N_k^{-1} U_k \\ I \end{pmatrix} B_k^{-1} V_k z_k.$$

The polynomial Q_{k+1} has degree n_{k+1} at most and it satisfies

$$(6) \quad \begin{aligned} c(\xi^i Q_{k+1}(\xi)) &= c(\xi^i P_k(\xi)) - c(\xi^i P_{k+1}(\xi)) \\ &= \begin{cases} 0 & \text{for } i = 0, \dots, n_k - 1 \\ c(\xi^i P_k(\xi)) & \text{for } i = n_k, \dots, n_k + m_k - 1 \end{cases} \end{aligned}$$

thanks to the orthogonality property of P_k and P_{k+1} . Moreover, since the first row of U_k is zero,

$$Q_{k+1}(0) = 0.$$

5. compute the coefficients of q_k according to (11) and (13) and set

$$z_{k+1} = q_k(A)z_k - C_{k+1}z_{k-1},$$

6. if $r_{k+1} = 0$, then $x_{k+1} = x$ and stop,

7. set $n_{k+1} = n_k + m_k$,

8. if $n_{k+1} < n$, then replace k by $k + 1$ and return to 3.

Since the most important quantities computed at each step are m_k , r_k and z_k , this algorithm has been called the MRZ. Obviously this name is also a joke of the first and third authors (the French ones, of course) concerning the initials of the second author (the Italian lady). We looked for a possible meaning of these three initials. Since the recurrence relation for computing the polynomials $P_k^{(1)}$ (that is in fact the z_k 's) has a varying length (depending on m_k) it is quite similar to a zoom lens on a camera and thus the letters MRZ stand for *Method of Recursive Zoom*.

6 Discussion

In the Lanczos type methods previously used, such as BIODIR, BIOMIN, BIORES and others, a breakdown can occur when dividing by a zero scalar product. The occurrence of such a situation is due to the fact that, in these methods, the polynomials P_k are required to be regular, a requirement no longer mandatory in the MRZ. Jumping over those singular polynomials was made possible by using the generalized recurrence relation of Draux [12] between regular orthogonal polynomials. This recurrence relation, which was also given by Struble [24], but with a nonconstructive proof, and which can be directly obtained from (2) or (3) as in [8], is the basis for the derivation of two quite similar breakdown-free methods by Gutknecht [15] called nongeneric BIORES algorithm and nongeneric BIODIR algorithm, respectively. In the first of these two methods the polynomials P_k are initially required to be monic polynomials of exact degree k and then renormalized by imposing the consistency condition $P_k(0) = 1$. Except for the formulae (8) and (11) for computing the coefficients of w_k and q_k the MRZ is equivalent to the nongeneric BIODIR algorithm. However our derivation, which was done independently, seems to be simpler and more elegant. Moreover it can be very easily extended to the other Lanczos type algorithms to avoid breakdown as, for example, in the CGS algorithm [7]. Let us mention that, in these algorithms, the only possible breakdown which can occur is the so-called incurable hard one corresponding to $(y, A^n z_k) = 0$ where n is the dimension of the system. Such a breakdown is due to a very unfortunate choice of the starting vectors x_0 and y and the algorithm has to be restarted with another choice.

The very important questions concerning the practical implementation of our method with as few computations and storage as possible and the treatment of near-breakdown is discussed in [10, 11].

The simplicity of our approach using orthogonal polynomials instead of linear algebra techniques also allows us to derive algorithms for avoiding near-breakdown in Lanczos methods [10, 11], in the CGS [9] and in a new class of methods, called CGM [5], which includes the Bi-CGSTAB of Van der Vorst [25] as a particular case.

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