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A Generalized Lanczos Scheme

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Abstract. It is shown in this paper how the Lanczos algorithm can be generalized so that it applies to both symmetric and skew-symmetric matrices and corresponding generalized eigenvalue problems.

1. Introduction. The Lanczos scheme, designed for the computation of approximate eigenvalues of a symmetric matrix A (or order n), can be used also for the computation of eigenvalues of the product matrix CB, where C is symmetric and B is symmetric positive definite. This can be done simply by choosing another inner product, thus avoiding the necessity of constructing an LL^T-decomposition of B. The algorithm in this form is closely related to an algorithm published by Widlund [1], for the solution of certain nonsymmetric linear systems.

The generalized eigenvalue problem $Cx = \lambda Bx$ can be reduced to the above form by $CB^{-1}y = \lambda y$. In this case the new Lanczos scheme is attractive if fast solvers are available for the solution of linear systems of the form $By = z$. The generalized algorithm is also applicable when C is skew-symmetric. This is achieved by introducing a minus sign in the appropriate place.

2. The Generalized Lanczos Scheme. Let A be of the form $A = CB$, where B is symmetric positive definite and C is either symmetric or skew-symmetric.

Then choose an arbitrary vector v_1, with $(v_1, v_1)_B = 1$, and form $u_1 = Av_1$. Rows $\{v_j\}$, $\{\alpha_j\}$, $\{\beta_j\}$, and $\{\gamma_j\}$ are then generated by

$$\alpha_j = \left(v_j, Av_j\right)_B, \quad w_j = u_j - \alpha_j v_j, \quad \gamma_{j+1} = \left(w_j, w_j\right)_B^{1/2},$$

$$\beta_{j+1} = \tau\gamma_{j+1}, \quad v_{j+1} = \frac{1}{\gamma_{j+1}} w_j,$$

$$u_{j+1} = Av_{j+1} - \beta_{j+1}v_j \quad \text{for } j = 1, 2, \dots, m \ \left(\text{as far as } \gamma_j \neq 0\right),$$

where $(x, y)_B = (x, By)$, with B symmetric and positive definite, and $\tau = 1$ if $C = C^T$, $\tau = -1$ if $C = -C^T$.

For $B = I$ and $\tau = 1$ we have the Lanczos scheme in the form as proposed by Paige [2]. The constants α_j, β_j, and γ_j define a tridiagonal matrix T_m:

$$T_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & \varnothing \\ \gamma_2 & \alpha_2 & \beta_3 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \beta_m \\ \varnothing & & & \gamma_m & \alpha_m \end{pmatrix}.$$

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THEOREM. *If either $C = C^T$ or $C = -C^T$ and if B is a positive definite symmetric matrix and $A = CB$, then the generalized Lanczos scheme applied to A generates a tridiagonal matrix T_m, where limit-values of the eigenvalues of T_m, for increasing m, should be equal to the eigenvalues of A; but they may differ by a certain amount depending on the precision of computation.*

Proof. (i) For $C = C^T$ and $B = I$, the result is well known (Paige [2]).

(ii) For $C = -C^T$ and $B = I$ the proof is as follows: It is only necessary to establish that the generated row $\{v_k\}$, $k = 1,\ldots,m$, is an orthonormal row. The proof is by induction. Let $\{v_k\}$, $k = 1,\ldots,j$, be an orthonormal row. Then we have for v_{j+1} the relation

$$\gamma_{j+1}v_{j+1} = Cv_j - \beta_j v_{j-1} - \alpha_j v_j,$$

where we assume that $\gamma_{j+1} \neq 0$, since in that case the recurrence relation terminates.

For $k < j - 1$,

$$\begin{aligned}(\gamma_{j+1}v_{j+1}, v_k) &= (Cv_j - \beta_j v_{j-1} - \alpha_j v_j, v_k) = -(v_j, Cv_k)\\ &= -(v_j, \gamma_{k+1}v_{k+1} + \beta_k v_{k-1} + \alpha_k v_k) = 0.\end{aligned}$$

For $k = j - 1$,

$$(\gamma_{j+1}v_{j+1}, v_{j-1}) = (Cv_j, v_{j-1}) - \beta_j(v_{j-1}, v_{j-1}) = (Cv_j, v_{j-1}) - \beta_j.$$

Since $\beta_j = -\gamma_j = -(\gamma_j v_j, v_j) = -(Cv_{j-1}, v_j) = (Cv_j, v_{j-1})$, it follows that $(\gamma_{j+1}v_{j+1}, v_{j-1}) = 0$.

For $k = j$,

$$(\gamma_{j+1}v_{j+1}, v_j) = (Cv_j, v_j) - \alpha_j = 0.$$

Finally we have

$$\begin{aligned}(v_{j+1}, v_{j+1}) &= \frac{1}{\gamma_{j+1}^2}(Av_j - \beta_j v_{j-1} - \alpha_j v_j, Av_j - \beta_j v_{j-1} - \alpha_j v_j)\\ &= \frac{1}{\gamma_{j+1}^2}(u_j - \alpha_j v_j, u_j - \alpha_j v_j) = \frac{1}{\gamma_{j+1}^2}(w_j, w_j) = 1.\end{aligned}$$

Thus the row $\{v_k\}$, $k = 1,\ldots,j + 1$, is an orthonormal row.

(iii) When $C = C^T$ and B is symmetric positive definite, B can be written as $B = LL^T$, where L is lower triangular. (Note that the LL^T-decomposition is not required during actual computation).

Since the eigenvalues of CB are equal to those of L^TCL, the original Lanczos scheme can be applied to L^TCL (with the normal euclidean inner product). In this case we then have the relations

$$\alpha_j = (v_j, L^TCLv_j) \quad \text{and} \quad u_{j+1} = (L^TCLv_{j+1} - \beta_{j+1}v_j).$$

It follows that

$$Lu_{j+1} = LL^TCLv_{j+1} - \beta_{j+1}Lv_j.$$

If we replace x by $L^T\tilde{x}$, then this equation can be rewritten as

$$\begin{aligned}LL^T\tilde{u}_{j+1} &= LL^TCLL^T\tilde{v}_{j+1} - \beta_{j+1}LL^T\tilde{v}_j,\\ \tilde{u}_{j+1} &= CB\tilde{v}_{j+1} - \beta_{j+1}\tilde{v}_j = A\tilde{v}_{j+1} - \beta_{j+1}\tilde{v}_j.\end{aligned}$$

The other Lanczos relations follow from

$$\alpha_j = \left(L^TCLv_j, v_j\right) = \left(L^TCLL^T\tilde{v}_j, L^T\tilde{v}_j\right) = \left(CB\tilde{v}_j, B\tilde{v}_j\right) = \left(A\tilde{v}_j, \tilde{v}_j\right)_B,$$

$$\beta_{j+1}^2 = \gamma_{j+1}^2 = \left(w_j, w_j\right) = \left(L^T\tilde{w}_j, L^T\tilde{w}_j\right) = \left(B\tilde{w}_j, \tilde{w}_j\right) = \left(\tilde{w}_j, \tilde{w}_j\right)_B.$$

The relations $\tilde{w}_j = \tilde{u}_j - \alpha_j\tilde{v}_j$ and $\tilde{v}_{j+1} = \tilde{w}_j/\gamma_{j+1}$ are obvious. The vectors $\tilde{w}_j$, $\tilde{v}_j$, and $\tilde{u}_j$ produce the desired result.

(iv) The remaining case $A = CB$, where $C = -C^T$ and B is symmetric positive definite, follows from the previous ones (with $\tau = -1$).

The last part of the theorem, concerning the accuracy of the limit-values of the matrices T_m follows from Paige [2].

Remarks. 1. If $C = -C^T$, we have that $\alpha_j = 0$ for all j.

2. The above scheme allows for the computation of the eigenvalues of CB, which are equal to those of BC, without the explicit need for an LL^T-factorization of the matrix B. This makes the generalized schemes very attractive, especially if B has a sparse structure. However, it should be mentioned that eigenvectors cannot be computed by these schemes directly, since then an LL^T-factorization is required for a proper transformation. Eigenvectors may be computed by a Raleigh-quotient iteration scheme, once one has a fast solver for systems like $Bx = y$.

3. We should like to mention briefly certain aspects of programming. For the generalized problem, the adapted schemes require only one extra matrix-vector multiplication and only one additional vector to store Bw_j. Remember that Bv_j can be computed from $Bv_j = Bw_j/\gamma_{j+1}$. The matrices A, B, and C do not have to be represented in the usual way as two-dimensional arrays of numbers, but as rules to compute the products Ax, Bx and Cx for any given x. This allows us to take full advantage of any sparsity structure.

4. If C is skew-symmetric, then the generated matrices T_m are also skew-symmetric. Eigenvalues of a tridiagonal skew-symmetric matrix can be computed as follows. The matrix iT_m is Hermitian and has real eigenvalues. Since, in the computation of the eigenvalues with Sturm-sequence, only squares of off-diagonal elements are involved, these eigenvalues can be computed without any complex computation. Once the eigenvalues of $|\,T_m\,|$ have been computed, they should be multiplied by i so that they represent the eigenvalues of T_m.

5. For practical algorithms for the selection of good eigenvalue approximations from the eigenvalues of T_m for those of A see Cullum and Willoughby [3], Parlett and Reid [4], or van Kats and van der Vorst [5].

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