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Abstract

We study transformations by unitary similarity of a nonderogatory matrix to certain rank structured matrices. This kind of transformations can be described in a unified framework that involves Krylov matrices. The rank structures here addressed are preserved by QR iterations, and every iterate can be associated with a suitable Krylov matrix.

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1 Introduction

We investigate the transformation, by unitary similarity, of a square matrix in various kind of rank structured matrices, such as combinations of banded matrices, inverses of banded matrices and matrices of definite rank. These matrices can be characterized by rank properties of certain subblocks, and for this reason belong to the wide class of rank structured matrices. Recently, rank structured matrices received a great deal of attention, in particular for the design of methods for computing polynomial roots and eigenvalues by means of the QR algorithm, see [5, 9]. The reason is that these structures are essentially preserved throughout the steps of the algorithm, allowing substantial reductions of space and time complexities.

Krylov matrices are the tool that we use for studying transformations into rank structured matrices. Krylov matrices appear in the theory of nonstationary methods, such as CG and GMRES, used for the solution of large sparse linear systems, see [14, 10]. In addition, Krylov matrices allow to explain the behavior of methods such as Lanczos for the computation of the tridiagonal matrix similar to a given Hermitian matrix [10]. In [7], the author uses a kind of generalized Krylov matrix to show that it is possible to transform, by unitary similarity, a symmetric matrix in the sum of a prescribed diagonal matrix and a semiseparable matrix. Here, we show how various other structures can be the target of the transformation.

The paper is organized as follows. In Section 2 we recall some basic facts about banded matrices and their inverses. In Section 3 we introduce Krylov matrices and use them in order to obtain various transformation of a nonderogatory matrix to matrices having particular structures. In Section 4 we extend the definition of Krylov matrices, with the main intent of including r-semiseparable matrices within the various structures concerned. In Section 5 we show how the QR algorithm fits in the theoretical framework here discussed.

2 Preliminaries on banded matrices and their inverses

Banded matrices are of widespread use in numerical linear algebra. Their inverses have also been thoroughly studied [3, 6, 12]. For example, the inverses of tridiagonal matrices arise in particular applications, see [8], and have been also proposed as alternative to tridiagonal matrices for eigenvalue computation, because reduction to semiseparable form could show additional convergence behavior with respect to tridiagonalization [4, 16, 2].

In order to set the ground for the future developments, we adapt here for our purposes two definitions and an important result from [1, 13].

Definition 1 *Let $A = (a_{ij})$ be square matrix of order n an let k be an integer. The matrix A is called upper k-banded if $a_{ij} = 0$ for $j - i < k$; it is called strictly upper k-banded if in addition $a_{ij} \neq 0$ for $j - i = k$.*

For the readers familiar with MATLAB‡ we note that a matrix A is upper k-banded if A and $\mathrm{triu}(A, k)$ are equal. For example an upper triangular matrix is a 0-banded matrix, and an upper Hessenberg matrix is a (-1)-banded matrix. Note that an upper k-banded matrix with $k \geq n$ is the zero matrix, while with $k \leq 1 - n$ is a full matrix. For brevity, we refer to upper k-banded matrices simply as k-banded.

It is useful to observe that if A is k-banded and B is h-banded then $A + B$ is $\min\{k,\, h\}$-banded and AB is $(k + h)$-banded.

Definition 2 *Let k be an integer such that $0 \leq k \leq n - 1$. A matrix S is called a lower k-semiseparable matrix if there exist two $n \times k$ matrices X and Y, called generators, and an upper k-banded matrix U such that*

$$S = XY^* + U.$$

As for banded matrices we refer lower k-semiseparable matrices simply as k-semiseparable. It can be shown that the nonsingularity of S implies that U is strictly banded. Moreover, if a banded matrix is nonsingular then $k \leq 0$. Now we can state the promised result [1, 13].

Theorem 1 *A nonsingular matrix is strictly k-banded matrix if and only if its inverse is $(-k)$-semiseparable.*

‡MATLAB is a registered trademark of The MathWorks, Inc.

The theorem does not longer hold if the word "strictly" is dropped. In this more general situation, the inverse is rank structured as well, but not more representable by means of generators in a straightforward way. Asplund in [1] names the inverse Green's matrix and does not address the problem of its representation. In [15] the authors consider the tridiagonal case and point out the lack of numerical robustness of the representation of the inverse by means of generators. They also propose a new general strategy for the representation of the inverse involving Given's rotation matrices.

3 Transformations via Krylov matrices

Let A be a square matrix of order n. The matrices of the form

$$K = [v, Av, \cdots, A^{n-1}v] \tag{1}$$

are known as Krylov matrices of A and form a linear space of dimension n. This space contains nonsingular matrices if and only if A is nonderogatory, see [11]. Now, let $p(x) = (-1)^n(x^n - \sum_{i=0}^{n-1} p_{i+1}x^i)$ be the characteristic polynomial of A. The p_i appear in the Frobenius matrix

$$F = \begin{pmatrix} 0 & & & p_1 \\ 1 & 0 & & p_2 \\ & \ddots & \ddots & \vdots \\ 0 & & 1 & p_n \end{pmatrix}. \tag{2}$$

It can be easily proved that $AX = XF$ if and only if X is a Krylov matrix of A. More generally, if M is a nonsingular matrix then the solutions of the equation

$$AX = XM^{-1}FM, \tag{3}$$

have the form $X = KM$. We refer to these matrices as M-Krylov matrices of A.

Let Q be unitary and R upper triangular such that $X = KM = QR$. If K is nonsingular, then R is nonsingular and

$$Q^*AQ = RM^{-1}FMR^{-1}. \tag{4}$$

Appropriate choices of M force Q^*AQ to assume particular structures. Let us consider two simple examples. We denote with Z the down shift matrix, and with e_i for $i = 1 : n$ the canonical vectors so that for the Frobenius matrix we can write $F = Z + pe_n^*$, where $p = (p_i)$ for $i = 1 : n$.

- $M = I$.
  Then RFR^{-1} is upper Hessenberg, or (-1)-banded according to Definition 1. If A is Hermitian $Q^*AQ = RFR^{-1}$ must be Hermitian and hence tridiagonal.

- $M = J$ where J is the reversion matrix.
  Then
  $$M^{-1}FM = J(Z + pe_n^*)J = Z^* + Jpe_1^*.$$
  It turns out that $M^{-1}FM$ is 1-semiseparable, and the same can be said of the matrix $RJFJR^{-1}$. If A is Hermitian the matrix $Q^*AQ = RM^{-1}FMR^{-1}$ must be Hermitian 1-semiseparable.

These simple examples suggest to perform a more systematic analysis of the structure of Q^*AQ depending on M. First of all we consider the case where $M = PL$ where $P = I$ or $P = J$ and L is nonsingular and lower triangular. Then

$$Q^*AQ \quad = \quad RL^{-1}P^*FPLR^{-1}. \tag{5}$$

In order to proceed it is necessary to make some additional assumptions on L. One possibility is to assume that L is strictly $(-k)$-banded. From Theorem 1 we have that L^{-1} is k-semiseparable. It follows that

$$L^{-1} = S + U$$

where S is a rank k matrix and U is k-banded. From equation (5) we obtain

$$\begin{aligned} Q^*AQ &= R(S+U)P^*FPLR^{-1} \\ &= RSP^*FPLR^{-1} + RUP^*FPLR^{-1} \\ &= RSP^*FPLR^{-1} + RUP^*(Z + pe_n^*)PLR^{-1} \\ &= RSP^*FPLR^{-1} + RUP^*pe_n^*PLR^{-1} + RUP^*ZPLR^{-1}. \end{aligned}$$

If $P = I$ the last two summands in the preceding sum made up a (-1)-banded matrix (all the factors are banded and the band of the product can be obtained summing up the band of the factors) while the first summand has rank not exceeding k. We observe that if L is Toeplitz the same conclusion can be reached directly from (5) without regard to k, since L and Z commute.

If $P = J$ the first two summands in the preceding sum made up a matrix of rank not exceeding $k + 1$ an the last summand is 1-banded.

The following theorem summarizes the results obtained so far.

Theorem 2 *Let A be a nonderogatory matrix and let $M = PL$ where L is a nonsingular lower triangular strictly $(-k)$-banded, for a given $k \geq 0$, and P is a permutation matrix. Let X be a nonsingular M-Krylov matrix of A. Let $X = QR$ being Q unitary and R upper triangular. If $P = I$ then Q^*AQ is the sum of a (-1)-banded matrix and a matrix whose rank does not exceed k. If $P = J$ then Q^*AQ is the sum of a 1-banded and a matrix whose rank does not exceed $k + 1$.*

Remark: It is worth noting that all the claims in Theorem 2 remain true if we interchange the roles of L and L^{-1}, that is if L is lower triangular k-semiseparable.

Clearly, if L is $(1-n)$-banded Theorem 2 becomes useless. Note that the claim of this theorem are somehow the best possible. To illustrate this, consider the following examples. Let $A = F$, $L = P = I$, which corresponds to have $k = 0$, then, choosing $v = e_1$, we have $K = I$, and Q^*AQ is indeed an upper Hessenberg matrix. Moreover, if $A = JFJ$, $L = I$ and $P = J$, then, choosing $v = e_n$, we have $K = J$ and $Q^*AQ = Z^* + Jpe_1^*$ is the sum of a 1-banded and a rank one matrix as stated in the theorem.

We end this section by studying the case where $M = JL$, being L a special unit lower triangular matrix, whose columns obey to a given recurrence. In this way, we generalize an idea presented in [7].

Let $B = (b_{ij})$ be a lower triangular $(-k)$-banded matrix, $k \geq 0$, that is a lower triangular matrix vanishing below the lower k-th diagonal. Let us define a unit lower triangular matrix L by means of the following recurrence

$$\begin{cases} Le_n = e_n, \\ Le_{j-1} = Z^*Le_j - \sum_{i=j}^{\min\{n,j+k-1\}} b_{ij}Le_i, \quad j = n : -1 : 2. \end{cases} \tag{6}$$

The relations (6) can be expressed in matrix form as

$$L(Z^* + we_1^*) = Z^*L - LB,$$

where $w = L^{-1}(Z^*L - LB)e_1$. Thus

$$L^{-1}Z^*L = B + Z^* + we_1^*. \tag{7}$$

Now

$$M^{-1}FM = L^{-1}J(Z + pe_n^*)JL = L^{-1}Z^*L + L^{-1}Jpe_1^*L,$$

and the equation (7) implies

$$\begin{aligned} M^{-1}FM &= B + Z^* + we_1^* + L^{-1}Jpe_1^*L \\ &= B + Z^* + (w + L^{-1}Jp)e_1^*. \end{aligned}$$

Thus $RM^{-1}FMR^{-1}$ is the sum of a $(-k)$-banded and a matrix of rank one. For convenience we state this fact explicitly.

Theorem 3 *Let A, X, Q and R be defined as in Theorem 2. Let $M = JL$ where L is a unit lower triangular matrix whose columns satisfy the k-terms recurrence (6). Then Q^*AQ is the sum of a $(-k)$-banded and a matrix whose rank is one, or equivalently is the sum of a $(-k)$-banded plus a 1-semiseparable matrix.*

In the case where B is diagonal, i.e. $k = 0$, the transformed matrix can be interpreted as the sum of a diagonal matrix B and a 1-semiseparable matrix. The paper [7] focuses on this kind of reduction in the case where A is Hermitian.

4 Unitary transformations to rank structures

In order to extend the transformations analyzed in Section 3, we define a generalized Krylov matrix as a matrix having the form

$$K = [V, AV, A^2V, \dots, A^mV(:, 1 : h)],$$

where V is an $n \times r$ matrix and $n = mr + h$, with $h \le r$.

If the Frobenius canonical form [17] of A is given by the direct sum of s nonderogatory matrices, with $s \le r$, it is possible to prove that there exists V such that K is nonsingular. In this hypothesis let X be a nonsingular generalized Krylov matrix of A, and let

$$F = Z^r + UY^*,$$

where $U = X^{-1}AX(:, (n - r + 1)) : n)$ and $Y^* = [O, I_r]$, being I_r the $r \times r$ identity. Then $AX = XF$. We define here the generalized M-Krylov matrices of A as the solutions of equation $AX = XM^{-1}FM$, having the form $X = KM$. The same line of reasoning developed in Section 3 holds, leading to the following theorem.

Theorem 4 *Let A be such that its Frobenius canonical form is given by the direct sum of s nonderogatory matrices, with $s \le r$. Let X be a nonsingular generalized M-Krylov matrix of A, where $M = P$ is a permutation matrix. Let $X = QR$ being Q unitary and R upper triangular. If $P = I$ then Q^*AQ is strictly $(-r)$-banded. If $P = J$ then Q^*AQ is r-semiseparable.*

PROOF. Since R is nonsingular we have

$$Q^*AQ = RP^{-1}FPR^{-1} = RP^{-1}Z^rPR^{-1} + RP^{-1}UY^TPR^{-1}.$$

If $P = I$ then RZ^rR^{-1} is a strictly $(-r)$-banded matrix and RUY^*R^{-1} is a r-rank matrix with the first $n-r$ columns equal to zero. Thus Q^*AQ is strictly $(-r)$-banded.

If $P = J$ then $RJZ^rJR^{-1} = R(Z^*)^rR^{-1}$ and this implies that Q^*AQ is r-semiseparable. If A is nonsingular, Q^*AQ is the inverse of a strictly $(-r)$-banded matrix. ■

Theorem 4 shows how unitary transformations to $(-r)$-banded and to r-semiseparable matrices can be obtained via generalized Krylov matrices. We now will generalize Theorem 3 to obtain r-semiseparable plus $(-k)$-banded matrices.

Let $B = (b_{ij})$ be a lower triangular $(-k)$-banded matrix, $k \ge 0$. Let us define a unit lower triangular matrix L by means of the following recurrence:

$$\begin{cases} Le_j = e_j, & j = n : -1 : n - r + 1, \\ Le_{j-r} = (Z^r)^*Le_j - \sum_{i=j}^{\min\{n, j+k-1\}} b_{ij}Le_i, & j = n : -1 : r + 1, \end{cases} \qquad (8)$$

As in (6), the relations (8) can be expressed in matrix form as

$$L((Z^r)^* + WJ_rY^*J) = (Z^r)^*L - LB,$$

where J_r is the reversion matrix of order r, and $W = L^{-1}((Z^r)^*L - LB)JYJ_r$. Let X be a nonsingular generalized M-Krylov matrix of A, where $M = JL$. Following the same reasoning which leads to Theorem 3 we have

$$L^{-1}(Z^r)^*L = B + (Z^r)^* + WJ_rY^*J,$$

and

$$\begin{aligned} M^{-1}FM &= L^{-1}J(Z^r + UY^*)JL \\ &= L^{-1}(Z^r)^*L + L^{-1}JUY^*JL \\ &= B + (Z^r)^* + (WJ_r + L^{-1}JUJ_rL_rJ_r)Y^*J, \end{aligned}$$

where L_r is the leading diagonal $r \times r$ block of L. Thus $RM^{-1}FMR^{-1}$ is the sum of a $(-k)$-banded and a matrix of rank r, and Theorem 3 can be generalized to r-semiseparable matrices as follows.

Theorem 5 *Under the same hypothesis of Theorem 4, let $M = JL$ where L is a unit lower triangular matrix whose columns satisfy the recurrent relations (8). If $X = QR$ being Q unitary and R upper triangular, then Q^*AQ is the sum of a $(-k)$-banded and a matrix whose rank is r, or equivalently is the sum of a $(-k)$-banded plus an r-semiseparable matrix.*

5 QR steps

In this section we study how the matrices obtained at each step of QR algorithm are related to the initial matrix A. In particular, we show that these matrices are M-Krylov matrices of A.

Theorem 6 *Let A satisfy the hypotheses of Theorem 4. Let $X = QR$ be a generalized M-Krylov matrix of A and let $B = Q^*AQ$. Let σ be such that $B - \sigma I$ is nonsingular, and let B_1 be the matrix obtained by applying a QR step with shift σ to B, that is, $B - \sigma I = Q_1R_1$. Then $B_1 = Q_1^*Q^*AQQ_1$ and the matrix $X_1 = QQ_1R_1R$ is a generalized M-Krylov matrix of A. Moreover, $X_1 = (A - \sigma I)X$.*

Proof. Clearly $B_1 = Q_1^*BQ_1 = Q_1^*Q^*AQQ_1$, and moreover $B_1 = R_1BR_1^{-1} = R_1RM^{-1}FMR^{-1}R_1^{-1}$.

This implies that $X_1 = QQ_1R_1R$ is an M-Krylov matrix of A, since $AX_1 = X_1M^{-1}FM$. Moreover $X_1 = Q(B - \sigma I)R = QBR - \sigma X = AX - \sigma X = (A - \sigma I)X$. ■

A natural consequence of Theorem 6 is that, if the matrix B has one of the rank structures analyzed in the previous sections, B_1 maintains the same structure. This fact simply follows from the observation that both B and B_1 are obtained factorizing QR two different generalized M-Krylov matrices, X and X_1 respectively.

References

[1] E. Asplund. Inverses of matrices $\{a_{ij}\}$ which satisfy $a_{ij} = 0$ for $j > i + p$. *Math. Scand.*, 7:57–60, 1959.

[2] M. Van Barel, R. Vandebril, and N. Mastronardi. The Lanczos-Ritz values appearing in an orthogonal similarity reduction of a matrix into semiseparable form. Technical Report TW 360, Katholieke Universiteit Leuven, Department of Computer Science, May 2003.

[3] W.W. Barrett and P.J. Feinsilver. Inverses of banded matrices. *Lin. Alg.and its Appl.*, 41:111–130, 1981.

[4] R. Bevilacqua and G. M. Del Corso. Structural properties of matrix unitary reduction to semiseparable form. *Calcolo*, 2004. to appear.

[5] D. A. Bini, F. Daddi, and L. Gemignani. On the shifted QR iteration applied to Frobenius matrices. *ETNA*, 2004. to appear.

[6] Y. Eidelman and I. Gohberg. Inversion formulas and linear complexity algorithm for diagonal plus semiseparable matrices. *Comput. Math. Appl.*, 33:69–79, 1997.

[7] D. Fasino. Rational Krylov matrices and QR steps on Hermitian diagonal-plus-semiseparable matrices. *Numerical Linear Algebra and its Applications*, 2004. to appear.

[8] F. R. Gantmacher and M. G. Krein. *Oscillation matrices and kernels and small vibrations of mechanical systems.* AMS Chelsea publishing, 2002.

[9] L. Gemignani. A unitary Hessenberg QR-based algorithm via semiseparable matrices. sumitted, 2004.

[10] G. H. Golub and C. F. Van Loan. *Matrix Computations.* The Johns Hopkins University Press, Baltimore, 1996. Third Edition.

[11] R. A. Horn and C. R. Johnson. *Matrix Analysis.* Cambridge university Press, 1985.

[12] T. Kailath I. Gohberg and I. Koltrach. Linear complexity algorithms for semiseparable matrices. *Integral Equations and Operator Theory*, 8:780–804, 1985.

[13] P. Rózsa, R. Bevilacqua, P. Favati, and F. Romani. On band matrices and their inverses. *Lin. Alg.and its Appl.*, 150:287–295, 1991.

[14] Y. Saad. *Iterative methods for sparse linear sistems.* SIAM, Second Edition, 2003.

[15] R. Vandebril, M. Van Barel, and N. Mastronardi. A note on the representation and definition of semiseparable matrices. Technical Report TW 368, Katholieke Universiteit Leuven, Department of Computer Science, October 2003.

[16] R. Vandebril, M. Van Barel, and N. Mastronardi. An orthogonal similarity reduction of a matrix to a semiseparable form. Technical Report TW 355, Katholieke Universiteit Leuven, Department of Computer Science, February 2003.

[17] J. H. Wilkinson. *The Algebraic Eigenvalue Problem.* Oxford University Press, London, 1965.