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DECAY IN FUNCTIONS OF MULTI-BAND MATRICES

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Abstract. The Benzi–Golub result on decay properties for matrix functions of a banded Hermitian matrix is extended to the case of multi-band and certain other sparse multilevel matrices.

Key words. Matrix functions, multilevel matrices, multi-band matrices, polynomial approximation, exponential decay.

1. Introduction. Decay properties of the entries of inverses to banded diagonally dominant matrices are known for a long time: exponential decay away from the main diagonal is granted, the actual rate depending on the band-width [3]. Then, a similar observation was established for infinite Hermitian positive definite matrices [4], with some care to be taken about the constant factor when applied to finite matrices. Further, a far reaching generalization was made in [2]: same decay properties turn out to hold for a wide class of functions of a given banded Hermitian positive definite matrix, rather than only inverses. Importance of the latter result is amplified by a conspicuous growth of interest to computations with matrix functions [1, 5].

However, multidimensional problems naturally give rise to multilevel sparse matrices with a band-width depending on the matrix size. As a consequence, the decay rates of the previous results depend on the matrix size. Nevertheless, the same matrices usually can be viewed as multilevel multi-band matrices with the multi-band sizes independent of the order of matrix. In this paper we propose that the decay results for such matrices can be more suitably presented in the multi-index notation, for the decay takes place at every level of a given multilevel matrix.

We use a definition of multilevel matrix suggested in [10]: a matrix A of order n is said to have p levels of sizes $n_1, ..., n_p$ if $n = n_1 ... n_p$ and A is viewed as a block $n_1 \times n_1$ matrix with every block considered as a block $n_2 \times n_2$ matrix, the same construction of getting to matrices with smaller blocks being repeated hierarchically p times. The row and column indices of A are in the one-to-one correspondence with p-tuple indices:

$$i \leftrightarrow \mathbf{i} = (i_1, ..., i_p), \quad j \leftrightarrow \mathbf{j} = (j_1, ..., j_p),$$

where, by definition,

$$\begin{array}{rcl} i & = & (i_1 - 1)n_2...n_p + (i_2 - 1)n_3...n_p + ... + (i_{p-1} - 1)n_p + i_p, \\ j & = & (j_1 - 1)n_2...n_p + (j_2 - 1)n_3...n_p + ... + (j_{p-1} - 1)n_p + j_p. \end{array}$$

Thus, for the entries of A we shall write

$$a_{ij} = a_{\mathbf{ij}} = a(i_1, ...i_p; j_1, ..., j_p).$$

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In this case we say that A is a matrix of multi-order $\mathbf{n} = (n_1, ..., n_p)$.

A p-level matrix A is called multi-band of multi-width $\mathbf{m} = (m_1, ..., m_p)$ if it is granted that

$$a(i_1, ..., i_p; j_1, ..., j_p) = 0$$

whenever

$$|i_l - j_l| > m_l/2$$

at least for one value of $l \in \{1, ..., p\}$. Each number m_l is assumed odd and referred to as the band-width of level l.

Multi-band matrices are sparse with a special sparsity pattern. This pertains to a more general type of linear structure expounded in [7].

We present certain conditions under which the entries of a p-level matrix $B = f(A)$ are estimated in the following way:

$$|b(i_1, ..., i_p; j_1, ..., j_p)| \leq c q^{\max_l |i_l - j_l|}, \quad 0 < q < 1.$$

Note that exponential decrease is ascertained in the estimate rather than entries, and the estimate is not necessarily sharp. In many cases, however, c does not depend on the multi-order. This makes the estimate very useful for proof and construction of low-parametric approximations to typical matrix functions of A.

2. Main results. Consider a sequence $S_0 \subset S_1 \subset ...$ of non-empty subsets of

$$S = \{(i, j) : i, j = 1, 2, ...\}.$$

For any matrix A, denote by $\mathrm{NZ}(A)$ the set of all index pairs $(i, j) \in S$ such that $a_{ij} \neq 0$.

Define $||A||_C$ as the maximal in modulus entry of A.

LEMMA 2.1. *Given a matrix A, assume that $\mathrm{NZ}(A^k) \subset S_k$ for $k = 0, 1, ...$, and consider a matrix B and a function $E(d)$ with the following property: for any $d = 0, 1, ...$ there exists a polynomial $p_d(x)$ such that $\deg(p_d) \leq d$ and*

$$||B - p_d(A)||_C \leq E(d).$$

Then

$$|b_{ij}| \leq E(d)$$

whenever

$$(i, j) \notin S_d.$$

Proof. All nonzero entries of $p_d(A)$ occupy positions $(i, j) \in S_d$. Hence, from $(i, j) \notin S_d$ we conclude that $|b_{ij}| = |(B - p_d(A))_{ij}| \leq E(d)$. □

LEMMA 2.2. *Let A be a p-level multi-band matrix with level band-widths $m_1, ..., m_p$. Then*

$$\mathrm{NZ}(A^k) \subset S_k,$$

where

$$S_k = \{(i,j) = (\mathbf{i},\mathbf{j}) : |i_l - j_l| < (km_l - k + 1)/2\}.$$

Proof. It follows from the observation that the product AB of two matrices with band-widths $m(A)$ and $m(B)$ is a band matrix with the band-width $m(AB) = m(A) + m(B) - 1$. □

LEMMA 2.3. *Let A be a p-level multi-band matrix with level band-widths $m_1, ..., m_p$. Assume that a matrix B and polynomials $p_d(x)$ are such that* $\deg(p_d) \le d$ *and*

$$||B - p_d(A)||_C \le E(d)$$

with the monotonicity property

$$E(d+1) \le E(d), \quad d = 0, 1, \ldots .$$

Then B can be considered as p-level matrix with the same level sizes as those of A, and the entries of B outside the multi-band of A are bounded as follows:

$$|b_{ij}| = |b_{\mathbf{ij}}| \le E\left(t(i,j)\right),$$

where

$$t(i,j) = \max_{1 \le l \le p} \left\lceil \frac{2|i_l - j_l|}{m_l} \right\rceil .$$

Proof. Consider a position (i,j), choose level l and find a positive integer d such that

$$(dm_l - d + 1)/2 < |i_l - j_l| \le dm_l/2.$$

Then $(i,j) \notin S_d$, and hence,

$$|b_{ij}| \le E(d) \le E\left(\left\lceil \frac{2|i_l - j_l|}{m_l} \right\rceil\right),$$

Using monotonicity of $E(d)$ we diminish the right-hand side by maximizing the argument. □

These lemmas help us to derive estimates for the entries of those matrices B that can be approximated by a polynomial of a multi-band matrix A. The decay properties are determined by the behavior of approximation accuracy in regard with the degree of polynomial.

A simple polynomial approximation result for $B = (I+F)^{-1}$ is easily available in the case $||F||_2 < 1$. The latter inequality implies the convergence of the Neumann series

$$(I+F)^{-1} = \sum_{s=0}^{\infty} (-1)^s F^s.$$

Upon truncation down to $d+1$ terms, we obtain a polynomial

$$p_d(F) = \sum_{s=0}^{d} (-1)^s F^s$$

with the estimate

$$||B - p_d(A)||_C \leq c_\rho \rho^d, \quad c_\rho = \frac{\rho}{1-\rho}.$$

This leads us immediately to the following theorem.

THEOREM 2.4. *Let A be a p-level multi-band matrix with level band-widths $m_1, ..., m_p$, and assume that A is diagonally dominant in rows:*

$$\rho |a_{ii}| \geq \sum_{j \neq i} |a_{ij}|, \quad 1 \leq i \leq n, \quad 0 < \rho < 1.$$

Then the entries of A^{-1} outside the multi-band of A satisfy the bounds

$$|(A^{-1})_{ij}| \leq c \rho^{t(i,j)}, \quad t(i,j) = \max_{1 \leq l \leq p} \left[\frac{2|i_l - j_l|}{m_l} \right],$$

with

$$c = \left(\max_i |a_{ii}^{-1}| \right) \frac{\rho}{1-\rho}.$$

Proof. Let $D = \mathrm{diag}(A)$ denote the main diagonal of A. Then $D^{-1}A = I + F$ with $||F||_2 \leq ||F||_\infty \leq \rho$. It remains to note that $A^{-1} = (I+F)^{-1}D^{-1}$ and apply the above polynomial approximations to $(I+F)^{-1}$. □

Similar results can be obtained for matrices of the form $B = f(A)$, where the function f is well-approximated by polynomials around the spectrum of A. A rather straightforward generalization of Theorem 2.4 is as follows.

THEOREM 2.5. *Assume that $f(z)$ is analytic in a bounded simply connected domain with a piece-wise smooth boundary Γ, and a matrix A and a number $0 < \rho < 1$ are such that*

$$\rho |a_{ii} - z| \geq \sum_{j \neq i} |a_{ij}|, \quad 1 \leq i \leq n, \quad z \in \Gamma.$$

Let A be a p-level multi-band matrix with level band-widths $m_1, ..., m_p$. Then the entries of $f(A)$ outside the multi-band of A are bounded as follows:

$$|\{f(A)\}_{ij}| \leq c \rho^{t(i,j)}, \quad t(i,j) = \max_{1 \leq l \leq p} \left[\frac{2|i_l - j_l|}{m_l} \right],$$

with

$$c = \frac{2\pi\rho}{1-\rho} \max_{z \in \Gamma} \min_{1 \leq i \leq n} |a_{ii} - z|^{-1} \int_{z \in \Gamma} |f(z)| d|z|.$$

Proof. ¿From the Gershgorin theorem, all the eigenvalues of A are strictly inside the domain encircled by Γ. Hence,

$$f(A) = \frac{1}{2\pi \mathbf{i}} \int_\Gamma (A - zI)^{-1} f(\zeta) d\zeta.$$

Observe that $A - zI$ keep the multi-band structure of A for all z. Then, the claimed estimate follows by direct application of Theorem 2.4. □

A more sophisticated result can be obtained by direct adjustment of the method suggested in [2]. Note that the symmetry assumption of [2] is not crucial and can be replaced by the two requirements:

(a) A is diagonalizable: $A = P\Lambda P^{-1}$, where $\Lambda = \text{diag}(\lambda_1, ..., \lambda_n)$ is a diagonal matrix of the eigenvalues and P is the eigenvector matrix;
(b) all the eigenvalues belong to the interval $[a, b] \subset \mathbb{R}$.

Suppose that $f(z)$ is an analytic function in a domain around the interval $[a, b]$. Then

$$f(A) = Pf(\Lambda)P^{-1}.$$

Thus, the function approximation estimates are converted into matrix approximation estimates of the same appearance but with a factor of the form $||P||_2||P^{-1}||_2$.

As in [2], we can use the Bernstein ellipses Γ_ρ. By definition, Γ_ρ is the ellipse with foci at the points -1, 1 and the sum of half-axes $\rho + \rho^{-1}$. Let us agree that $0 < \rho < 1$. Let us assume that $f(z)$ with

$$z = \frac{a+b}{2} + \frac{b-a}{2}\zeta$$

is analytic as a function of ζ for all $\zeta \in \Gamma_\rho$. Then there exist polynomials $p_d(x)$ such that $\deg p_d \leq d$ and

$$|f(x) - p_d(x)| \leq c(f, \rho)\rho^d, \quad a \leq x \leq b. \tag{2.1}$$

It can be shown that $c(f, \rho)$ depends actually on the maximal modulus of $f(z)$ for $\zeta \in \Gamma_\rho$ and as well on the length of Γ_ρ and the very ρ.

THEOREM 2.6. *A be a p-level multi-band matrix with level band-widths $m_1, ..., m_p$, and let the requirements (a) and (b) be fulfilled. Assume that $f(z)$ admits polynomial approximations with the estimate (2.1). Then the entries of $f(A)$ outside the multi-band of A are bounded as follows:*

$$|\{f(A)\}_{ij}| \leq c\rho^{t(i,j)}, \quad t(i,j) = \max_{1 \leq l \leq p} \left[\frac{2|i_l - j_l|}{m_l}\right], \tag{2.2}$$

with

$$c = c(f)||P||_2||P^{-1}||_2.$$

3. Numerical Examples. Consider first one-level matrices. Set $q = 0.1$ and let A_n be of order n with the entries

$$a_{ij} = \begin{cases} \exp\{-q(i-j)^2\}, & i \neq j, \\ 2, & i = j. \end{cases}$$

Let A_{mn} be a matrix of order n and of band-width m with the same nonzero entries as A_n. Note that A_n is not diagonally dominant for $n \geq 5$, neither A_{mn} for $m \geq 2$.

First of all, we can regard A_{mn} as a banded approximation to A_n. In Table 1, we give approximation errors in the Frobenius norm for $||f(A)_{mn} - f(A)_n||_F$ for the following matrix functions:

$$f(A) = A, \quad f(A) = A^{-1}, \quad f(A) = \log(A), \quad f(A) = \exp\{-A\}.$$

Table 1 demonstrates the decay properties in functions of the dense matrix A_n. Formally, these are not covered by the above theorems. However, we see that A_n can

Band-width	7	9	11	13	15	17	19
A	8.E-02	2.E-03	2.E-05	1.E-07	3.E-10	4.E-13	2.E-16
A^{-1}	1.E-01	2.E-02	7.E-03	3.E-03	5.E-04	2.E-04	8.E-05
$\log(A)$	5.E-02	1.E-02	5.E-03	7.E-04	2.E-04	9.E-05	1.E-05
$\exp(-A)$	9.E-02	2.E-02	1.E-02	2.E-03	8.E-04	2.E-04	5.E-05

Table 1. One-level banded approximations for functions of A_{1000}.

Band-width	7	9	11	13	15	17	19
A^{-1}	8.E-02	2.E-02	9.E-03	3.E-03	5.E-04	3.E-04	7.E-05
$\log(A)$	6.E-02	2.E-02	6.E-03	8.E-04	4.E-04	1.E-04	2.E-05
$\exp(-A)$	8.E-02	3.E-02	1.E-02	2.E-03	9.E-04	2.E-04	7.E-05

Table 2. One-level banded approximations for functions of $A_{7,1000}$.

be approximated by a banded matrix A_{mn} and $f(A_n)$ can be then approximated by $f(A_{mn})$. The decay results for $m = 7$ are put in Table 2.

Now, with the same $q = 0.1$ consider two-level matrices with the entries

$$a_{i_1 i_2; j_1 l_2} = \begin{cases} \exp\{-q((i_1 - j_1)^2 + (i_2 - j_2)^2)\}, & i \neq j, \\ 4, & i = j. \end{cases}$$

Take the level sizes to be $n_1 = n_2 = 30$ and examine the decay properties at each level for the same matrix fucntions. Table 3–6 show the Euclidean lengths of two-level diagonals $i_1 - j_1 = k_1,\ k_2 = i_2 - j_2$ as functions of k_1, k_2.

k_1, k_2	0	1	3	5	7	9	11	12
0	1.E+02	3.E+01	1.E+01	2.E+00	2.E-01	8.E-03	1.E-04	1.E-05
1	3.E+01	2.E+01	1.E+01	2.E+00	2.E-01	7.E-03	1.E-04	1.E-05
3	1.E+01	1.E+01	4.E+00	9.E-01	8.E-02	3.E-03	5.E-05	5.E-06
5	2.E+00	2.E+00	9.E-01	2.E-01	1.E-02	6.E-04	1.E-05	1.E-06
7	2.E-01	2.E-01	8.E-02	1.E-02	1.E-03	5.E-05	9.E-07	8.E-08
9	8.E-03	7.E-03	3.E-03	6.E-04	5.E-05	2.E-06	3.E-08	3.E-09
11	1.E-04	1.E-04	5.E-05	1.E-05	9.E-07	3.E-08	6.E-10	6.E-11
12	1.E-05	1.E-05	5.E-06	1.E-06	8.E-08	3.E-09	6.E-11	6.E-12

Table 3. Decay in two-level diagonals: $f(A) = A$, $n_1 = n_2 = 30$.

The decay properties can serve as a base for some fast algorithms. A general scheme is proposed in [6], developing an approach considered for the approximate matrix inversion using Toeplitz-like structures in [9] and using tensor approximations in [8].

Given a two-level matrix A with the level band-widths m_1, m_2, in order to perform the inversion we can consider the approximate Newton-Schultz iteration as follows:

$$X_{k+1} = \mathcal{P}_{k_1,k_2}(X_k - X_k A X_k),$$

where $\mathcal{P}_{k_1,k_2}$ is a truncation operator that sets to zero all the entries outside the two-level band with band-width parameters k_1, k_2.

Consider the above matrix with level sizes $p = n_1 = n_2$, let the input band-width be $m = m_1 = m_2$ and set the truncation band-width parameter to $k = k_1 = k_2$. The

k_1, k_2	0	1	3	5	7	9	11	12
0	9.E+00	7.E-01	1.E-01	3.E-02	5.E-03	1.E-03	7.E-04	1.E-04
1	7.E-01	5.E-01	6.E-02	3.E-02	5.E-03	9.E-04	6.E-04	8.E-05
3	1.E-01	6.E-02	4.E-02	1.E-02	6.E-03	4.E-04	4.E-04	9.E-05
5	3.E-02	3.E-02	1.E-02	5.E-03	2.E-03	1.E-03	4.E-05	2.E-04
7	5.E-03	5.E-03	6.E-03	2.E-03	9.E-04	4.E-04	2.E-04	1.E-04
9	1.E-03	9.E-04	4.E-04	1.E-03	4.E-04	2.E-04	6.E-05	8.E-06
11	7.E-04	6.E-04	4.E-04	4.E-05	2.E-04	6.E-05	3.E-05	3.E-05
12	1.E-04	8.E-05	9.E-05	2.E-04	1.E-04	8.E-06	3.E-05	1.E-05

Table 4. Decay in two-level diagonals: $f(A) = A^{-1}$, $n_1 = n_2 = 30$.

k_1, k_2	0	1	3	5	7	9	11	12
0	4.E+01	4.E+00	1.E+00	5.E-02	1.E-02	5.E-03	9.E-04	6.E-04
1	4.E+00	3.E+00	8.E-01	6.E-02	1.E-02	5.E-03	9.E-04	5.E-04
3	1.E+00	8.E-01	9.E-02	6.E-02	3.E-03	3.E-03	9.E-04	3.E-04
5	5.E-02	6.E-02	6.E-02	9.E-03	7.E-03	2.E-04	5.E-04	4.E-05
7	1.E-02	1.E-02	3.E-03	7.E-03	1.E-03	9.E-04	2.E-05	1.E-04
9	5.E-03	5.E-03	3.E-03	2.E-04	9.E-04	1.E-04	1.E-04	6.E-05
11	9.E-04	9.E-04	9.E-04	5.E-04	2.E-05	1.E-04	2.E-05	1.E-05
12	6.E-04	5.E-04	3.E-04	4.E-05	1.E-04	6.E-05	1.E-05	2.E-05

Table 5. Decay in two-level diagonals: $f(A) = \log(A)$, $n_1 = n_2 = 30$.

initial guess X_0 is chosen as $X_0 = \alpha I$, below we set $\alpha = 0.05$. Table 7 shows the residual values $r_i = ||I - X_k A||_F$.

4. Conclusions. In this paper we presented a simple framework that allows us to revisit a proof of the Benzi–Golub result on decay properties for matrix functions of a banded Hermitian matrix and also extend this result to multilevel multi-banded matrices. It is worth stressing that our framework can be used with some sparisty patterns rather than bands. However, despite the generality of our theorems, we ought to note that practical usefulness of the presented decay estimates depend on the involved constants.

Some numerical examples are given to illustrate the multilevel decay property on typical matrix functions such as the inverse, exponent and logarithm. We show how the decay properties can be used in approximate computation of the inverse matrix by the Newton–Schultz iteration with a sparsification on every step so that the total number of nonzero entries is kept limited.

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k_1, k_2	0	1	3	5	7	9	11	12
0	1.E+00	2.E-01	8.E-03	8.E-03	4.E-03	1.E-03	2.E-04	4.E-04
1	2.E-01	1.E-01	7.E-03	7.E-03	4.E-03	1.E-03	2.E-04	4.E-04
3	8.E-03	7.E-03	2.E-02	2.E-03	2.E-03	1.E-03	2.E-04	4.E-04
5	8.E-03	7.E-03	2.E-03	4.E-03	8.E-04	7.E-04	4.E-04	2.E-04
7	4.E-03	4.E-03	2.E-03	8.E-04	1.E-03	2.E-04	2.E-04	3.E-05
9	1.E-03	1.E-03	1.E-03	7.E-04	2.E-04	3.E-04	5.E-05	1.E-04
11	2.E-04	2.E-04	2.E-04	4.E-04	2.E-04	5.E-05	9.E-05	4.E-05
12	4.E-04	4.E-04	4.E-04	2.E-04	3.E-05	1.E-04	4.E-05	3.E-06

Table 6. Decay in two-level diagonals: $f(A) = \exp\{-A\}$, $n_1 = n_2 = 30$.

iteration	1	2	3	4	5	6	7
$p = 50$	3.4E+01	2.5E+01	1.3E+01	3.4E+00	2.5E-01	1.4E-03	1.2E-04
$p = 100$	6.9E+01	4.9E+01	2.5E+01	6.8E+00	5.0E-01	2.7E-03	2.8E-04

Table 7. Residual values for the Newton-Schultz iteration, $m = 7,\ p = 21$.

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