Divide and conquer methods for functions of matrices with banded or hierarchical low-rank structure

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Matrix functions

Matrix functions arise in many applications, e.g.:

- Solution of PDEs (exponential, square root, fractional powers, ...)
  \[
  \begin{cases}
    \frac{dy}{dt} = Ay, \quad A \in \mathbb{R}^{n \times n} \\
    y(0) = c, \quad c \in \mathbb{R}^n
  \end{cases}
  \text{ has solution } y(t) = \exp(At) \cdot c.
  \]
- Electronic structure calculations (sign function)
- Network analysis (exponential for Estrada index)
- Statistical learning (logarithm, ...)
- Nonlinear matrix equations
- ...

Definition

Given function \( f \) and \( A = V \cdot \text{diag}(\lambda_1, \ldots, \lambda_n) \cdot V^{-1} \),

\[
f(A) := V \cdot \text{diag}(f(\lambda_1), \ldots, f(\lambda_n)) \cdot V^{-1}.
\]

(Generalization to non-diagonalizable matrices possible [Higham’2008])
(Approximate) preservation of structure

Example: Tridiagonal matrix $A = \text{tridiag}(-1, 2, -1)$.

Figure: $f(z) = \exp(z)$. Log of entries of $f(A)$: matrix function $f(A)$ is approximately banded.

Figure: $f(z) = z^{-1}$. Log of entries of $f(A)$: matrix function $f(A)$ is not (approximately) banded...

Figure: ... but $f(A) = A^{-1}$ has all off-diagonal blocks of rank 1!
Connection to polynomial/rational approximation

For now, assume $A$ banded.

If $f$ is well approximated by a small-degree polynomial $p$ on spectrum of $A$ then

$$f(A) \approx p(A) = \text{banded.}$$

If $f$ is well approximated by a small-degree rational function $r$ on spectrum of $A$ then

$$f(A) \approx r(A) = \text{HSS matrix.}$$

Generalizations to other formats such as hierarchically semiseparable (HSS) matrices are possible.
Existing methods for computing $f(A)$

- A priori polynomial approximation
  [Benzi/Boito/Razouk’2013], [Goedecker’1999], [Benzi/Razouk’2008], ...

- Iterations + thresholding
  [Németh/Scuseria’2000] (sign), [Bini et al.’2016] (Toeplitz matrices), ...

- A priori rational approximation
  [Gavrilyuk et al.’2002] (exponential), [Kressner/Šušnjara’2017] (spectral projectors), [Beckermann/Bisch/Luce’2021] (Markov functions of Toeplitz matrices), ...

- Iterations in HSS arithmetics + truncation strategies
  [Grasedyck et al.’2003] (sign), $\sqrt{\cdot}$, ...
Goal:
Compute \( f(A) \)
for matrix \( A \in \mathbb{R}^{n \times n} \)
with some low-rank structure.
We consider matrices which can be decomposed (recursively) as

\[ A = D_1 + D_2 + \text{low-rank} = D + R \]

e.g. banded matrices, HODLR/HSS matrices, adjacency matrices of graphs with community structure.

Divide-and-conquer idea for computing \( f(A) \):

\[ f(A) = \begin{bmatrix} f(D_1) \\ f(D_2) \end{bmatrix} + \text{correction}. \]
Low-rank updates

Nice fact: In many cases \( f(D + R) - f(D) \) is approximately low-rank!

Example: Singular value decay of \( f(A) - f(D) \) for
- \( A = \text{tridiag}(-1, 2, -1) \) of size \( 256 \times 256 \),
- \( D_1 = D_2 = \text{tridiag}(-1, 2, -1) \) of size \( 128 \times 128 \),
- \( R = A - D \) has rank 2.

\[ f(z) = \exp(z). \]

\[ f(z) = \sqrt{z}. \]

[Beckermann/Kressner/Schweitzer'2018], [Beckermann et al.'2021]
Low-rank updates: Algorithm

Let \( R = BJC^T \), with \( B, C \in \mathbb{R}^{n \times r} \) and \( J \in \mathbb{R}^{r \times r} \).

Choose rank \( m \) and approximate \( f(D + R) - f(D) \approx U_mX_m(f)V_m^T \), where:

- \( U_m \in \mathbb{R}^{n \times mr} \) orthonormal basis of \( \mathcal{K}_m(D, B) \) or \( q_m(D)^{-1}\mathcal{K}_m(D, B) \);
- \( V_m \in \mathbb{R}^{n \times mr} \) orthonormal basis of \( \mathcal{K}_m(D^T, C) \) or \( q_m(D^T)^{-1}\mathcal{K}_m(D^T, C) \);

**Definition**

- Polynomial Krylov subspace: \( \mathcal{K}_m(D, B) := \text{span} \begin{bmatrix} B, DB, D^2B, \ldots, D^{m-1}B \end{bmatrix} \).
- Rational Krylov subspace associated with \( q(z) = (z - \xi_1) \cdots (z - \xi_m) \) for prescribed poles \( \xi = (\xi_1, \ldots, \xi_m)^T \in \mathbb{C}^m \):
  \[
  \mathcal{RK}_m(D, B, \xi) := \text{span} \begin{bmatrix} q_m(D)^{-1}B, q_m(D)^{-1}DB, q_m(D)^{-1}D^2B, \ldots, q_m(D)^{-1}D^{m-1}B \end{bmatrix}.
  \]

\( X_m(f) \in \mathbb{R}^{mr \times mr} \) chosen in suitable way according to [Beckermann/Kressner/Schweitzer’2018], [Beckermann et al.’2021]
Divide-and-conquer algorithm

**Input:** Matrix $A$ with hierarchical low-rank structure, function $f$

**Output:** Approximation of $f(A)$, in HSS format

1. if $A$ is small then
2. Compute $f(A)$ in “dense” arithmetics, e.g. by Schur-Parlett’s algorithm
3. else
4. Decompose $A = D + R = \text{block-diagonal} + \text{low-rank}$
5. Compute $f(\text{diagonal blocks})$ recursively
6. Add correction $f(D + R) - f(D)$ computed by low-rank updates algorithm
7. end if

[C./Kressner/Massei’2021]
Convergence of D&C algorithm

Theorem ([C./Kressner/Massei’2021])

Let $A$ be symmetric and let $f$ be a function analytic on an interval $\mathbb{E}$ containing the eigenvalues of $A$. Suppose that we use rational Krylov subspaces with poles $\xi_1, \ldots, \xi_m$, closed under complex conjugation, for computing updates. Then the output $F_A$ of the D&C algorithm satisfies

$$\|f(A) - F_A\|_2 \leq 4 \cdot \text{recursion depth} \cdot \min_{r \in \Pi_m/q_m} \|f - r\|_E,$$

where $q_m(z) = \prod_{i=1}^m (z - \xi_i)$.

Main ingredient of the proof:
Each low-rank update is exact for rational functions $r \in \Pi_m/q_m$.

Nice fact: Convergence is related to best rational approximation, but does not need to explicitly find such rational function.
Numerical experiments (1)

Example from [Ilić/Turner/Simpson’2010]: Sampling from a Gaussian random field requires $A^{-1/2}$ for $A =$ covariance matrix; here $A$ is banded.

- D&C algorithm (extended Krylov subspaces for low-rank updates)
- Denman and Beavers iteration with HSS arithmetic (hm-toolbox [Massei/Robol/Kressner’2020])
- Matlab’s sqrtm

<table>
<thead>
<tr>
<th>$A$ Size</th>
<th>Band</th>
<th>D&amp;C Time</th>
<th>D&amp;C Err</th>
<th>sqrtm (HSS) Time</th>
<th>sqrtm (HSS) Err</th>
<th>Dense Time</th>
<th>$A^{-\frac{1}{2}}$ HSS rank</th>
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Numerical experiments (2)

For $A = \text{adjacency matrix of undirected graph}$, diagonal entries of $\exp(A)$ are subgraph centralities and $\frac{1}{n} \text{trace}(\exp(A))$ is the Estrada index.

- D&C algorithm (splitting vertices into 2 components using METIS algorithm, polynomial Krylov subspaces for the low-rank updates)
- mmq (Gauss quadrature to approximate each diagonal entry of $\exp(A)$, see [Golub/Meurant'2010])
- Matlab’s expm and eig

<table>
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<th>$A$ Size</th>
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<th>D&amp;C diagonal Err</th>
<th>mmq diagonal Time</th>
<th>mmq diagonal Err</th>
<th>expm Time</th>
<th>expm Err</th>
<th>D&amp;C trace Time</th>
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</tbody>
</table>

Test matrices from the SuiteSparse Matrix Collection.
Special case: Banded matrices (1)

Bases of polynomial Krylov subspaces inherit sparsity and have the form

\[ U_m = V_m = \begin{bmatrix} 0 \\ I \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \]
Special case: Banded matrices (2)

D&C algorithm simplifies a lot! \( \rightsquigarrow \) “block-diagonal splitting algorithm”

\[
A = \begin{bmatrix}
\end{bmatrix}
\]

Then,  

\[
f(A) \approx f \begin{bmatrix}
\end{bmatrix} + f \begin{bmatrix}
\end{bmatrix} - f \begin{bmatrix}
\end{bmatrix}.
\]

**Theorem ([C./Kressner/Massei’2021])**

For a matrix \( A \) with bandwidth \( b \), block size \( s \), let \( m := \lfloor s/2b \rfloor \), then

\[
\| f(A) - \text{approx} \|_2 \leq 10 \min_{p \in \Pi_m} \| f - p \| \text{numerical range of } A.
\]
Numerical example for banded matrices

The size of the blocks can be chosen adaptively.

Example: \( A \) is tridiagonal, \( \text{linspace}(2, 3, n) \) on the diagonal, \(-1\) on super- and sub-diagonals; \( f(A) = \sqrt{A} \).

**Figure:** \( \log |f(A)| \)

**Figure:** Sparsity pattern of the output
Computational complexity

Simplified assumption: low-rank updates converge in a fixed number of steps.

- General D&C algorithm: $O(k^2n \log n)$ for matrix of size $n$ and HSS rank $k$
- Block diagonal splitting algorithm: $O(nb^2)$ for a matrix of bandwidth $b$

**Figure:** $A = \text{tridiag}(-1, 2, -1)$, $f = \exp$. 
Trace & diagonal of matrix functions

Assume polynomial Krylov subspaces are used for the low-rank updates.

Figure: Convergence of low-rank updates algorithm \( f(A) - f(A - R) \), \( A \) and \( R \) symmetric, \( f = \exp \).

Figure: Convergence of block-diagonal splitting algorithm for the exponential of normalized non-symmetric pentadiagonal matrix \( A \).

Trace and/or diagonal converge faster! (And we proved it)
Summary & conclusions

1. Two new algorithms for approximating matrix functions:
   - A general D&C algorithm for matrices with hierarchical low-rank structure;
   - An algorithm that is specialized to banded matrices.

2. Convergence analysis: Links to best polynomial/rational approximation of \( f \) on a suitable region containing eigenvalues of \( A \).

3. Numerical tests: Generally faster than existing methods (for large \( n \)), with comparable accuracy.