Matrix decay phenomenon and its applications I

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Seminar on Numerical Analysis
January 23–27, 2023

Outline

January 25, 9:00. Decay phenomenon and sparse matrices

- Introduction;
- Decay characterization and applications;
- Upper bounds for banded matrices;
- Extension to sparse matrices;
- Application to network analysis.

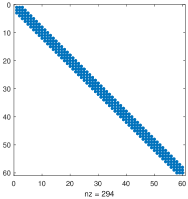
January 26, 9:00. Decay phenomenon and numerical applications

- Decay phenomenon and Krylov subspace methods;
- Applications to the (inexact) Arnoldi algorithm;
- Decay phenomenon and rational Krylov subspace methods;
- Decay phenomenon and linear ODEs.

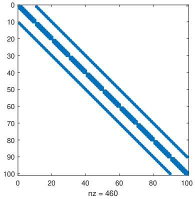
Introduction

Sparse matrices

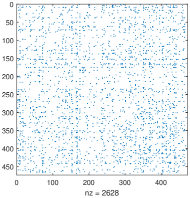
- Sparse matrix: small number of nonzero elements (the number of nonzero elements is $\mathcal{O}(n)$?);
- "A matrix is sparse if there is an advantage in exploiting its zeros" [Duff, Erisman, Reid, '86].



Banded matrix



Kronecker sum

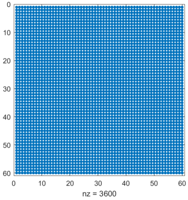


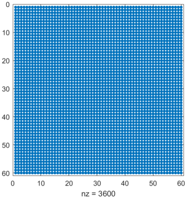
Graph (Erdos971)

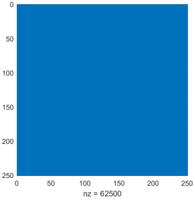
Localization and matrices

Sparsity does not take into account the elements' magnitude.

- There are dense matrices where only a small portion of its elements are non-negligible in magnitude;
- The elements with large magnitude are localized in a region of the matrix (e.g., diagonals);
- The magnitude usually tends to decay to zero as we move away from those regions;
- They are said to be localized, or that they exhibit decay.







Refer to: [Benzi, Localization in matrix computation, '16]

Localization and matrices

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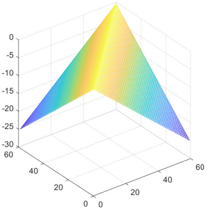
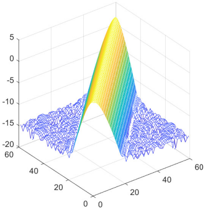
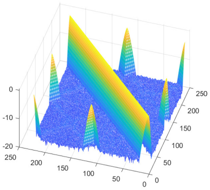






Refer to: [Benzi, Localization in matrix computation, '16]

Matrix functions

- Matrix exponential:

$$\exp(A) = \sum_{j=0}^{\infty} \frac{A^j}{j!} \, ;$$

- Matrix resolvent:

$$\begin{aligned} r_\alpha(A) &= (I - \alpha A)^{-1}, && (1/\alpha \notin \sigma(A)), \\ &\stackrel{?}{=} \sum_{j=0}^{\infty} \alpha^j A^j, && (1/\alpha < \rho(A)); \end{aligned}$$

- Other functions: inverse A^{-1}, square root $A^{1/2}$, ...

Refer to: [Higham, Functions of Matrices, '08].

Matrix function definition

Matrix function

Let $A \in \mathbb{C}^{n\times n}$ and f be an analytic function on some open $\Omega \subset \mathbb{C}$. Then

$$f(A) = \int_\Gamma f(z)\,(zI - A)^{-1}\,\mathrm{d}z,$$

with $\Gamma \subset \Omega$ a system of Jordan curves encircling each eigenvalue of A exactly once, with mathematical positive orientation.

When f is analytic other equivalent definitions exist[1]. Moreover,

$$f(z) = \sum_{j=0}^{\infty} \alpha_j z^j, \quad f(A) = \sum_{j=0}^{\infty} \alpha_j A^j,$$

if both the series converge ($|z| < 1$, $\rho(A) < 1$).

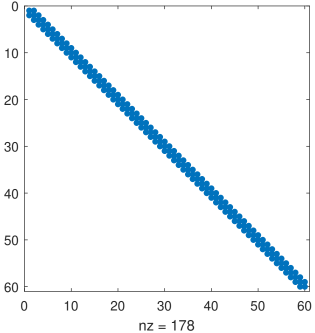
[1] [Higham, Functions of Matrices, '08]

Decay characterization and applications

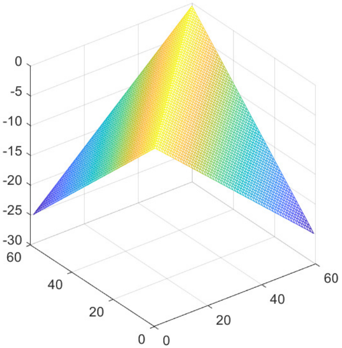
Banded matrices and decay - Example

$$A = \begin{bmatrix} 3 & 1 & 0 & \cdots & 0 \\ 1 & 3 & 1 & & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & 3 \end{bmatrix}$$

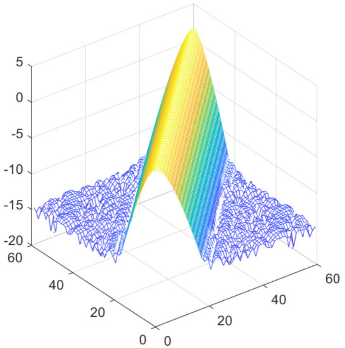
60×60 tridiagonal SPD matrix



Sparsity pattern of A



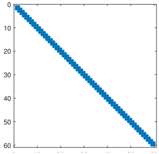
Magnitude of A^{-1} elements (log scale)

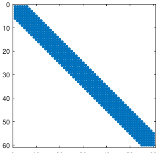


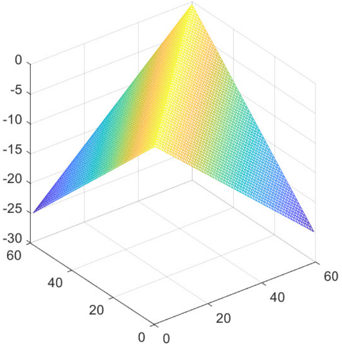
Magnitude of $\exp(A)$ elements (log scale)

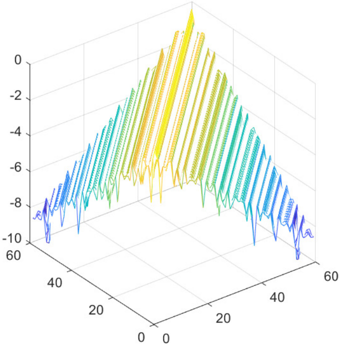
Function properties influence the decay behavior (pole vs entire)

Banded matrices and decay - Band length

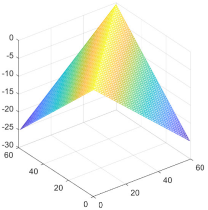
A^{-1}, $A =$ 

B^{-1}, $B =$ 

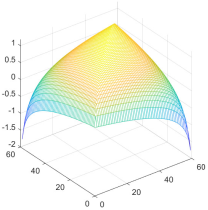




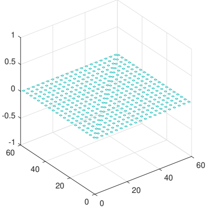
$[1.0027, 4.9973]$ $[0.0027, 3.9973]$ $[-0.9973, 2.9973]$



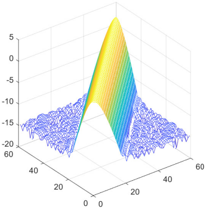
A^{-1}



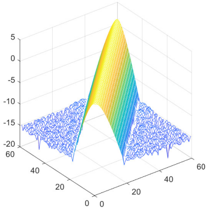
$(A - I)^{-1}$



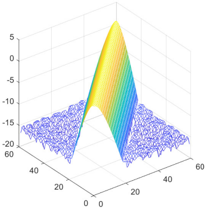
$(A - 2I)^{-1}$



$\exp(A)$



$\exp(A - I)$



$\exp(A - 2I)$

An application: matrix exponential approximations

- A_n is a sequence of banded matrices of increasing size n;
- $f(A_n)$ displays an off-diagonal decay whose rate is independent of n.

We want to compute $\exp(A_n)$ by polynomial approximation:

$$\exp(A_n) \approx p_k(A_n).$$

For instance, p_k can be given in terms of Chebyshev polynomials $T_k(z)$. As the T_k are orthogonal polynomials, we get the recurrences

$$T_{k+1}(A_n) = 2A_n T_k(A_n) - T_{k-1}(A_n), \quad k = 1, 2, \dots .$$

An application: matrix exponential approximations

The most expensive operation in the recurrences:

$$T_{k+1} = 2A_n T_k(A_n) - T_{k-1}(A_n), \quad k = 1, 2, \dots .$$

- A_n is banded;
- $T_k(A_n)$ shows a decay. It can be approximated by a banded matrix $B_{n,k} \approx T_k(A_n)$;
- The bandwidth of $B_{n,k}$ is independent from n.

Therefore

$$A_n T_k(A_n) \approx A_n B_{n,k},$$

Note that the cost of performing $A_n B_{n,k}$ is $\mathcal{O}(n)$ as n increases.

For certain sequences of matrices A_n, it is possible to derive $\mathcal{O}(n)$ methods for matrix function approximation [Benzi, Razouk, '07].

Other applications

- Linear systems: $Ax = b$, with A, b localized. Compute only the parts of x where the information is localized, e.g., by Gaussian elimination ([Duff, Erisman, Reid, '86]), Monte Carlo ([Benzi, Evans, Hamilton, Pasini, Slattery, '17]), quadrature ([Golub, Meurant, '10], [Bonchi, Esfandiar, Gleich, Greif, Lakshmanan, '12]), ...
- Preconditioner construction: e.g., based on banded approximation of inverse ([Concus, Golub, Meurant, '85]), decay in the inverse triangular factors ([Benzi, Tuma, '00]), ...
- Eigenvalue problems: since spectral projectors can be expressed as matrix functions ([Razouk, '08], [Benzi, Rinelli, '22])
- Error bound for Krylov subspace approximations: Using the structure of the Arnoldi upper-Hessenberg matrix ([Ye, '13], [Wang, Ye, '16], [P., Simoncini, '19]), ...
- ...

References (incomplete list...)

Early works on the decay property: [Demko, '77], [Demko, Moss, Smith, '84], [Eijkhout, Polman, '88], [Freund, '89], [Meurant, '92], [Benzi, Golub, '99]

Surveys and theses: [Razouk, '08], [Benzi, '16], [Schimmel, '19], [Benzi, '20]

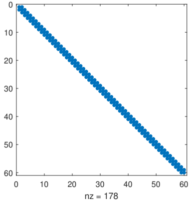
Matrix functions: [Iserles, '00], [Del Buono, Lopez, Peluso, '05], [Benzi, Razouk, '07], [Benzi, Boito, Razouk, '13], [Benzi, Boito, '14], [Schweitzer, '21], [Benzi, Rinelli, '22], [Boito, Eidelman, Gemignani, '22]

Applications to numerical methods: [Simoncini, Szyld, '03], [Simoncini '05], [Ye, '13], [Wang, '15], [Dinh, Sidje, '17], [Wang, Ye, '17], [Kürschner, Freitag, '20], [P., Simoncini, '19], [Frommer, Schimmel, Schweitzer, '21]

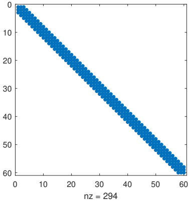
Sparse and structured matrices: [Mastronardi, Ng, Tyrtyshnikov, '10], [Canuto, Simoncini, Verani, '14], [Benzi, Simoncini, '15], [Frommer, Schimmel, Schweitzer, '18], [P., Tudisco, '18]

Upper bounds for banded matrices

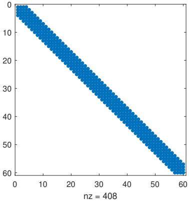
Bandwidth 1 and Polynomials



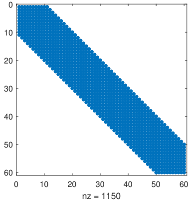
A



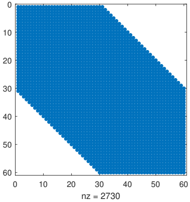
A^2



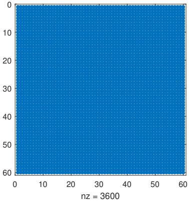
A^3



A^{10}

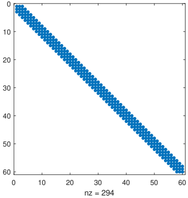


A^{30}

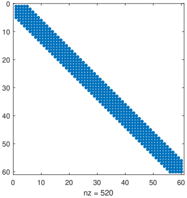


A^{59}

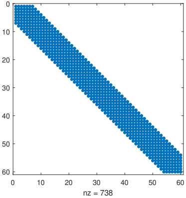
Bandwidth 2 and Polynomials



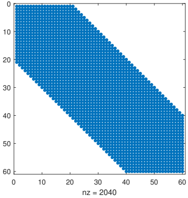
C



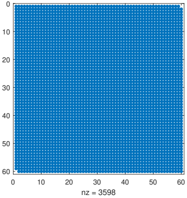
C^2



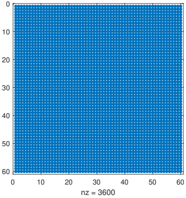
C^3



C^{10}



C^{29}



C^{30}

Banded matrices

Notation

$\mathcal{B}_n(\beta, \gamma)$ is the set of banded matrices $A \in \mathbb{C}^{n \times n}$ with upper bandwidth $\beta \geq 0$ and lower bandwidth $\gamma \geq 0$, i.e.,

$$(A)_{k,\ell} = 0, \qquad \text{for } \ell - k > \beta \text{ or } k - \ell > \gamma.$$

If $A \in \mathcal{B}_n(\beta, \gamma)$ with $\beta, \gamma \neq 0$, for

$$\xi := \begin{cases} \lceil (\ell - k)/\beta \rceil, & \text{if } k < \ell \\ \lceil (k - \ell)/\gamma \rceil, & \text{if } k \geq \ell \end{cases},$$

then

$$(A^m)_{k,\ell} = 0, \qquad \text{for every } m < \xi.$$

Banded matrices and decay - Polynomial expansion

If it is possible to expand the matrix function into a series of polynomials

$$f(A) = \sum_{j=0}^{\infty} \alpha_j p_j(A),$$

then,

$$f(A)_{k,\ell} = \sum_{j=\boxed{\xi}}^{\infty} \alpha_j p_j(A)_{k,\ell}.$$

Assuming $|\alpha_j| \longrightarrow 0$ quick enough, and $|p_j(A)_{k,\ell}|$ bounded, then $|f(A)_{k,\ell}|$ decays to zero as $|k-\ell|$ increases.

Banded matrices and decay - a-priori bounds

Using the previous observations, one can derive upper bounds in the form

$$|(f(A))_{k,\ell}| \leq c\rho^{|k-\ell|},$$

where $\rho \in (0,1), c > 0$ depend on properties of A, f. In the non-symmetric case, the Field of Values

$$W(A) = \{\boldsymbol{v}^* A \boldsymbol{v} \mid \boldsymbol{v} \in \mathbb{C}^n, ||\boldsymbol{v}|| = 1\},$$

can provide the necessary spectral information.

We now show an a-priori bound for a function of a (non-Hermitian) matrix based on this approach; see [P. Simoncini, '19] (no use of the Crouzeix's conjecture), c.f. [Benzi, Boito, '14], [Benzi, '20].

The a-priori bound

Joint work with V. Simoncini (University of Bologna)

The bound takes the general form:

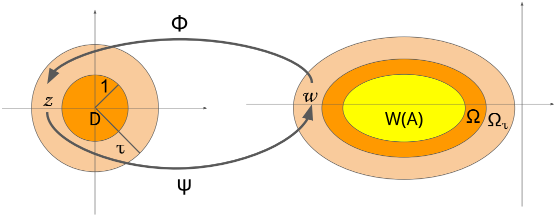
$$|(f(A))_{k,\ell}| \leq p(\xi) \left(\frac{1}{\tau(\xi)} \right)^{\xi},$$

where $p(\xi) \to p > 0$, and $\tau(\xi) > 1$ depends on f and $W(A)$.

Faber polynomials - Definition

Let Ω be a continuum with connected complement, ϕ is the relative conformal map satisfying the following conditions

$$\phi(\infty) = \infty, \qquad \lim_{z \to \infty} \frac{\phi(z)}{z} = d > 0.$$



Faber polynomials - Definition

Consider the Laurent expansion of ϕ:

$$\phi(z) = dz + a_0 + \frac{a_1}{z} + \frac{a_2}{z^2} + \dots.$$

Then, the nth power of ϕ can be expanded as

$$(\phi(z))^n = dz^n + a_{n-1}^{(n)} z^{n-1} + \dots + a_0^{(n)} + \frac{a_{-1}^{(n)}}{z} + \frac{a_{-2}^{(n)}}{z^2} + \dots.$$

The Faber polynomial of degree n for the domain Ω is defined as

$$\Phi_n(z) = dz^n + a_{n-1}^{(n)} z^{n-1} + \dots + a_0^{(n)}, \qquad \text{for } n \geq 0.$$

When $\Omega = [-1, 1]$, they are the Chebyshev polynomials.

See [Suetin, '98].

Properties of Faber polynomials

- If f is analytic on Ω then

$$f(z) = \sum_{j=0}^{\infty} f_j \Phi_j(z), \qquad \text{for } z \in \Omega;$$

- If the spectrum of A, $\sigma(A)$, is contained in Ω, then

$$f(A) = \sum_{j=0}^{\infty} f_j \Phi_j(A);$$

- If Ω is convex and contains $W(A)$, then ([Beckermann, '05])

$$||\Phi_j(A)|| \leq 2.$$

Bound derivation - Idea

Assume $A \in \mathcal{B}(\beta, \gamma)$, Φ_j define on the domain $\Omega \supset W(A)$, then

$$f(A)_{k,\ell} = \sum_{j=0}^{\infty} f_j \Phi_j(A)_{k,\ell} = \sum_{j=\xi}^{\infty} f_j \Phi_j(A)_{k,\ell}$$

with $\xi = \lceil (\ell - k)/\beta \rceil$ for $k < \ell$, $\xi = \lceil (k - \ell)/\gamma \rceil$ for $k > \ell$. Thus

$$|f(A)_{k,\ell}| \leq \sum_{j=\xi}^{\infty} |f_j| \, |\Phi_j(A)_{k,\ell}| \leq \sum_{j=\xi}^{\infty} |f_j| \, \|\Phi_j(A)\|$$
$$\leq 2 \sum_{j=\xi}^{\infty} |f_j|.$$

Approximating $|f_j|$, we obtain the bound (it depends on f, Ω, ξ).

The bound

Theorem

Let $A \in \mathcal{B}_n(\beta, \gamma)$ with $W(A) \subset \Omega$. Moreover, let ϕ be the conformal map of Ω, ψ be its inverse and G_τ the set with border $\Gamma_\tau = \{w \; : \; |\phi(w)| = \tau\}$. Assume that, for $\tau > 1$, f is analytic on G_τ and bounded on Γ_τ. Then

$$\left|(f(A))_{k,\ell}\right| \leq 2\frac{\tau}{\tau - 1} \max_{z \in \Gamma_\tau} |f(z)| \left(\frac{1}{\tau}\right)^{\xi}.$$

For the given f, Ω and ξ, τ must be chosen so to minimize

$$\max_{z \in \Gamma_\tau} |f(z)| \left(\frac{1}{\tau}\right)^{\xi}$$

Exponential function

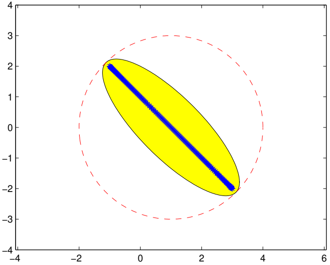
Corollary

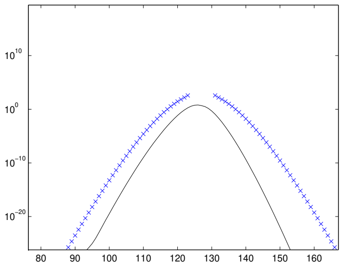
Let $A \in \mathcal{B}_n(\beta, \gamma)$ with $W(A) \subset \Omega$, with Ω's boundary a horizontal ellipse with semi-axes $a \geq b > 0$ and center $c = c_1 + ic_2 \in \mathbb{C}$, $c_1, c_2 \in \mathbb{R}$. Then for $\xi > b$

$$\left| \left(e^A \right)_{k,\ell} \right| \lesssim 2e^{c_1} \left(e \frac{a+b}{2\xi} \right)^{\xi}, \quad \xi > b.$$

A similar bound is derived in a different way in [Wang, Ye, '16].

Example - 127-th column of $\exp(A)$

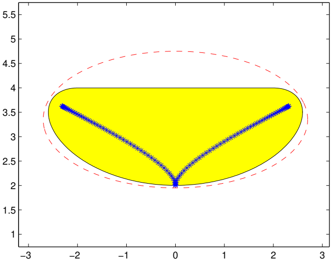


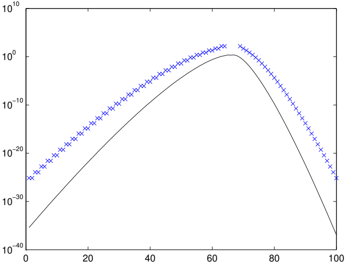


$$A = \mathrm{Toeplitz}(-i, \underline{i}, -2) \in \mathbb{C}^{n \times n},\ n = 200$$

Condition number of the eigenvector matrix: $4.0e + 29$

Example - 67-th column of exp(A)





$A = \mathrm{Toeplitz}(i, \underline{3i}, -i, -i) \in \mathbb{C}^{n \times n},\ n = 100$

Condition number of the eigenvector matrix $5.5e+13$

Since $z^{-\frac{1}{2}}$ is defined in $\mathbb{C}^+$, Γ_τ must be in $\mathbb{C}^+$.

Corollary

Let $A \in \mathcal{B}_n(\beta, \gamma)$ with $W(A) \subset \Omega \subset \mathbb{C}^+$. Ω's boundary is a horizontal ellipse with semi-axes $a \geq b > 0$ and center $c \in \mathbb{C}$. Then, for any $\varepsilon \in \mathbb{R}$ with $0 < \varepsilon \leq |c| - \sqrt{a(a+b)}$

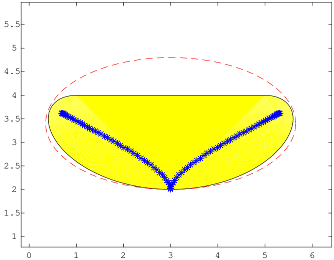
$$\left| \left(A^{-\frac{1}{2}} \right)_{k,\ell} \right| \lesssim \frac{2}{\sqrt{\varepsilon}} p_2(\varepsilon) \left(\frac{a+b}{|c| - \varepsilon} q_2(\varepsilon) \right)^{\xi}$$

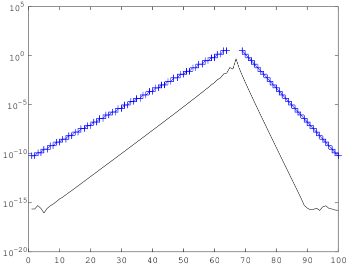
with

$$p_2(\varepsilon) = \frac{\left| c(1-\varepsilon/|c|) + \sqrt{c^2(1-\varepsilon/|c|)^2 - (a^2-b^2)^2} \right|}{\left| c(1-\varepsilon/|c|) + \sqrt{c^2(1-\varepsilon/|c|)^2 - (a^2-b^2)^2} \right| - (a+b)}.$$

$$q_2(\varepsilon) = \frac{1}{|1 + \sqrt{1 - (a^2-b^2)/(c(1-\varepsilon/|c|))^2}|}$$

Example - 67-th column of $A^{-\frac{1}{2}}$

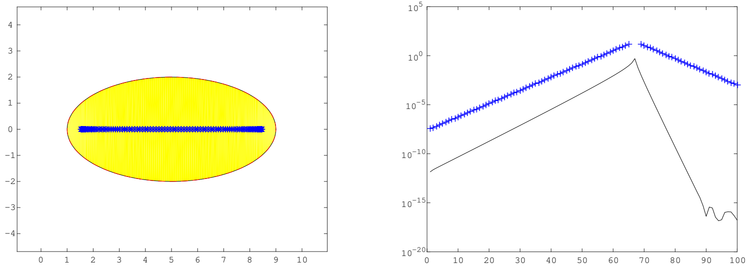




$A = \mathrm{Toeplitz}(i, \underline{7+3i}, -i, -i) \in \mathcal{B}_{100}(1,2)$, $\varepsilon = 0.05$

Condition number of the eigenvector matrix: $5.5e + 13$

Example - 67-th column of $A^{-\frac{1}{2}}$



$A = \mathrm{Toeplitz}(i, \underline{3 + 3i}, -i, -i) \in \mathcal{B}_{100}(1, 2)$, $\varepsilon = 0.05$

Condition number of the eigenvector matrix: $1.2e + 24$

Summarizing

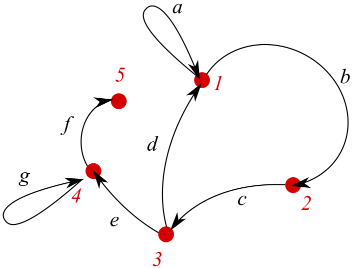
- We presented a family of bounds for the decay of functions of banded matrices;
- The bounds depend on the shape of the matrix field of values and on the domain of analyticity of the function;
- The better we approximate the field of values, the better the bound.

More details: P., Simoncini, *Inexact Arnoldi residual estimates and decay properties for functions of non-Hermitian matrices*, BIT (2019).

Extension to sparse matrices

Sparse matrices and decay: A graph interpretation

Any graph $G = (V, E)$ is represented by its adjacency matrix A.
Vice versa, any matrix A represents a (weighted) graph.



$$A = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 1 & 1 & & & \\ & & 1 & & \\ 1 & & & 1 & \\ & & & 1 & 1 \\ & & & & \end{bmatrix} \end{array}$$

$V = \{1, 2, \ldots, 5\}, \; E = \{a, b, \ldots, g\}$

$$(A^m)_{k,\ell} = 0, \text{ if } \operatorname{dist}(k, \ell) > m$$

$\operatorname{dist}(k, \ell)$ is the geodesic distance from k to ℓ.

Graphs and Polynomials

A

	1	2	3	4	5
1	*	*			
2			*		
3	*			*	
4				*	*
5					

A^2

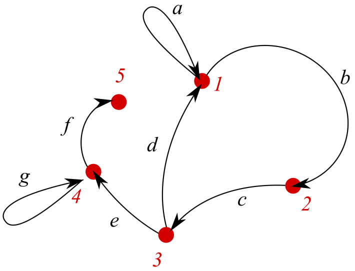
*	*	*		
*			*	
*	*		*	*
			*	*

A^3

*	*	*	*	
*	*		*	*
*	*	*	*	*
			*	*

A^4

	1	2	3	4	5
1	*	*	*	*	*
2	*	*	*	*	*
3	*	*	*	*	*
4				*	*
5					



A-priori bound for sparse matrices

For banded matrices we, generally, have bounds of the form:

$$|(f(A))_{k,\ell}| \lesssim c \left(\frac{1}{\tau}\right)^{\xi}.$$

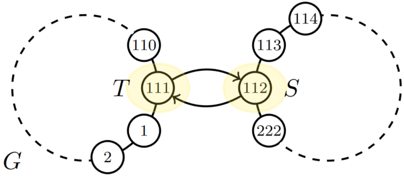
Using $(A^m)_{k,\ell} = 0$, if $\text{dist}(k,\ell) > m$, they can be extended to the sparse case as follows:

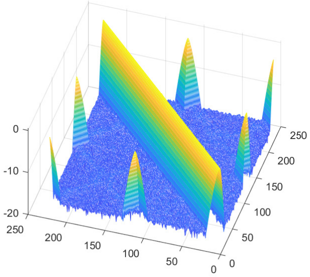
$$|(f(A))_{k,\ell}| \lesssim c \left(\frac{1}{\tau}\right)^{\text{dist}(k,\ell)}.$$

[Benzi, Razouk, '07]

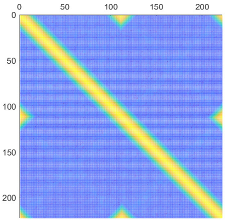
Decay phenomenon and graphs: An example

$$
\begin{array}{r}
1\\ 2\\ \vdots\\ 111\\ 112\\ \vdots\\ 221\\ 222
\end{array}
\begin{bmatrix}
 & 1 & & 1 & & & & \\
1 & & \ddots & & & & & \\
 & \ddots & & 1 & & & & \\
1 & & 1 & & 1 & & & \\
 & & & 1 & & 1 & & 1 \\
 & & & & 1 & & \ddots & \\
 & & & & & \ddots & & 1 \\
 & & & & 1 & & 1 &
\end{bmatrix}
$$





$= \exp(A) =$

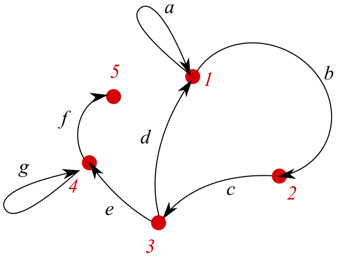


Application to network analysis

Counting walks in graphs

A walk from k to ℓ is a path from the node k to the node ℓ that admits repeated edges (it is said to be closed when $k = \ell$).

$$(A^n)_{k,\ell} = \text{number of walks of length } n \text{ from } k \text{ to } \ell.$$



$1 \longrightarrow 4$:

- length 3: b, c, e
- length 4: a, b, c, e
- length 6: b, c, d, b, c, e
- length 7: b, c, d, b, c, e, g
- ...

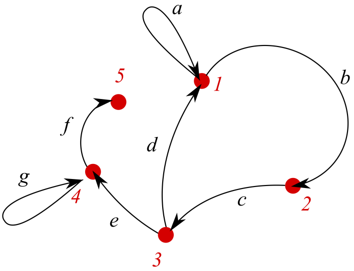
Matrix powers and walks

$$\begin{array}{c} 1\\2\\3\\4\\5 \end{array} \begin{bmatrix} 1 & 1 & & & \\ & & 1 & & \\ 1 & & & 1 & \\ & & & 1 & 1 \\ & & & & \end{bmatrix} \quad \begin{bmatrix} 1 & 1 & 1 & & \\ 1 & & & 1 & \\ 1 & 1 & & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix} \quad \begin{bmatrix} 2 & 1 & 1 & 1 & \\ 1 & 1 & & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}$$

$A \qquad A^2 \qquad A^3$

$$\begin{array}{c} 1\\2\\3\\4\\5 \end{array} \begin{bmatrix} 3 & 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 2 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}$$

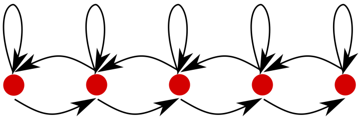
A^4



Tridiagonal matrix

$$\underbrace{\begin{bmatrix} 1 & 1 & & & \\ 1 & 1 & 1 & & \\ & 1 & 1 & 1 & \\ & & 1 & 1 & 1 \\ & & & 1 & 1 \end{bmatrix}}_{A} \quad \underbrace{\begin{bmatrix} 2 & 2 & 1 & & \\ 2 & 3 & 2 & 1 & \\ 1 & 2 & 3 & 2 & 1 \\ & 1 & 2 & 3 & 2 \\ & & 1 & 2 & 2 \end{bmatrix}}_{A^2} \quad \underbrace{\begin{bmatrix} 4 & 5 & 3 & 1 & \\ 5 & 7 & 6 & 3 & 1 \\ 3 & 6 & 7 & 6 & 3 \\ 1 & 3 & 6 & 7 & 5 \\ & 1 & 3 & 5 & 4 \end{bmatrix}}_{A^3}$$

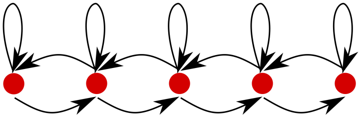
$$\underbrace{\begin{bmatrix} 9 & 12 & 9 & 4 & ? \\ 12 & 18 & 16 & 10 & 4 \\ 9 & 16 & 19 & 16 & 9 \\ 4 & 10 & 16 & 18 & 12 \\ ? & 4 & 9 & 12 & 9 \end{bmatrix}}_{A^4}$$



Tridiagonal matrix

$$\underbrace{\begin{bmatrix} 1 & 1 & & & \\ 1 & 1 & 1 & & \\ & 1 & 1 & 1 & \\ & & 1 & 1 & 1 \\ & & & 1 & 1 \end{bmatrix}}_{A} \qquad \underbrace{\begin{bmatrix} 2 & 2 & 1 & & \\ 2 & 3 & 2 & 1 & \\ 1 & 2 & 3 & 2 & 1 \\ & 1 & 2 & 3 & 2 \\ & & 1 & 2 & 2 \end{bmatrix}}_{A^2} \qquad \underbrace{\begin{bmatrix} 4 & 5 & 3 & 1 & \\ 5 & 7 & 6 & 3 & 1 \\ 3 & 6 & 7 & 6 & 3 \\ 1 & 3 & 6 & 7 & 5 \\ & 1 & 3 & 5 & 4 \end{bmatrix}}_{A^3}$$

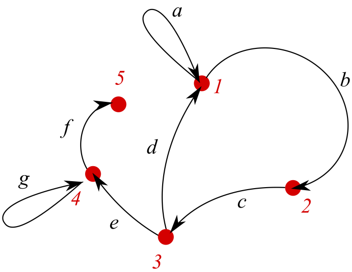
$$\underbrace{\begin{bmatrix} 9 & 12 & 9 & 4 & {\color{red}1} \\ 12 & 18 & 16 & 10 & 4 \\ 9 & 16 & 19 & 16 & 9 \\ 4 & 10 & 16 & 18 & 12 \\ {\color{red}1} & 4 & 9 & 12 & 9 \end{bmatrix}}_{A^4}$$



Subgraph centrality: counting closed walks

$$\underbrace{\begin{bmatrix} \boxed{1} & 1 & & & \\ & & 1 & & \\ 1 & & & 1 & \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}_{A} \quad \underbrace{\begin{bmatrix} \boxed{1} & 1 & 1 & & \\ 1 & & & 1 & \\ 1 & 1 & & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}_{A^2} \quad \underbrace{\begin{bmatrix} \boxed{2} & 1 & 1 & 1 & \\ 1 & 1 & & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}_{A^3}$$

$$\underbrace{\begin{bmatrix} \boxed{3} & 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 2 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}_{A^4}$$



Subgraph centrality: counting closed walks

$$\underset{A}{\begin{bmatrix} \boxed{1} & 1 & & & \\ & & 1 & & \\ 1 & & & 1 & \\ & & & 1 & 1 \\ & & & & \end{bmatrix}} + \underset{A^2}{\begin{bmatrix} \boxed{1} & 1 & 1 & & \\ 1 & & & 1 & \\ 1 & 1 & & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}} + \underset{A^3}{\begin{bmatrix} \boxed{2} & 1 & 1 & 1 & \\ 1 & 1 & & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}$$

$$+ \underset{A^4}{\begin{bmatrix} \boxed{3} & 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 2 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}$$

$$SC(1) = 1 + 1 + 2 + 3 + \dots$$

Divergent!

Subgraph centrality: counting closed walks

$$
\alpha_1 \underbrace{\begin{bmatrix} \boxed{1} & 1 & & & \\ & & 1 & & \\ 1 & & & 1 & \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}_{A} + \alpha_2 \underbrace{\begin{bmatrix} \boxed{1} & 1 & 1 & & \\ 1 & & & 1 & \\ 1 & 1 & & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}_{A^2} + \alpha_3 \underbrace{\begin{bmatrix} \boxed{2} & 1 & 1 & 1 & \\ 1 & 1 & & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ & & & 1 & 1 \\ & & & & \end{bmatrix}}_{A^3} + \dots
$$

$$
\begin{aligned}
SC(1) &= \alpha_0 + \alpha_1 + \alpha_2 + 2\alpha_3 + 3\alpha_4 + \dots \\
&= \alpha_0 + \alpha_1 A_{1,1} + \alpha_2 (A^2)_{1,1} + \alpha_3 (A^3)_{1,1} + \alpha_4 (A^4)_{1,1} + \dots \\
&= \left(\sum_{j=0}^{\infty} \alpha_j A^j \right)_{1,1} = f(A)_{1,1}
\end{aligned}
$$

It is a matrix function when the series converges.

[Estrada, Rodriguez-Velazquez, '05]

Exponential and resolvent indexes

Usually, the following functions are considered:

$$\exp(A) = \sum_{n=0}^{\infty} \frac{1}{n!} A^n, \qquad r_\alpha(A) = \sum_{n=0}^{\infty} \alpha^n A^n = (I - \alpha A)^{-1}.$$

Subgraph centrality references (incomplete list)

[Arrigo, Higham, Noferini, Wood, '22]
[Arrigo, Durastante, '21]
[Benzi, Boito, '20]
[Arrigo, Higham, '17]
[Aprahamian, Higham, Higham, '16]
[Benzi, Klymko, '13]
[Benzi, Estrada, Klymko, '13]
[Estrada, Hatano, Benzi, '12]
[Estrada, '12]
[Estrada, Higham, '10]
[Estrada, Hatano, '08]
[Newman, Barabasi, Watts, '06]
[Estrada, Rodríguez-Velázquez, '05]
...

Application: Stability under sparse perturbation

Joint work with F. Tudisco (GSSI Gran Sasso Science Institute).

Consider $G = (V, E)$ with adjacency matrix A. Let us add, remove or simply modify the edges in the set δE, obtaining

$$\widetilde{G} = (V, \widetilde{E}),$$

with $\widetilde{E} \subset E \cup \delta E$ and with adjacency matrix $\widetilde{A} = A + \delta A$.
We have derived bounds for

$$|f(A)_{k,\ell} - f(A + \delta A)_{k,\ell}|$$

which enlighten the dependency on the distance that separates either k or ℓ from the nodes touched by the edges in δE.

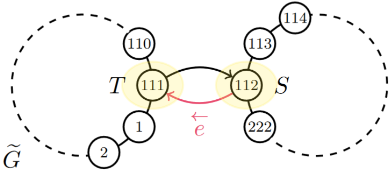
Motivations

- Computing the entries of $f(A)$ is a costly operation.
- Often only the first most important nodes are needed.
- Typically modifying a few marginal edges does not change the ranking of the most important ones.
- The distance of important nodes from those with marginal role is usually large.

If δA is low-rank, efficient techniques for updating $f(A)$ can be found in [Beckermann, Kressner, Schweitzer (2018)].

Example: The bridge

$$
\begin{array}{c}
1 \\ 2 \\ \vdots \\ 111 \\ 112 \\ \vdots \\ 221 \\ 222
\end{array}
\begin{bmatrix}
 & 1 & & 1 & & & & \\
1 & & \ddots & & & & & \\
 & \ddots & & 1 & & & & \\
1 & & 1 & & 1 & & & \\
 & & & \boxed{1} & & 1 & & 1 \\
 & & & & 1 & & \ddots & \\
 & & & & & \ddots & & 1 \\
 & & & & 1 & & 1 &
\end{bmatrix}
$$



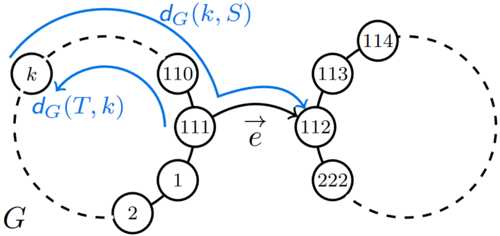
- Adding e, the number of walks in the graph significantly increases;
- The far a node k is from the bridge, the longer the walks passing through e;
- Therefore, we expect $SC(k)$ to significantly varies only for nodes close to the bridge.

Lemma

Let $S = \{s | (s,t) \in \delta E\}$ and $T = \{t | (s,t) \in \delta E\}$ be respectively the sets of sources and tips of δE, then

$$(\widetilde{A}^n)_{k\ell} = (A^n)_{k\ell}, \quad \text{for } k \notin S \text{ and } \ell \notin T,$$

for every $n \leq d_G(k,S) + d_G(T,\ell) =: \delta$.



Remark: $d_G(k,S), d_G(T,\ell)$ are distances in the original network G.

Polynomial approximation

If both the matrix and the perturbed matrix functions can be expanded in the same series of Faber polynomials:

$$f(A) = \sum_{j=0}^{\infty} f_j \Phi_j(A), \quad f(\widetilde{A}) = \sum_{j=0}^{\infty} f_j \Phi_j(\widetilde{A}),$$

then we get

$$f(\widetilde{A})_{k,\ell} - f(A)_{k,\ell} = \sum_{j=\boxed{\delta+1}}^{\infty} f_j(\Phi(\widetilde{A})_{k,\ell} - \Phi_j(A)_{k,\ell}).$$

Using the same approach seen for the decay property of banded matrices, we derived the following bound.

The bound

Theorem

Let $W(A)$ and $W(\tilde{A})$ contained in a convex continuum E with connected complement whose boundary is Γ. Moreover, let ϕ be the conformal mapping of E, ψ be its inverse and G_τ the set with border $\Gamma_\tau = \{w \;:\; |\phi(w)| < \tau\}$. Let us assume that $\tau > 1$, f is analytic in G_τ and f is bounded on Γ_τ. Then

$$\left| \left(f(A) - f(\tilde{A}) \right)_{k\ell} \right| \leq \mu_\tau(f) \frac{2}{\pi} \frac{\tau}{\tau - 1} \left(\frac{1}{\tau} \right)^{\delta+2},$$

with $\delta = d_G(k, S) + d_G(T, \ell)$ and

$$\mu_\tau(f) = \int_{\Gamma_\tau} |f(\psi(z))| \, \mathrm{d}z \, .$$

Corollaries

Let $\delta = d_G(k,S) + d_G(T,\ell)$. If the boundary of Ω is a horizontal ellipse with semi-axes $a \geq b > 0$ and center c, then for $\delta > b-1$

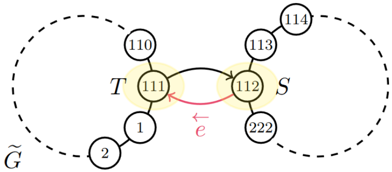
$$\left|\left(\exp(A) - \exp(\tilde{A})\right)_{k\ell}\right| \leq \frac{4e^{\Re(c)}p(\delta)}{p(\delta) - (a+b)/(\delta+1)} \left(\frac{a+b}{\delta+1}\frac{e^{q(\delta)}}{p(\delta)}\right)^{\delta+1},$$

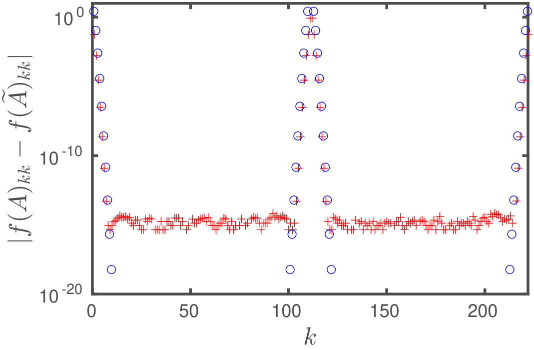
with $q(t) = 1 + \frac{a^2-b^2}{t^2+t\sqrt{t^2+a^2-b^2}}$ and $p(t) \approx 2$.
Moreover, for $0 < \epsilon < |\alpha^{-1} - c| - a$ and $\delta > 0$

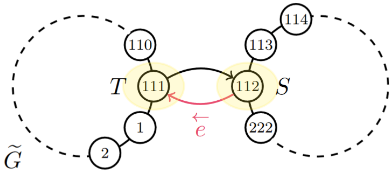
$$\left|\left(r_\alpha(A) - r_\alpha(\tilde{A})\right)_{k\ell}\right| \leq \frac{4}{1 - \frac{a+b}{(|\alpha^{-1}-c|-\varepsilon)p_\varepsilon}} \frac{1}{\varepsilon} \left(\frac{a+b}{|\alpha^{-1}-c|-\varepsilon}\frac{1}{p_\varepsilon}\right)^{\delta+1},$$

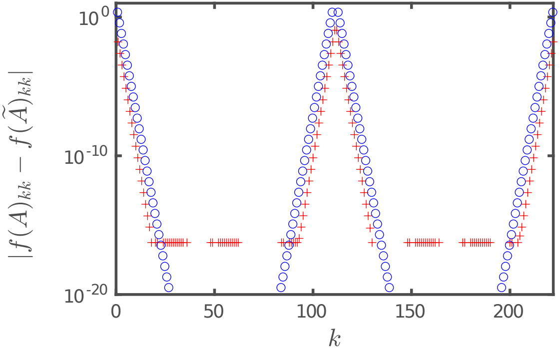
where $p_\varepsilon \leq 2$.

Two circles: exponential-centrality



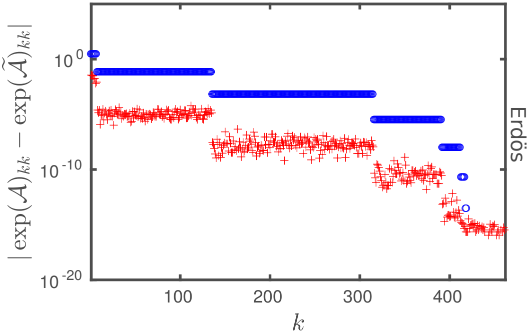



110
111
112
113
114
1
2
222
T
S
$\overleftarrow{e}$
$\widetilde{G}$

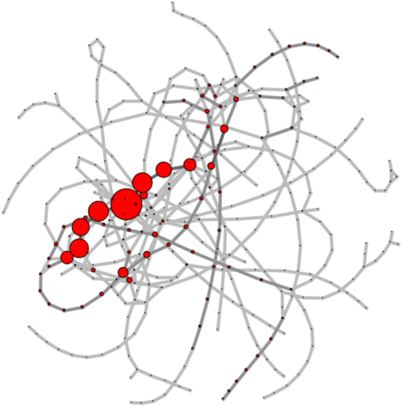

10^0
10^{-10}
10^{-20}
0
50
100
150
200
k
$|f(A)_{kk} - f(\widetilde{A})_{kk}|$

Normalized Pajek/Erdos971: exponential-centrality

We added all the missing edges between the 10 nodes with smallest centrality $\exp(A)_{kk}$

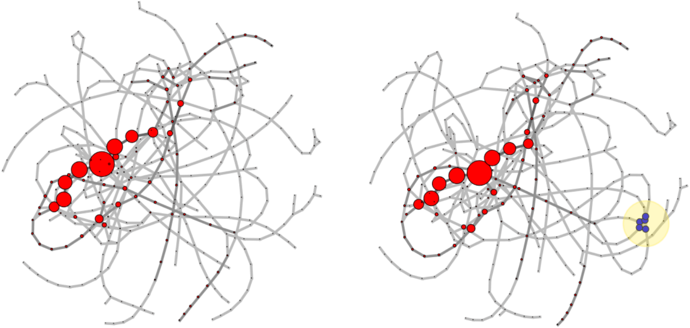


London train connections

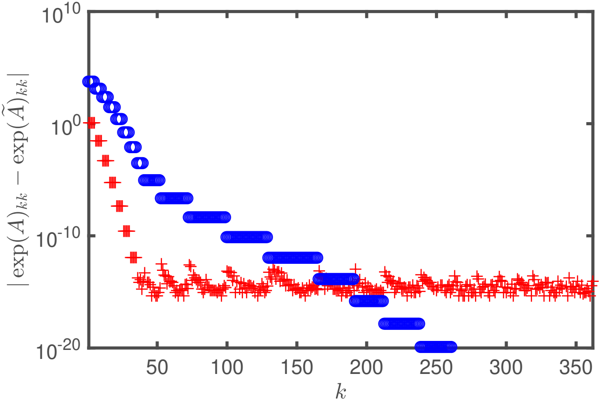


The nodes are the train stations, and the edges are the existing routes between them (overground, underground, DLR, etc.)
[De Domenico, Solé-Ribalta, Gómez, Arenas, '14].

We added all the missing edges between the 5 nodes with smallest centrality $\exp(A)_{kk}$

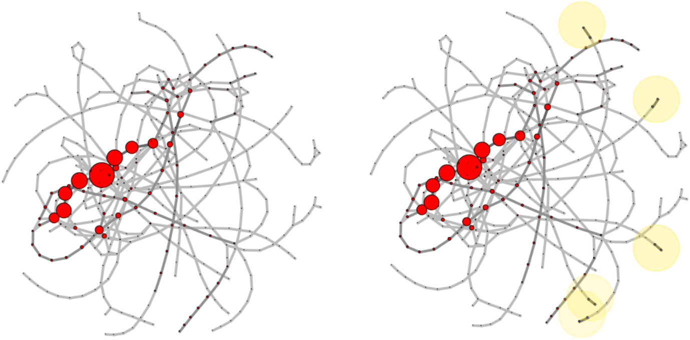


London train network 1: Exponential-centrality

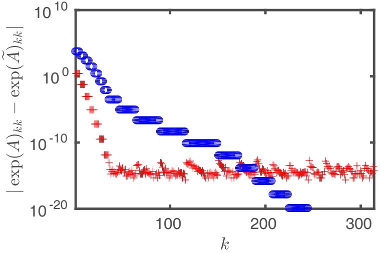


London train network 2

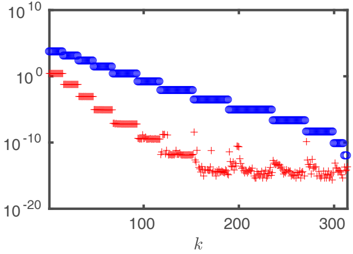
We modified the last 5 and 15 nodes changing their weights.



London train network 2: Exponential-centrality



Last 5 nodes.



Last 15 nodes.

Remarks

- The bounds show that the variation of $f(A)_{k\ell}$ decays exponentially with respect to $d_G(k, S) + d_G(T, \ell)$, the sum of the distances that separates k and ℓ from the set of nodes touched by the perturbed edges in S, T.
- The bounds depend on $W(A)$, $W(\widetilde{A})$ and we gave strategies for their estimation.
- We also proposed a strategy that allows to compute the distances between nodes simultaneously with the computation of the entries of $f(A)$ by Lanczos algorithm.

More details: P., Tudisco, *On the stability of network indices defined by means of matrix functions*, SIMAX (2018).

Conclusions

- We have introduced the decay phenomenon;
- We have discussed its characterization in terms of matrix and function properties;
- We have shown how to predict it;
- We have seen an application to network analysis.

Tomorrow: Decay phenomenon and . . .

- (Inexact) Arnoldi's method;
- Rational Krylov subspace method;
- A new approach for linear ODEs.

Conclusions

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Tomorrow: Decay phenomenon and ...

- (Inexact) Arnoldi's method;
- Rational Krylov subspace method;
- A new approach for linear ODEs.

Thank you for your attention!

Matrix decay phenomenon and its applications II

Stefano Pozza

Charles University, Prague

Seminar on Numerical Analysis
January 23–27, 2023

Outline

January 25, 9:00. Decay phenomenon and sparse matrices

- Introduction;
- Decay characterization and applications;
- Upper bounds for banded matrices;
- Extension to sparse matrices;
- Application to network analysis.

January 26, 9:00. Decay phenomenon and numerical applications

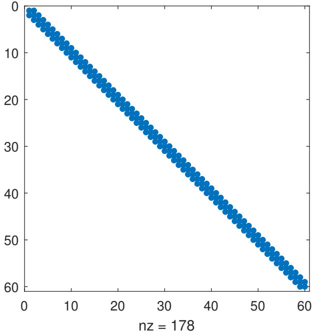
- Decay phenomenon and Krylov subspace methods;
- Applications to the (inexact) Arnoldi algorithm;
- Decay phenomenon and rational Krylov subspace methods;
- Decay phenomenon and linear ODEs.

Decay phenomenon

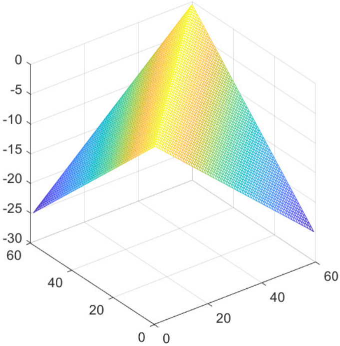
Banded matrices and decay - Example

$$A = \begin{bmatrix} 3 & 1 & 0 & \cdots & 0 \\ 1 & 3 & 1 & & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & 3 \end{bmatrix}$$

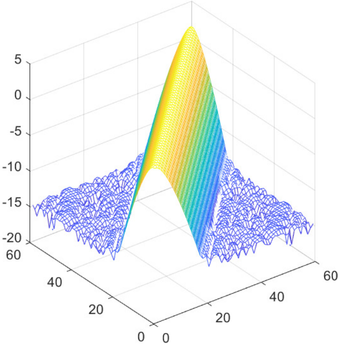
60×60 tridiagonal SPD matrix



Sparsity pattern of A



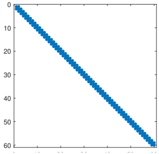
Magnitude of A^{-1} elements (log scale)

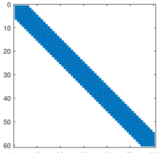


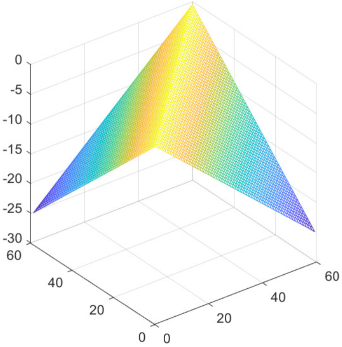
Magnitude of $\exp(A)$ elements (log scale)

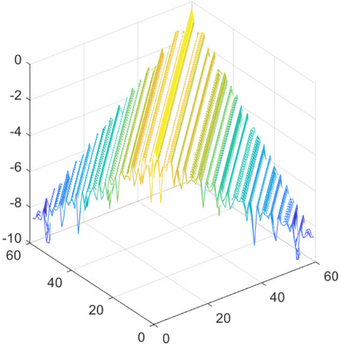
Function properties influence the decay behavior (pole vs entire)

Banded matrices and decay - Band length

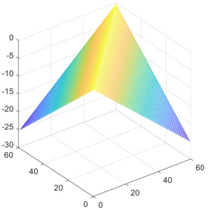
A^{-1}, $A =$ 

B^{-1}, $B =$ 

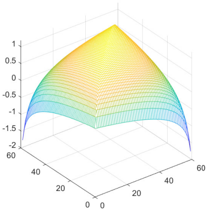




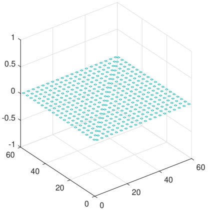
$[1.0027, 4.9973]$ | $[0.0027, 3.9973]$ | $[-0.9973, 2.9973]$



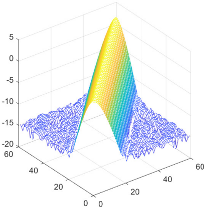
A^{-1}



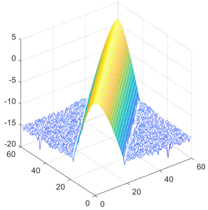
$(A - I)^{-1}$



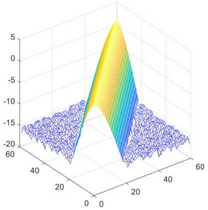
$(A - 2I)^{-1}$



$\exp(A)$



$\exp(A - I)$



$\exp(A - 2I)$

By expanding a matrix function into a series of polynomials

$$f(A) = \sum_{j=0}^{\infty} \alpha_j p_j(A),$$

we derived upper bounds in the form

$$|(f(A))_{k,\ell}| \leq c\rho^{|k-\ell|},$$

where $\rho \in (0,1), c > 0$ depend on properties of A, f (and ρ can depend on $|k-\ell|$). To compute the a-priori bound we need to approximate the Field of Values

$$W(A) = \{\boldsymbol{v}^* A \boldsymbol{v} \mid \boldsymbol{v} \in \mathbb{C}^n, ||\boldsymbol{v}|| = 1\}.$$

Decay phenomenon and Krylov subspace methods

Model reduction

A possible way to approximate $f(A)\boldsymbol{v}$ is by projecting the problem onto a small subspace, such as the Krylov subspace:

$$\mathcal{P}_m(A, \boldsymbol{v}) := \mathrm{span}\{\boldsymbol{v}, A\,\boldsymbol{v}, \dots, A^{m-1}\,\boldsymbol{v}\}\,.$$

Given a basis U_m of $\mathcal{P}_m(A, \boldsymbol{v})$, we can define the reduced matrix

$$T_m = U_m^* A U_m.$$

Then we have the model reduction:

$$f(A)\boldsymbol{v} \approx U_m f(T_m)\boldsymbol{w}, \quad \boldsymbol{w} = U_m^* \boldsymbol{v}.$$

If m is small, computing $f(T_m)\boldsymbol{w}$ is computationally cheaper.

E.g., [Higham, Functions of Matrices, '08]

Arnoldi's method

Given a matrix $A \in \mathbb{R}^{N \times N}$ and a vector $\boldsymbol{v} \neq 0$, Arnoldi's method produces the orthogonal matrix

$$U_m = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m],$$

forming a basis of $\mathcal{P}_m(A, \boldsymbol{v})$.

Starting with $\boldsymbol{u}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|$, Arnoldi's method is a Gram-Schmidt orthogonalization process defined by the recurrences

$$t_{j+1,j}\boldsymbol{u}_{j+1} = A\boldsymbol{u}_j - \sum_{i=1}^{j} t_{i,j}\boldsymbol{u}_i, \quad j = 1, \ldots, m.$$

$$t_{i,j} = \boldsymbol{u}_i^* A\boldsymbol{u}_j, \quad t_{j+1,j} = \|\boldsymbol{u}_{j+1}\|.$$

E.g., [Saad, Iterative Methods for Sparse Linear Systems, '03]

Arnoldi's method

The recurrences have the matrix form:

$$AU_m = U_m T_m + t_{m+1,m} \boldsymbol{u}_{m+1} \boldsymbol{e}_m^T,$$

with T_m the $m \times m$ upper Hessenberg matrix with entries $t_{i,j}$ ($\boldsymbol{e}_m$ the mth vector of the canonical basis). By orthogonality we get

$$T_m = U_m^* A \, U_m.$$

The matrix T_m plays two roles in the algorithm:

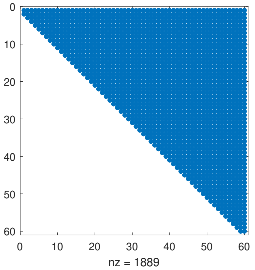
- It represents the orthogonalization process (coefficients $t_{i,j}$);
- It represents the action of A in the Krylov subspace $\mathcal{P}_m(A, \boldsymbol{v})$, i.e.,

$$U_m T_m U_m^* = U_m U_m^* A \, U_m U_m^*.$$

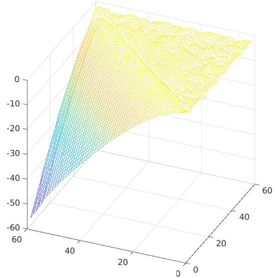
T_m can be used for matrix-function approximation

$$f(A)\boldsymbol{v} \approx U_m f(T_m)\boldsymbol{e}_1,$$

$f(\lambda) = \lambda^{-1} \to$ FOM.



Sparsity pattern of T_{60}



$\exp(T_{60})$ (log scale)

Decay bounds

It is possible to derive a-priori decay bound for $f(T_m)$.

- We know the band length;
- We know f;
- We can derive the necessary spectral information from the input matrix since $W(T_m) \subseteq W(A)$.

Applications: Decay bounds can be used, e.g., for:

- Devise new relaxed approaches (inexact Arnoldi);
- Stopping criteria for iterative solvers in matrix function evaluations and matrix equation solving.

E.g., [Güttel, Schweitzer,'21], [Kürschner, Freitag,'20], [P. , Simoncini,'19].

Matrix function approximation

Joint work with V. Simoncini (University of Bologna)

Let $\mathbf{y}(x) = f(xA)\mathbf{v}$ be the solution to the differential equation

$$\mathbf{y}^{(d)}(x) = A\,\mathbf{y}(x), \quad \mathbf{y}(0) = \mathbf{v}, \quad x \geq 0,$$

with $\mathbf{y}^{(d)}$ the dth derivative. Consider the approximation

$$\mathbf{y}(x) \approx \mathbf{y}_m(x) = U_m f(xT_m)\,\mathbf{e}_1.$$

The differential equation residual is given by:

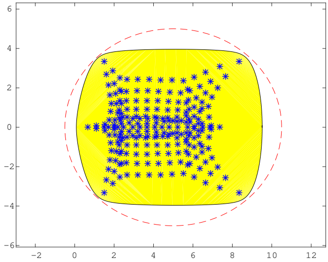
$$\mathbf{r}_m(x) = A\,\mathbf{y}_m(x) - \mathbf{y}_m^{(d)}(x) = \mathbf{u}_{m+1}\,t_{m+1,m}\,\mathbf{e}_m^T f(xT_m)\,\mathbf{e}_1.$$

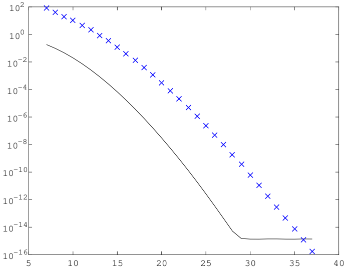
Residual bound

For simplicity, let us fix $x = 1$,

- $|\mathbf{e}_m^T f(T_m)\,\mathbf{e}_1|$ decays as m increases;
- We can bound $|\mathbf{e}_m^T f(T_m)\,\mathbf{e}_1|$ a-priori, and hence

$$\|\mathbf{r}_m\| \leq |t_{m+1,m}||\mathbf{e}_m^T f(T_m)\,\mathbf{e}_1|.$$





$A =$ pde225f (Matrix Market), $f(A) = e^{-A}$, $\mathbf{v} = (1, \ldots, 1)^T/\sqrt{n}$.

Applications to the inexact Arnoldi method

Inexact Arnoldi

Joint work with V. Simoncini (University of Bologna)

In inexact Arnoldi, A is assumed to be not known exactly. Then, the matrix-vector product can only be approximated:

$$A\mathbf{u}_k \approx A\mathbf{u}_k + \mathbf{w}_k,$$

with accuracy $\|\mathbf{w}_k\| < \epsilon$. Then the the original recurrences become

$$(A + E)U_m = U_m T_m + t_{m+1,m}\boldsymbol{u}_{m+1}\boldsymbol{e}_m^T, \quad E = [\mathbf{w}_1, \ldots, \mathbf{w}_m]U^*.$$

We can define the quantities $(x = 1)$

$$\mathbf{r}_m = A\mathbf{y}_m - \mathbf{y}_m^{(d)} \quad \text{and} \quad \rho_m = |t_{m+1,m}\mathbf{e}_m^T f(T_m)\mathbf{e}_1|.$$

However, $\mathbf{r}_m$ cannot be computed exactly!

A strategy for the inexact Arnoldi

Observe that

- T_m is upper-Hessenberg;
- Assuming ϵ small enough, $W(A+E)$ is not much larger than $W(A)$ since $W(A+E) \subset W(A) + W(E)$.

Therefore, by using the same bound seen before, we expect $\rho_m = |t_{m+1,m}\mathbf{e}_m^T f(T_m)\mathbf{e}_1|$ to decay.

Since

$$\|\mathbf{r}_m\| \leq |\|\mathbf{r}_m\| - \rho_m| + \rho_m,$$

if $|\|\mathbf{r}_m\| - \rho_m|$ is small, then $\|\mathbf{r}_m\|$ decays too.

A strategy for the inexact Arnoldi method

Note that ([Simoncini, '05], [Simoncini, Szyld, '03]),

$$\left| \|\mathbf{r}_m\| - \rho_m \right| \leq \|[\mathbf{w}_1, \ldots, \mathbf{w}_m] f(tH_m)\mathbf{e}_1\| \leq \sum_{j=1}^{m} \|\mathbf{w}_j\| \, |\mathbf{e}_j^T f(T_m)\mathbf{e}_1|,$$

Therefore, $\left| \|\mathbf{r}_m\| - \rho_m \right|$ is small as long as

$$\|\mathbf{w}_j\| \, |\mathbf{e}_j^T f(T_m)\mathbf{e}_1| \leq \mathrm{toll}/m$$

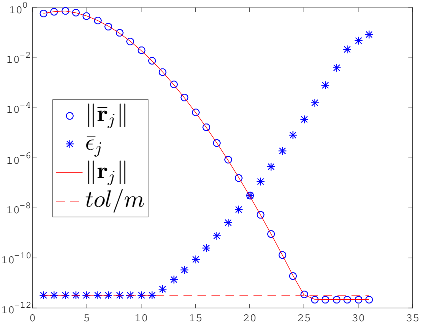
As a consequence,

- we can relax the accuracy of each iteration $\epsilon_j = \|w_j\|$;
- ϵ_j can be set a-priori using the bound for $|\mathbf{e}_j^T f(T_m)\mathbf{e}_1|$.

The smaller is ρ_m the larger is the accuracy ϵ_j.

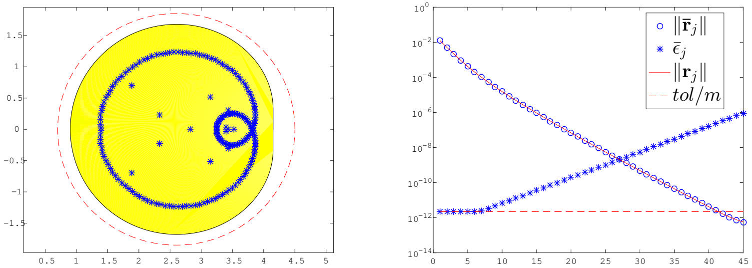
Example - $e^{-A}\mathbf{v}$

- $\|\mathbf{r}_j\| \longrightarrow$ constant accuracy strategy, $\epsilon_j = \mathrm{toll}/m$, for every j;
- $\|\bar{\mathbf{r}}_j\| \longrightarrow$ previously presented strategy for $\bar{\epsilon}_j$.



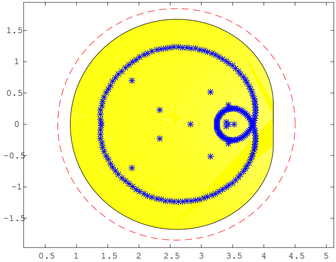
Matrix pde225 (Matrix Market), $\mathbf{v} = (1, \ldots, 1)^T/\sqrt{n}$.

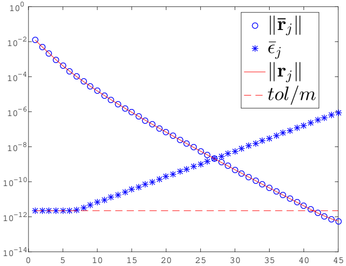
Example - $\exp(-\sqrt{A})\mathbf{v}$



$A = \text{Toeplitz}(-1, 1, \underline{3}, 0.1) \in \mathcal{B}_{200}(1, 2)$, $\mathbf{v} = (1, \ldots, 1)^T/\sqrt{n}$.

Example - $\exp(-\sqrt{A})\mathbf{v}$





$$A = \mathrm{Toeplitz}(-1, 1, \underline{3}, 0.1) \in \mathcal{B}_{200}(1, 2),\ \mathbf{v} = (1, \ldots, 1)^T/\sqrt{n}.$$

More details: S. Pozza, V. Simoncini, *Decay bounds for functions of banded non-Hermitian matrices*, BIT, 2019.

Decay phenomenon and rational Krylov subspace methods

Rational Krylov Subspace Method

Setting $\boldsymbol{\sigma} = [\sigma_1, \ldots, \sigma_{m-1}]$ with $\sigma_j \notin \lambda(A)$, the rational Krylov subspace is defined as

$$\mathcal{K}_m(A, \boldsymbol{v}, \boldsymbol{\sigma}) := \mathrm{span}\left\{ \boldsymbol{v}, (A - \sigma_1 I)^{-1} \boldsymbol{v}, \ldots, \prod_{j=1}^{m-1} (A - \sigma_j I)^{-1} \boldsymbol{v} \right\}.$$

RKSM produces the orthogonal matrix $V_m = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m]$ basis of $\mathcal{K}_m(A, \boldsymbol{v}, \boldsymbol{\sigma})$. RKSM is a Gram-Schmidt orthogonalization:

$$h_{j+1,j} \boldsymbol{v}_{j+1} = (A - \sigma_j I)^{-1} \boldsymbol{v}_j - \sum_{i=1}^{j} h_{i,j} \boldsymbol{v}_i, \quad j = 1, \ldots, m,$$

$$h_{i,j} = \boldsymbol{v}_i^* (A - \sigma_j I)^{-1} \boldsymbol{v}_j, \quad h_{j+1,j} = \|\boldsymbol{v}_{j+1}\|.$$

RKSM matrices

RKSM recurrences have the matrix form:

$$A\,V_m H_m = V_m K_m - h_{m+1,m}(A - \sigma_m I)\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T,$$

with H_m the Hessenberg matrix with entries $h_{i,j}$, and

$$K_m = (I + H_m \operatorname{diag}(\sigma_1, \dots, \sigma_m));$$

see, e.g., [Ruhe, '94], [Güttel, '13], [Güttel, Knizhnerman, '13].
The information about the orthogonalization are carried by H_m.
The reduced-order matrix is defined as

$$J_m := V_m^* A V_m = K_m\, H_m^{-1} - h_{m+1,m} V_m^* (A - \sigma_m I)\, \boldsymbol{v}_{m+1} \boldsymbol{e}_m^T\, H_m^{-1},$$

which is the projection of A onto $\mathcal{K}_m(A, \boldsymbol{v}, \boldsymbol{\sigma})$.

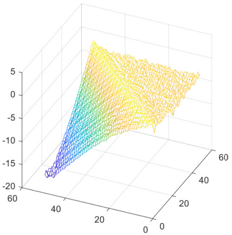
Reduced-order matrix applications

RKSM can be used for the approximation of matrix function

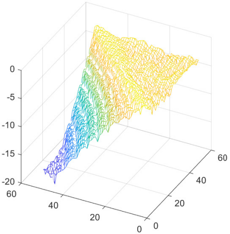
$$f(A)\boldsymbol{v} \approx V_m f(J_m)\boldsymbol{e}_1;$$

Another application is the Lyapunov matrix equation. See, e.g., [Guttel, '13] [Knizhnerman, Simoncini,'11], [Simoncini,'15-'16].

J_m is generally full. Nevertheless, J_m, and $f(J_m)$ exhibit a decay.



J_{60}



$\exp(J_{60})$

?

See also [Fasino, '05], semiseparable + diag

The hidden sparsity structure of J_m

Given the rational function

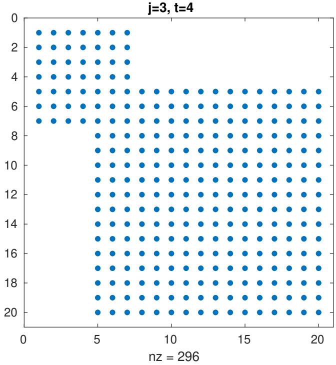
$$s_j^{(t)}(x) := \frac{q_j(x)}{(x-\sigma_t)\cdots(x-\sigma_{t+j-1})},$$

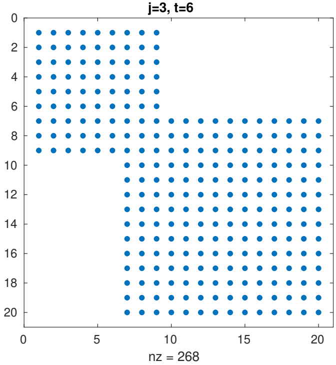
with $t \geq 1$ and $q_j(x)$ a polynomial of degree at most j. If the indexes k, ℓ are such that $k \geq t+2$ and $\ell \leq t$, then

$$\left(s_j^{(t)}(J_m)\right)_{k,\ell} = 0, \quad j = 1, \dots, k-t-1.$$

- The hidden sparsity structure of J_m is a consequence of V_m orthogonality.
- In Arnoldi's method, the connection between the orthogonalization process and the sparsity pattern of T_m is evident.

The hidden sparsity structure of J_m





Sparsity pattern of $s_j^{(t)}(J_m)$ for J_{20} and Hermitian matrix A.

A-priori decay bound

To derive a-priori decay bounds for $f(J_m)$ we exploit:

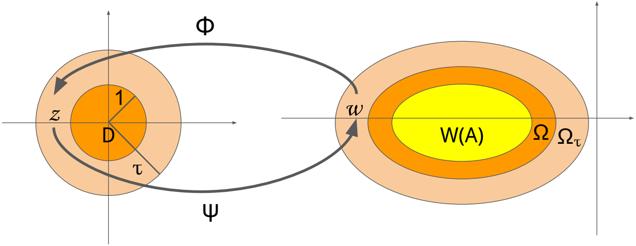
- The hidden sparsity structure of J_m;
- Rational function approximation. Specifically, rational Faber-Dzhrbashyan functions M_j, ([Dzhrbashyan,'57], [Suetin,'98], [Beckermann, Reichel,'09]);
- The domain of analyticity of f;
- Information on the field of values of A since $W(J_m) \subseteq W(A)$.

Our results are based on Faber-Dzhrbashyan expansions:

$$f(J_m) = \sum_{j=0}^{\infty} \alpha_j M_j(J_m).$$

See also [Druskin, Knizhnerman, Simoncini, '11], [Knizhnerman, Simoncini, '11]

Let $\Omega \supseteq W(A)$ be a convex compact set and let ϕ and ψ be the related conformal map and its inverse, s.t. $\phi(\infty) = \infty$, and $\lim_{z\to\infty} \phi(z)/z = d > 0$.



Upper bounds

Assume $\tau > 1$, $k - \ell > 1$, and f analytic on Ω_τ. Then

$$|f(J_m)_{k,\ell}| \leq 3\frac{\tau}{\tau - 1} \max_{|z|=\tau} |f(\psi(z))| \prod_{t=\ell}^{k-2} \frac{\tau + |\phi(\sigma_t)|}{|\phi(\sigma_t)|\tau + 1} := B(k, \ell).$$

Setting the coefficients

$$\alpha_j = \frac{1}{2\pi i} \int_{|z|=\tau} \frac{f(\psi(z))}{z} \prod_{t=\ell}^{k-2} \frac{z - \phi(\sigma_t)}{\overline{\phi(\sigma_t)}z - 1} \frac{\phi(\sigma_t)}{|\phi(\sigma_t)|} \left(-\frac{1}{z}\right)^{j-k+\ell+2} dz.$$

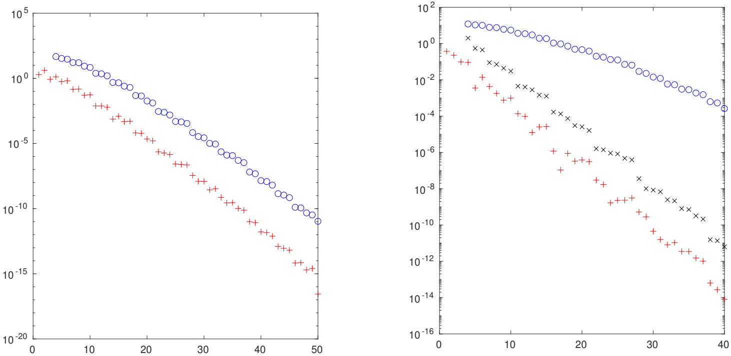
and a positive integer s, we have the following more refined bound

$$|f(J_m)_{k,\ell}| \leq 3 \left(\sum_{j=0}^{s-1} |\alpha_{j+k-\ell-1}| + \frac{B(k, \ell)}{\tau^s} \right).$$

Remarks

- $B(k, \ell)$ depends on the parameter τ;
- For each k, ℓ, we can choose a nearly optimal τ;
- For $f(\lambda) = \lambda$, the bound shows that J_m elements decays in the matrix lower part (wannabe Hessenberg);
- The better Ω approximate $W(A)$ the better is the bound;

Numerical tests: Symmetric case, 2D Laplacian



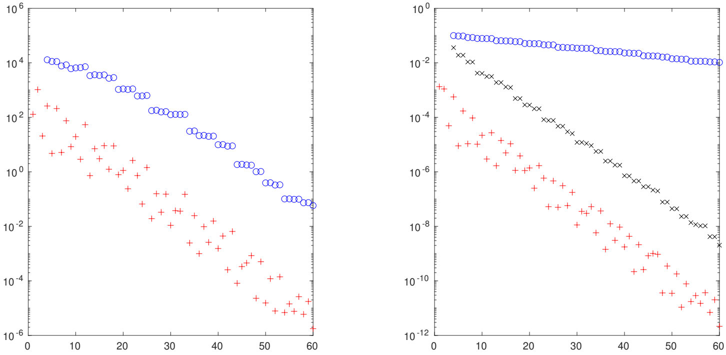
$|(J_{50})_{:,2}|$ (+), $B(k,\ell)$ (∘)

$|(\exp(J_{50}))_{:,2}|$ (+), $B(k,\ell)$ (∘), refined bound (+)

$A = L \otimes I + I \otimes L$, $L = \mathrm{tridiag}(-1, 2, -1)$, $n = 1600$, $\boldsymbol{v}$ random, $\lambda(A) \subseteq [-7.9883, -0.0117]$.

(+): coefficients α_j computed by MatLab `integral` , $s \leq 27$.

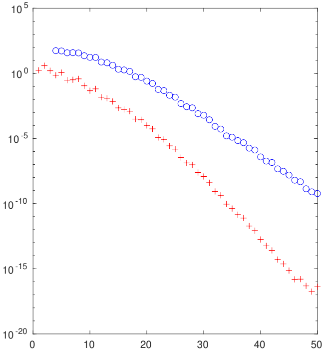
Numerical tests: Symmetric case



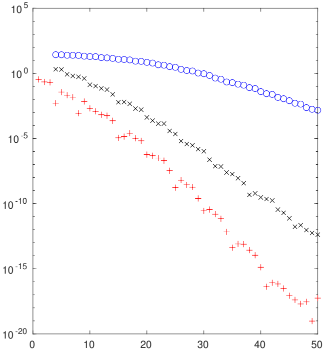
$|(J_{60})_{:,2}|$ $\quad$ $|((J_{60} - 100i\, I)^{-1})_{:,2}|$

`flowmeter0` , Oberwolfach Model Reduction Benchmark Collection (dynamical systems). Symm., $n = 9669$, $\lambda(A) \subset [-2.08 \cdot 10^3, -1.31 \cdot 10^{-4}]$. $s \leq 53$.

Numerical tests: Non-symmetric case



$|(J_{60})_{:,2}|$



$|((J_{60} - 100i\,I)^{-1})_{:,2}|$

A is obtained from the centered finite difference discretization of $L(u) = -\Delta u + 35u_x + 35u_y$, on the unit square, with homogeneous Dirichlet boundary conditions. Non-symmetric, $n = 784$. $s \leq 20$.

Lyapunov equation

Another application is the Lyapunov matrix equation

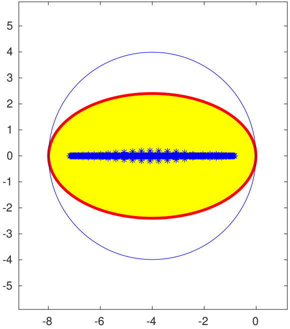
$$AX + XA^H = \boldsymbol{c}\boldsymbol{c}^H.$$

that can be approximated by solving the reduced-order equation

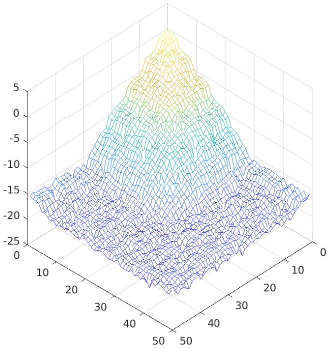
$$J_m Y_m + Y_m J_m^H = \boldsymbol{e}_1 \boldsymbol{e}_1^T, \quad X \approx V_m Y_m V_m^H,$$

$$Y_m = \frac{i}{2\pi} \int_{-i\infty}^{+i\infty} (wI - J_m)^{-1} \boldsymbol{e}_1 \boldsymbol{e}_1 (wI + J_m)^{-1} \,\mathrm{d}w.$$

Y_m decay can be used to estimate the residual.

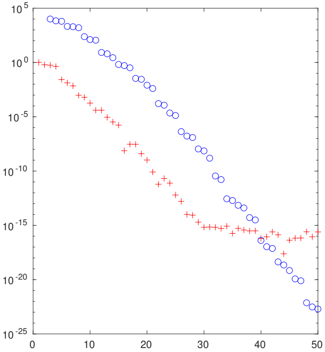


Field of values of A (yellow area), eigenvalues of A ($*$)

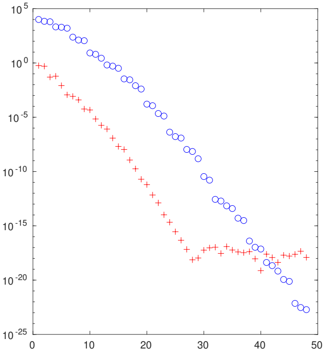


$|Y_{50}|$, solution of the reduced-order Lyapunov equation (log scale)

Numerical tests: Y_m Lyapunov non-symmetric eq.



$|(Y_{50})_{:,3}|$



$\mathrm{diag}(|Y_{50}|)$

See also [Kürschner, Freitag, 2020].

Remarks

- The matrix $T_m = U_m^* A U_m$ from Arnoldi's method is upper-Hessenberg, hence characterized by a decay phenomenon.
- In RKSM, the matrix $J_m = V_m^* A V_m$ is generally a full matrix.
- Despite having lost the band structure, J_m is still characterized by a decay phenomenon in its lower part.
- We explained and described this decay phenomenon by deriving effective a-priori bounds.
- We derived similar bounds for Lyapunov matrix equations.

More details: P., Simoncini, *Functions of rational Krylov space matrices and their decay properties*, Numerische Mathematik, 2021.

Decay phenomenon and linear ODEs

Non-autonomous linear ODEs

Consider the following ordinary differential equation

$$\partial_t y(t) = \tilde{f}(t)y(t), \quad y(0) = 1, \quad t \in [0, 1],$$

with $\tilde{f}(t)$ a given analytic function over $[0, 1]$.

- We present a new approach for the solution of linear ODEs.
- The new method is meant for large systems of non-autonomous linear ODEs.
- For the sake of simplicity, here, we consider the simpler case where the time-dependent coefficient $\tilde{f}(t) \in \mathbb{C}$.

Joint work with N. Van Buggenhout (Charles University) and P-L. Giscard (ULCO, Calais).

ODE solution expansion

Consider the (shifted) normalized Legendre polynomials $p_0(t), p_1(t), p_2(t), \dots$, i.e., polynomials s.t.

$$\int_0^1 p_k(\tau) p_\ell(\tau) d\tau = \begin{cases} 0, & \text{if } k \neq \ell \\ 1, & \text{if } k = \ell \end{cases}$$

The solution $y(t)$ is an analytic function over $[0, 1]$, as such, we can expand it into the series

$$y(t) = \sum_{j=0}^{\infty} u_j p_j(t), \quad t \in [0, 1].$$

ODE solution expansion

Let us define the truncated expansion

$$y_m(t) := \sum_{j=0}^{m} u_j p_j(t), \quad t \in [0,1].$$

Then the error is bounded by

$$\max_{t\in[0,1]} |y(t) - y_m(t)| \leq \sum_{j=m+1}^{\infty} |u_j| \frac{\sqrt{2j+1}}{2}.$$

- As $y(t)$ is analytic, the coefficients $|u_j|$ asymptotically converge to zero faster than geometric (decay).
- For m large enough, $|u_{m+1}|$ is a good approximation of the truncation error.

ODE solution by $\star$-product

The new approach is based on the so-called $\star$-product. Given two distributions $g_1(t,s), g_2(t,s)$ from a certain class,

$$(g_1 \star g_2)(t,s) := \int_{-\infty}^{+\infty} g_1(t,\tau) g_2(\tau,s)\, d\tau.$$

Then, the ODE solution can be expressed as [P., Giscard, '22]

$$y(t) = \left(\Theta(t-s) \star (1_\star - \tilde{f}(t)\Theta(t-s))^{-\star}\right)(t,0),$$

with

$$\Theta(t-s) = \begin{cases} 1, & t \geq s, \\ 0, & t < s \end{cases}.$$

(Replacing $\tilde{f}$ with a matrix, we can solve an ODE system.)

$\star$-product discretization

By using the Legendre polynomials, the $\star$-product expression can be discretized. This leads to transforming the $\star$-product algebra into a matrix algebra.

$$
\begin{array}{lcl}
\tilde{f}(t)\Theta(t-s) & & F_m \\
r(t,s) = p(t,s) \star q(t,s) & \text{discr.} & R_m = P_m Q_m \\
p + q & \longrightarrow & P_m + Q_m \\
1_\star = \delta(t-s) & & I_m, \text{ identity matrix} \\
p^{-\star}(t,s) & & P_m^{-1} \\
(1_\star - p)^{-\star}(t,s) & & (I_m - P_m)^{-1}
\end{array}
$$

[P., Van Buggenhout, '22]

ODE solution by discretized $\star$-product

Then, the $\star$-solution of the ODEs can also be discretized.

$$y(t) = \left(\Theta(t-s) \star \left(1_\star - \tilde{f}(t)\Theta(t-s)\right)^{-\star}\right)(t,0)$$

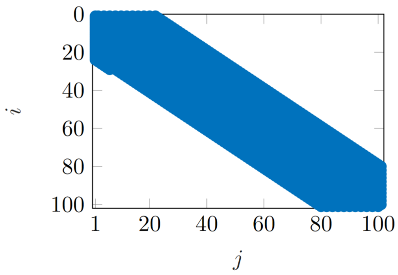
$\downarrow$ *discr.*

$$\mathbf{u}_m \approx H_m (I_m - F_m)^{-1} \mathbf{e}_1$$

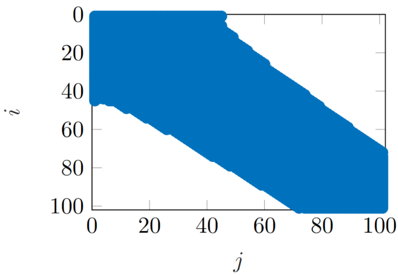
$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ \vdots \end{bmatrix} \approx \begin{bmatrix} & * & & & & \\ * & & * & & & \\ & * & & * & & \\ & & * & & * & \\ & & & * & & \ddots \\ & & & & \ddots & \end{bmatrix} \begin{bmatrix} * & * & * & * & * & \dots \\ * & * & * & * & * & \ddots \\ * & * & * & * & * & \ddots \\ * & * & * & * & * & \ddots \\ * & * & * & * & * & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

decay $\uparrow$ decay $\uparrow$ banded by truncation

Example- $\tilde{f}(t) = \cos(4t)$



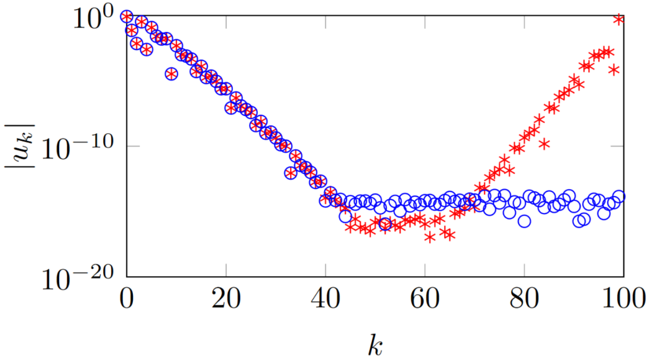
F_{100}



$H_{100}(I_{100} - F_{100})^{-1}$

Sparsity pattern of the matrices after truncation ($tol = 2e - 16$)

Example- $\tilde{f}(t) = \cos(4t)$



Legendre coefficients of the solution $u(t)$; computed by the $\star$-approach ($*$), computed via chebfun knowing that $u(t) = \exp(\cos(4t) - 1)$.

Remarks

- There is a clear relation between the decay of the resolvent of the discretized matrix and the decay of the Legendre coefficients $u_0, u_1 \dots$;
- We need to determined m a-priori. This means that we need to know how many $u_0, u_1 \dots$ are needed before solving the linear system;
- A-priori bound on the decay of $(I_m - F_m)^{-1}$ may provide an estimate for m.

More details:

- P., Van Buggenhout, *A $\star$-product solver with spectral accuracy for non-autonomous ordinary differential equations*, PAMM, '23.
- P., Van Buggenhout, *The $\star$-product approach for linear ODEs: A numerical study of the scalar case*, PAMM, '23.

Conclusion

The decay phenomenon appears in:

- Network/graph analysis;
- Krylov subspace methods (Hessenberg matrix);
- Rational Krylov subspace methods (hidden structure);
- Legendre polynomial expansion of and ODE solution (from a matrix point of view);
- Many other applications.

Its understanding requires combining tools from:

- Polynomial and rational approximation;
- Linear algebra;
- Graph Theory.

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Thank you for your attention!