PhD days - Numerical Analysis

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What is numerical analysis?

Many words (sometimes improperly) used as synonym

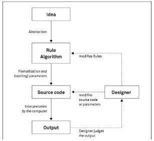
- Scientific computing
- Numerical mathematics
- Computational mathematics
- Numerical methods
- Numerical computation
- Mathematical software

A possible definition by Nick Trefethen:

Numerical analysis is the study of algorithms for the problems of continuous mathematics.

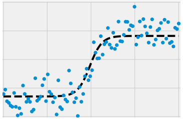
What we aim to do/study

Design algorithms



Identify important mathematical quantities and propose how to approximate them

Efficiency

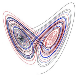


Time and memory consumption, use of modern computational architectures

Accuracy

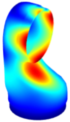
Error bounds, and stability analysis

Convergence



Prove that approximated quantities converge to the truth as resolution increases

Applications



Collaborate with researchers from other areas on specific applications

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What is NLA about

NLA concerns the development, analysis, testing and evaluation of numerical algorithms for linear systems, eigenvalue problems, matrix functions, and other core LA tasks.

Our favourite topics:

- High performance computing
- Eigenvalue problems, especially in structural engineering
- Multilinear algebra (a.k.a. tensors)
- Randomized linear algebra
- Structured matrix problems

Less beaten paths:

- Analysis of accuracy and stability of algorithms
- Mixed precision algorithms

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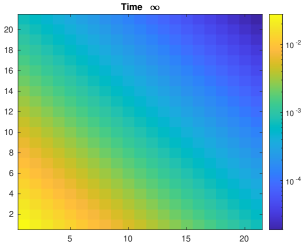
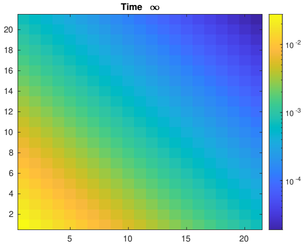
Matrix-analytic methods for Markov chains

3 Past projects: Example 1

$$\boxed{\pi_{ij} := \lim_{t\to\infty} \mathbb{P}(X_t = (i, j))}$$

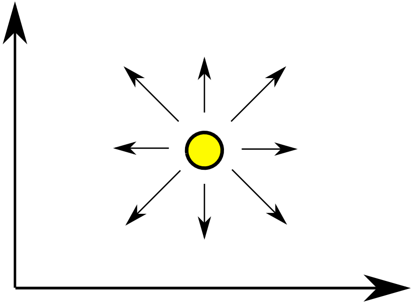




Matrix-analytic methods for Markov chains

Framework:

- Random walk on 2D lattices (phase – level),
- Discrete time,
- Each transition depends only on the current position (independent on time),
- Bounded transitions (Quasi-Birth-Death).



Goal:

- Compute the stationary distribution π, i.e.:

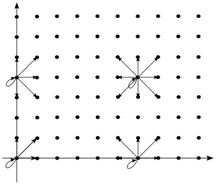
$$\pi_j := \lim_{n\to\infty} \mathbb{P}(X_n = j), \quad \forall j \in \mathbb{N}^2,$$

Applications:

- Queuing models,
- Populations growth.

Matrix-analytic methods for Markov chains

3 Past projects: Example 1



For Quasi-Birth-Death processes the transition probability matrix looks like

$$P = \begin{bmatrix} B_0 & B_1 & & & \\ A_{-1} & A_0 & A_1 & & \\ & A_{-1} & A_0 & A_1 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \qquad B_i, A_i \in \mathbb{R}^{\mathbb{N}\times\mathbb{N}},\ i = -1, 0, 1.$$

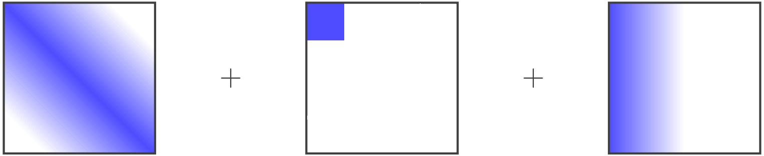
Finding π requires to solve $\boxed{A_{-1} + A_0 X + A_1 X^2 = X}$ $\rightsquigarrow$ infinite matrix arithmetic.

Matrix-analytic methods for Markov chains

We have introduced and studied the class of semi-infinite matrices of the form

$$\begin{bmatrix} a_0 & a_1 & a_2 & \dots \\ a_{-1} & a_0 & a_1 & \ddots \\ a_{-2} & a_{-1} & a_0 & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{bmatrix} \quad + \quad E \quad + \quad \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \vdots \end{bmatrix} \begin{bmatrix} v_1 & v_2 & v_3 & \dots \end{bmatrix}$$

with the following decay properties.



Idea: the matrices within this class form a Banach algebra and **are representable at any arbitrary precision with a finitely large set of parameters**.

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4 Past projects: Example 2

Let $f(z) = z^{-\alpha}$, $\alpha \in (0, 1)$.

Problem: Given a symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$ with eigenvalues in $[\lambda_{\text{min}}, \lambda_{\text{max}}] \subset \Omega$ and $v \in \mathbb{R}^n$ compute

$$x := f(A)v.$$

$$\text{Reminder:} \quad A = Q \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} Q^* \Rightarrow f(A) = Q \begin{bmatrix} f(\lambda_1) & & \\ & \ddots & \\ & & f(\lambda_n) \end{bmatrix} Q^*.$$

Settings: A is large and structured $\rightsquigarrow$ we do not want to form $f(A)$ explicitly but we are allowed to compute matvecs and solve (shifted) linear systems with A.

Applications: Fractional diffusion, Matrix Transform Method

Rational approximation for matrix functions

Let $\mathcal{U} \subset \mathbb{R}^n$ be a ℓ-dimensional subspace ($\ell \ll n$) with an orthogonal basis $U = [u_1 | \dots | u_\ell]$ and $A_\ell = U^* A U$, $v_\ell = U^* v$ be the projections of A and v on $\mathcal{U}$.

- **Linear systems**

$$x = A^{-1} v \approx x_\ell := U A_\ell^{-1} v_\ell.$$

- **Matrix functions**

$$x = f(A) v \approx x_\ell := U f(A_\ell) v_\ell.$$

Rational approximation for matrix functions

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If we use the **Krylov subspace** $\mathcal{U} = \mathcal{K}_\ell(A, v) := \text{span}\{v, Av, \dots, A^{\ell-1} v\}$ then,

$$||x - x_\ell||_2 \leq 2 \cdot \min_{p(z) \in \mathcal{P}_{\ell-1}} \max_{z \in [\lambda_{\text{min}}, \lambda_{\text{max}}]} |p(z) - f(z)|,$$

where $\mathcal{P}_\ell := \{\text{poly of degree} \leq \ell\}$.

Rational approximation for matrix functions

Rational Krylov subspace. Given $\Sigma_\ell := \{\sigma_1, \dots, \sigma_\ell\} \subset \mathbb{C}$ it is defined as[1]

$$\begin{aligned}\mathcal{RK}_\ell(A, v, \Sigma_\ell) :&= q_\ell(A)^{-1}\mathcal{K}_{\ell+1}(A, v) = \left\{ \frac{p(A)}{q_\ell(A)} v : \ p(z) \in \mathcal{P}_\ell \right\} \\ &= \operatorname{span}\{v, (\sigma_1 I - A)^{-1} v, \dots, (\sigma_\ell I - A)^{-1} v\}\end{aligned}$$

where $q_\ell(z) := \prod_j (z - \sigma_j)^{-1}$.

If $\mathcal{U} = \mathcal{RK}_\ell(A, v, \Sigma_\ell)$ we get a problem of rational approximation with fixed poles

$$||x - x_\ell||_2 \le 2 \cdot \min_{r(z) \in \frac{\mathcal{P}_\ell}{q_\ell(z)}} \max_{z \in [\lambda_{\min}, \lambda_{\max}]} |r(z) - f(z)|.$$

[1] last equality is valid only for distinct poles

Rational approximation for matrix functions

Goal. Provide selection strategies for Σ_ℓ and estimates of the error $||x - x_\ell||_2$.

Idea: Exploit the integral formulation of $z^{-\alpha} = \frac{\sin(\alpha\pi)}{\pi} \int_0^\infty \frac{t^{-\alpha}}{z+t} dt$ we get:

$$\int_0^\infty (A + tI)^{-1} v \, d\mu(t) = f(A)v \quad \approx \quad Uf(A_\ell)v_\ell = \int_0^\infty U(A_\ell + tI)^{-1} v_\ell \, d\mu(t).$$

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Outcome:

Theorem

Let $f(z) = z^{-\alpha}$, $\alpha \in (0, 1)$, *U be an orthogonal basis of* $\mathcal{RK}_\ell(A, v, \Sigma_\ell^*)$ *and* $x_\ell = Uf(A_\ell)v_\ell$. *Then*

$$||f(A)v - x_\ell||_2 \leq 8f(\lambda_{min})||v||_2 \rho^\ell,$$

where $\rho := \exp\left(-\frac{\pi^2}{\log\left(16\frac{\lambda_{max}}{\lambda_{min}}\right)}\right)$.

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5 New directions

Approximation via exponential sums

Goal: Study both theoretically, and computationally the problem of finding an approximation of $f : \mathbb{C} \to \mathbb{C}$ as

$$f(z) \approx \sum_{j=1}^{k} \alpha_j \exp(\beta_j z), \qquad \alpha_j, \beta_j \in \mathbb{C}.$$

- Fixed a compact region $\Omega \subset \mathbb{C}$, and a norm, how do the approximation error decay with respect to k? What is the role of the regularity of f?
- The interpolation problem has been already studied (Prony's method); what is the best computational way to deal with the least squares approximation problem?

Approximation via exponential sums

- For functions defined via an integral transform, study the connection with the rational approximation of the integrand.
  For instance in the case $f(z)$ is the Laplace transform of $\varphi(z)$

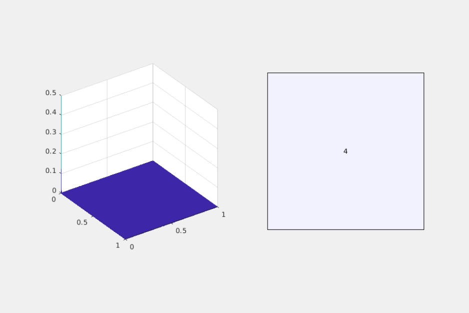
$$f(z) = \int_0^\infty \varphi(t)e^{-zt}dt \approx \int_0^\infty \sum_{j=1}^k \frac{\alpha_j}{z-\beta_j} e^{-zt}dt = \sum_{j=1}^k \alpha_j \exp(\beta_j z),$$

  where $\sum_{j=1}^k \frac{\alpha_j}{z-\beta_j}$ is a rational approximation of $\varphi(z)$.
- In the case $f(z) = \frac{1}{z}$ exploit exponential sums for preconditioning linear systems with Kronecker structure like $(A_1 \otimes I + I \otimes A_2)x = b$, by means of the relation:

$$\exp(A_1 \otimes I + I \otimes A_2) = \exp(A_1) \otimes \exp(A_2).$$

New directions: dynamical hierarchical structures in PDEs

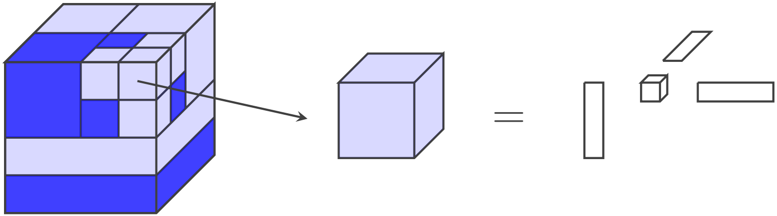
- The solution of certain PDEs on 2D domains are rank-structured.
- For evolutionary problems, such as the Burgers equation, the structure is time dependent.



Blue blocks: Full rank submatrices, **Grey blocks**: Low-rank submatrices

New directions: dynamical hierarchical structures in PDEs

Why not extending this framework to tensors?



Research questions/challenges:

- Various possibilities for the representation of the low-rank blocks: Tucker, Tensor Train, Hierarchical Tucker, ...
- How to identify an advantageous partitioning in an efficient way.
- Under which circumstances we can mitigate the curse of dimensionality?