Krylov Subspace Methods and Matrix Functions

new directions in design, analysis, and applications

Tyler Chen

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`chen.pw/slides`

About me

I am a numerical linear algebraist who likes working with nearby communities (theoretical computer science, computational science, optimization, etc.)

Academic history:

- Currently an Assistant Professor / Courant Instructor at New York University
  - Sponsor: Chris Musco
- PhD in Applied Math at University of Washington
  - Advisors: Anne Greenbaum and Tom Trogdon
- B.S. in Math and Physics at Tufts University, minor in Studio Art

My research program

Focus: design and analysis of practically fast and theoretically justified (randomized) algorithms for fundamental linear algebra tasks

Goal: develop tools to support the advancement of knowledge in current scientific applications

Mode: collaboration with a range of fields, and involvement and training of (underrepresented) students

Hope: provide conceptually simple insights into key problems

I am interested in diverse linear algebra problems

Compressed sensing/operator learning[1]

- $O(s/\epsilon)$ matrix-vector product algorithms for relative approximation with an s-row sparse matrix (no dimension dependence and matching lower bounds!)

Stochastic Optimization[2]

- First proof of $O(\sqrt{\kappa})$ convergence of minibatch stochastic gradient descent with heavy-ball momentum

Spectrum approximation[3]

- Sharp analysis of stochastic Lanczos quadrature algorithm proving spectrum approximation in Wasserstein distance in $\tilde{O}(\mathrm{nnz}(\mathbf{A})/\epsilon)$ time

Numerical Analysis/Random Matrix Theory[4]

- First proof of forward stability of Lanczos algorithm on random matrices

[1] Amsel, T. C., Halikias, Keles, Musco, and Musco 2024.
[2] Bollapragada, T. C., and Ward 2022.
[3] T. C., Trogdon, and Ubaru 2021.
[4] T. C. and Trogdon 2023.

What is a matrix function?

An $n \times n$ symmetric matrix $\mathbf{A}$ has real eigenvalues and orthonormal eigenvectors:

$$\mathbf{A} = \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^\top.$$

The matrix function $f(\mathbf{A})$, induced by $f : \mathbb{R} \to \mathbb{R}$ and $\mathbf{A}$, is the matrix:

$$f(\mathbf{A}) = \sum_{i=1}^{n} f(\lambda_i) \mathbf{u}_i \mathbf{u}_i^\top.$$

Typically $\mathbf{A}$ is sparse while $f(\mathbf{A})$ is dense.

What do we want?

In this talk, think of the dimension n as big! E.g. $n = 10^6$ or 10^{12}.

- For reference, if $n = 10^6$:
  - matrix requires 8 terabytes of storage (not even enough disk space)
  - 100 vectors require 0.8 gigabytes of storage (can store in RAM)

We can't store $f(\mathbf{A})$, but we might instead compute:

$$f(\mathbf{A})\mathbf{b}, \qquad \mathbf{b}^\mathsf{T} f(\mathbf{A})\mathbf{b}, \qquad \operatorname{tr}(f(\mathbf{A})) = \sum_{i=1}^{n} f(\lambda_i).$$

Example. If $f(x) = x^{-1}$, then $f(\mathbf{A}) = \mathbf{A}^{-1}$ and $f(\mathbf{A})\mathbf{b} = \mathbf{A}^{-1}\mathbf{b}$ is the solution to the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$.

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Why do we care?

Applications in many fields: quantum physics/chemistry,[5] biology,[6] statistics/data science,[7] network science,[8] machine learning,[9] high performance computing,[10] etc.

Common functions: inverse, exponential, square root, sign function.

[5] Eshof, Frommer, Lippert, Schilling, and Vorst 2002; Weiße, Wellein, Alvermann, and Fehske 2006; Schnalle and Schnack 2010.

[6] Estrada 2000.

[7] Barry and Pace 1999; Gardner, Pleiss, Weinberger, Bindel, and Wilson 2018; Jin and Sidford 2019.

[8] Avron 2010; Dong, Benson, and Bindel 2019.

[9] Ghorbani, Krishnan, and Xiao 2019; Papyan 2019; Granziol, Wan, and Garipov 2019; Yao, Gholami, Keutzer, and Mahoney 2020.

[10] Polizzi 2009; Li, Xi, Erlandson, and Saad 2019.

Example application: high performance computing

State of the art parallel eigensolvers such as FEAST and EVSL work by splitting the spectrum of $\mathbf{A}$ into pieces, which can each be solved on different machines in parallel.[11]

Let $\mathbb{1}[a \le x \le b] = 1$ if $x \in [a,b]$ and 0 otherwise. Then.

$$\text{number of eigenvalues in } [a,b] = \operatorname{tr}(\mathbb{1}[a \le \mathbf{A} \le b]).$$

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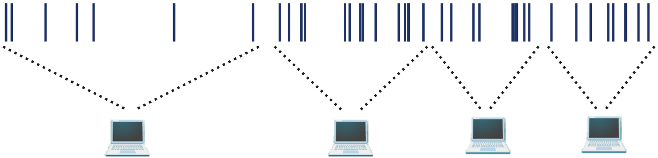

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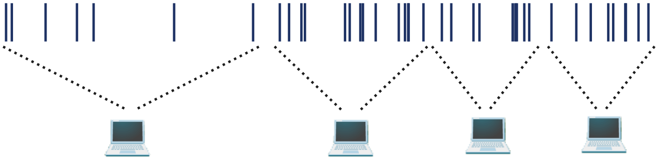

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Part I: Rethinking how we think about existing algorithms

Many linear algebra algs are extremely effective in practice, but have limited theory.

- Analysis of Minibatch-SGD with Heavyball Momentum[12]
- Analysis of Stochastic Lanczos Quadrature and Kernel Polynomial Method[13]
- Stability of Lanczos-based methods[14]
- Analysis of Lanczos-FA[15]

[12] Bollapragada, T. C., and Ward 2022.
[13] T. C., Trogdon, and Ubaru 2021; T. C., Trogdon, and Ubaru 2022.
[14] T. C. and Trogdon 2023; T. C. 2023.
[15] T. C., Greenbaum, Musco, and Musco 2022; Xu and T. C. 2022; Amsel, T. C., Greenbaum, Musco, and Musco 2023.

Krylov subspace methods[16]

Krylov subspace methods are among the most widely used algorithms for solving large linear systems $\mathbf{Ax} = \mathbf{b}$; i.e. approximating $\mathbf{A}^{-1}\mathbf{b}$.

KSMs work by iteratively constructing a basis for the Krylov subspace:

$$\mathcal{K}_k(\mathbf{A}, \mathbf{b}) = \operatorname{span}\{\mathbf{b}, \mathbf{Ab}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^{k-1}\mathbf{b}\}.$$

Elements of the Krylov subspace are polynomials of $\mathbf{A}$ applied to $\mathbf{b}$:

$$c_0\mathbf{b} + c_1\mathbf{Ab} + \cdots + c_{k-1}\mathbf{A}^{k-1}\mathbf{b} = p(\mathbf{A})\mathbf{b},$$

where $p(x) = c_0 + c_1 x + \cdots + c_{k-1}x^{k-1}$.

[16] IEEE Top 10 algorithms of 20th century!

Error bounds for linear system solvers

The convergence of KSMs used to approximate $\mathbf{A}^{-1}\mathbf{b}$ are well understood.

Popular KSMs for linear systems, like Conjugate Gradient, efficiently compute iterates $\mathbf{x}_k$ which satisfy strong error guarantees:

$$
\begin{aligned}
\|\mathbf{A}^{-1}\mathbf{b} - \mathbf{x}_k\| &= \operatorname*{argmin}_{\mathbf{x}\in\mathcal{K}_k(\mathbf{A},\mathbf{b})} \|\mathbf{A}^{-1}\mathbf{b} - \mathbf{x}\| && \text{optimality} \\
&\lesssim \min_{\deg(p)<k} \max_{x\in\operatorname{spec}(\mathbf{A})} |x^{-1} - p(x)| && \text{bound on eigenvalues} \\
&\lesssim \exp\left(-\frac{2k}{\sqrt{\lambda_{\max}/\lambda_{\min}}} \right). && \text{bound on spectral interval}
\end{aligned}
$$

We also have very good techniques for posteriori error estimates; entire books![17]

[17] Meurant and Tichy 2024.

The Lanczos method for matrix function approximation

The Lanczos algorithm[18] iteratively constructs a basis $\mathbf{Q}_k = [\mathbf{q}_0, \ldots, \mathbf{q}_{k-1}]$ for the Krylov subspace and a symmetric tridiagonal matrix matrix $\mathbf{T}_k$ of recurrence coefficients.

Given a function $f(x)$, we define the Lanczos-FA iterate

$$\mathsf{lan\text{-}FA}_k(f) = \mathbf{Q}_k f(\mathbf{T}_k)\mathbf{Q}_k^\mathsf{T}\mathbf{b}.$$

Fact. If $f(x) = x^{-1}$ and $\mathbf{A}$ is positive definite, then $\mathsf{lan\text{-}FA}_k(f)$ is mathematically equivalent to the CG iterate (so we have error bounds and estimates).

For other functions the algorithm is still widely used, and performs remarkably well in practice. However, less theory is known about the error.

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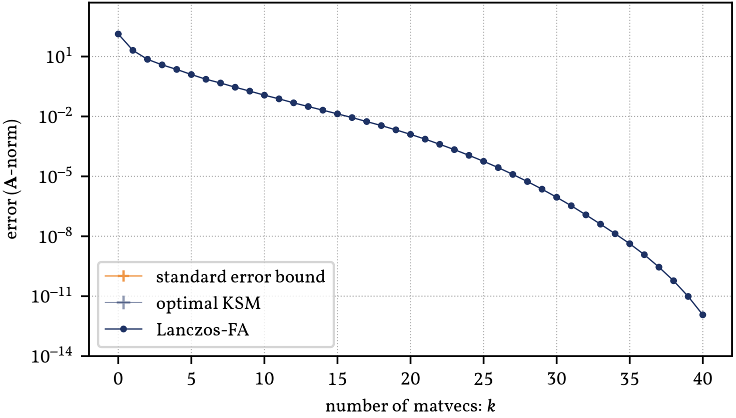
Why does Lanczos-FA work so well? example: matrix square root)

Amazingly, despite being the method of choice for 30+ years, we still don't know why Lanczos-FA works so well!



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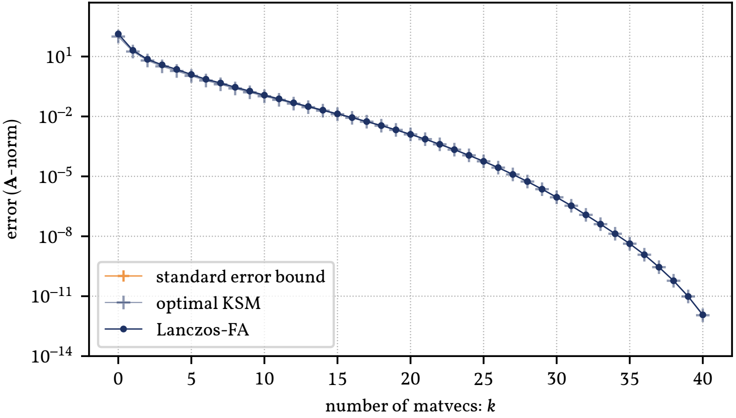

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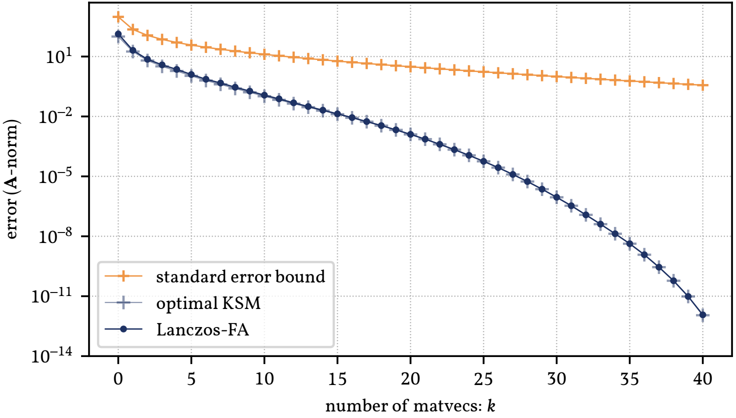

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Key question:

Why does Lanczos-FA work so well?

A reduction to linear systems

Theorem (T. C., Greenbaum, Musco, and Musco 2022). Suppose f is analytic on an neighborhood of the eigenvalues of $\mathbf{A}$ and $\mathbf{T}_k$. Let Γ be a contour containing the eigenvalues of $\mathbf{A}$ and $\mathbf{T}_k$. Then, there is a function $C(w,z)$ (which can be computed using limited information about $\mathbf{A}$) such that, for any fixed w,

$$\|f(\mathbf{A})\mathbf{b} - \mathsf{lan\text{-}FA}_k(f)\| \leq \underbrace{\left(\frac{1}{2\pi} \oint_\Gamma |f(z)||C(w,z)|\mathrm{d}z \right)}_{\text{integral term}} \underbrace{\|\mathsf{err}_k(w)\|}_{\text{linear system error}}.$$

This decouples the error into:

- an integral term we can bound or approximate numerically
- and an error term for CG (which we know a lot about)

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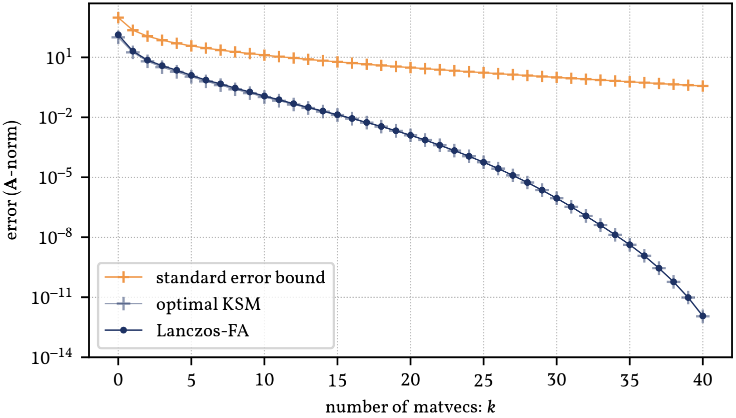

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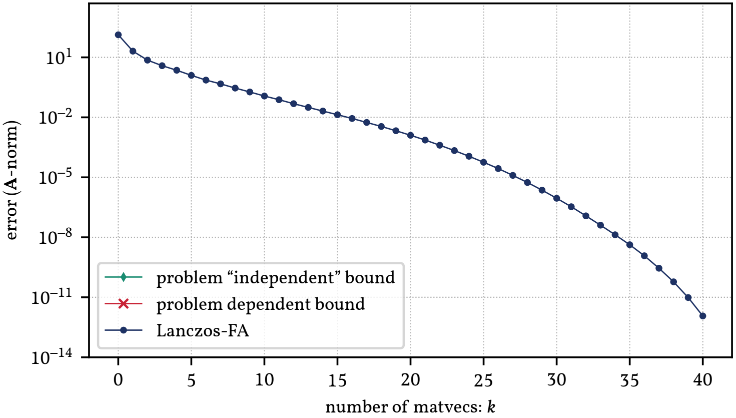

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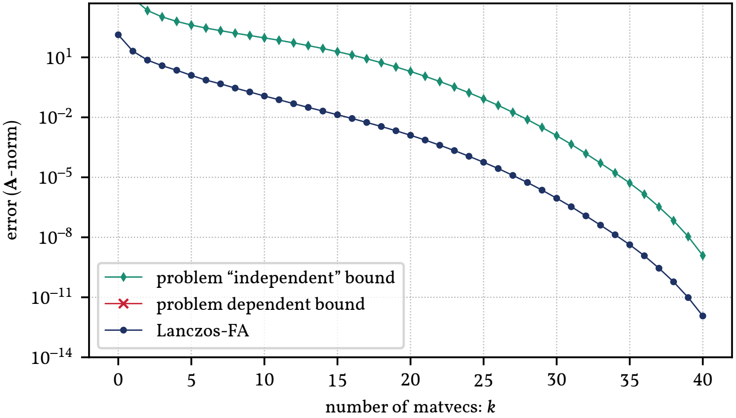

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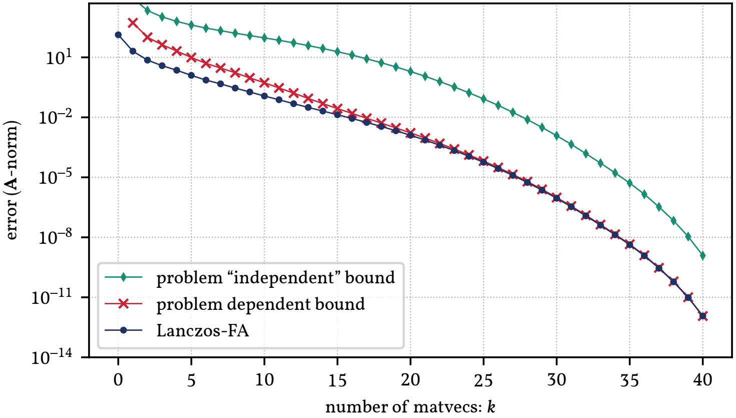

A reduction to linear systems

From Cauchy integral formula:

$$f(x) = -\frac{1}{2\pi \boldsymbol{i}} \oint_\Gamma \frac{f(z)}{x - z}\, \mathrm{d}z.$$

This gives matrix versions:

$$f(\mathbf{A})\mathbf{b} = -\frac{1}{2\pi \boldsymbol{i}} \oint_\Gamma f(z)(\mathbf{A} - z\mathbf{I})^{-1}\mathbf{b}\, \mathrm{d}z.$$

$$\textsf{lan-FA}_k(f) = -\frac{1}{2\pi \boldsymbol{i}} \oint_\Gamma f(z)\mathbf{Q}(\mathbf{T} - z\mathbf{I})^{-1}\mathbf{Q}^\mathsf{T}\mathbf{b}\, \mathrm{d}z.$$

Define $\textsf{err}_k(z) = (\mathbf{A} - z\mathbf{I})^{-1}\mathbf{b} - \mathbf{Q}(\mathbf{T} - z\mathbf{I})^{-1}\mathbf{Q}^\mathsf{T}\mathbf{b}$. Then,

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Some basic facts and a key lemma

Lemma 1. The CG residual to $\mathbf{A}\mathbf{x} = \mathbf{b}$ is in the direction of the Lanczos vector $\mathbf{q}_k$.

Lemma 2. For any z, $\mathcal{K}_k(\mathbf{A} - z\mathbf{I}, \mathbf{b}) = \mathcal{K}_k(\mathbf{A}, \mathbf{b})$.

Define the residual and error for the iterate $\mathbf{x}_k(z) = \mathbf{Q}_k(\mathbf{T}_k - z\mathbf{I})\mathbf{Q}_k^\top\mathbf{b}$:

$$\mathsf{res}_k(z) = \mathbf{b} - (\mathbf{A} - z\mathbf{I})\mathbf{x}_k(z), \qquad \mathsf{err}_k(z) = (\mathbf{A} - z\mathbf{I})^{-1}\mathbf{b} - \mathbf{x}_k(z).$$

Corollary. With $h_{w,z}(x) = (x - w)/(x - z)$, we have

$$\mathsf{res}_k(z) = c(w,z)\mathsf{res}_k(w), \qquad \mathsf{err}_k(z) = c(w,z)h_{w,z}(\mathbf{A})\mathsf{err}_k(w).$$

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An error bound

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There’s still more!

Generalizations of T. C., Greenbaum, Musco, and Musco 2022:

- Xu and T. C. 2022: block Lanczos algorithm[19]
- Simunec 2023: rational Krylov methods

In Amsel, T. C., Greenbaum, Musco, and Musco 2023, we show that Lanczos-FA is nearly-optimal for certain classes of functions.

We have made progress over the past several years, but the remarkable performance of Lanczos-FA still defies understanding!

[19] Work with an undergrad at UW!

Part II: Designing better algorithms

We can improve existing linear algebra algorithms and design new ones.

- High performance Conjugate Gradient algorithms[20]
- Memory efficient / optimal KSMs[21]
- Krylov-aware low-rank approximation and trace estimation[22]
- Spectrum-adaptive Kernel Polynomial Method[23]

[20] T. C. and Carson 2020.
[21] T. C., Greenbaum, Musco, and Musco 2023.
[22] T. C. and Hallman 2023; Persson, T. C., and Musco 2023.
[23] T. C. 2023.

Low-rank approximation

Since $f(\mathbf{A})$ is dense, we can't store it explicitly if n is big. If we need access to $f(\mathbf{A})$ for some application, we might try to get a low-rank approximation:

$$f(\mathbf{A}) \approx \mathbf{W}\mathbf{X}\mathbf{W}^\top, \text{ where } \mathbf{W} \text{ is } n \times k \text{ and } \mathbf{X} \text{ is } k \times k, \text{ and } k \ll n.$$

KSMs like Lanczos-FA essentially give black-box matrix-vector products with matrix functions: $\mathbf{b} \mapsto f(\mathbf{A})\mathbf{b}$.

This lets us run existing matrix-free low-rank approximation algorithms.

Randomized low-rank approximation

Suppose we wish to obtain a low-rank approximation to a symmetric matrix $\mathbf{B}$.

- Compute a (low-dimension) subspace $\mathbf{K}$
- Project $\mathbf{X}$ onto $\mathbf{K}$

Algorithm 1 Randomized SVD (two-sided)

1: Sample a standard Gaussian $n \times k$ matrix $\mathbf{\Omega}$
2: Form $\mathbf{K} = \mathbf{B\Omega}$ ▷ k matvecs with $\mathbf{B}$
3: Compute $\mathbf{W} = \textsc{orth}(\mathbf{K})$
4: Form $\mathbf{X} = \mathbf{W}^\mathsf{T}\mathbf{BW}$ ▷ k matvecs with $\mathbf{B}$
5: **return** $\mathbf{WXW}^\mathsf{T}$

The result $\mathbf{WXW}^\mathsf{T}$ is a nearly optimal rank k approximation to $\mathbf{B}$.[24]

Algorithms of this flavor are widely used in all areas of computational science.

[24] Halko, Martinsson, and Tropp 2011; Tropp and Webber 2023.

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Key question:

How to do low-rank approximation of matrix functions?

Randomized SVD for matrix functions (black-box version)

Algorithm 3 Low-rank approximation for matrix functions

1: Sample a standard Gaussian $n \times k$ matrix $\mathbf{\Omega}$
2: Form $\mathbf{K} \approx f(\mathbf{A})\mathbf{\Omega}$ from $\mathcal{K}_s(\mathbf{A}, \mathbf{\Omega})$ $\triangleright$ $(s-1)k$ matvces with $\mathbf{A}$
3: Compute $\mathbf{W} = \textsc{orth}(\mathbf{K})$
4: Form $\mathbf{X} \approx \mathbf{W}^\top f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W})$ $\triangleright$ rk matvces with $\mathbf{A}$
5: **return** $\mathbf{W}\mathbf{X}\mathbf{W}^\top \approx \mathbf{W}\mathbf{W}^\top f(\mathbf{A})\mathbf{W}\mathbf{W}^\top$

As we send $s, r \to \infty$, algorithm converges to the exact randomized SVD.

Look into black box

The main costs are matvecs with $\mathbf{A}$:

1. comptuing $\mathbf{K} \approx f(\mathbf{A})\boldsymbol{\Omega}$ from $\mathcal{K}_s(\mathbf{A}, \boldsymbol{\Omega})$ and
2. computing $\mathbf{X} \approx \mathbf{W}^\top f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W})$, where $\mathbf{W} = \textsc{orth}(\mathbf{K})$.

Note that:

- We can instead take: $\mathbf{K} \approx f(\mathbf{A})^q\boldsymbol{\Omega}$ or even $\mathbf{K} \approx [\boldsymbol{\Omega}, f(\mathbf{A})\boldsymbol{\Omega}, \ldots, f(\mathbf{A})^q\boldsymbol{\Omega}]$.
- Best error if we use the whole Krylov subspace: $\mathbf{K} = [\boldsymbol{\Omega}, \mathbf{A}\boldsymbol{\Omega}, \ldots, \mathbf{A}^s\boldsymbol{\Omega}]$.

But wait…

- If $\mathbf{K}$ (and hence $\mathbf{W}$) has more columns, approximating $\mathbf{X} \approx \mathbf{W}^\top f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W})$ is ostensibly more expensive.

Look into black box

The main costs are matvecs with $\mathbf{A}$:

1. comptuing $\mathbf{K} \approx f(\mathbf{A})\mathbf{\Omega}$ from $\mathcal{K}_s(\mathbf{A}, \mathbf{\Omega})$ and
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Krylov subspaces of Krylov subspaces are Krylov subspaces

In general, if $\mathbf{K}$ (and hence $\mathbf{W}$) have sk columns, approximating $\mathbf{X} \approx \mathbf{W}^\top f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W})$ is ostensibly s-times expensive than if $\mathbf{K}$ has k columns.

Theorem. Suppose $\mathbf{Q}_s = [\boldsymbol{\Omega}\ \mathbf{A}\boldsymbol{\Omega} \cdots \mathbf{A}^{s-1}\boldsymbol{\Omega}]$. Then, $\mathcal{K}_{s+r}(\mathbf{A}, \boldsymbol{\Omega}) = \mathcal{K}_{r+1}(\mathbf{A}, \mathbf{Q}_s)$.

Proof.

$$\begin{aligned}
\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{Q}_s) &= \operatorname{range}\left(\begin{bmatrix} \mathbf{Q}_s & \mathbf{A}\mathbf{Q}_s & \cdots & \mathbf{A}^r\mathbf{Q}_s \end{bmatrix}\right) \\
&= \operatorname{range}\left(\begin{bmatrix} \boldsymbol{\Omega} & \mathbf{A}\boldsymbol{\Omega} & \cdots & \mathbf{A}^{s-1}\boldsymbol{\Omega} \\ & \mathbf{A}\boldsymbol{\Omega} & \mathbf{A}^2\boldsymbol{\Omega} & \cdots & \mathbf{A}^{s}\boldsymbol{\Omega} \\ & & \mathbf{A}^r\boldsymbol{\Omega} & \mathbf{A}^{r+1}\boldsymbol{\Omega} & \cdots & \mathbf{A}^{s+r-1}\boldsymbol{\Omega} \end{bmatrix}\right) \\
&= \operatorname{range}\left(\begin{bmatrix} \boldsymbol{\Omega} & \mathbf{A}\boldsymbol{\Omega} & \cdots & \mathbf{A}^{s+r-1}\boldsymbol{\Omega} \end{bmatrix}\right) = \mathcal{K}_{s+r}(\mathbf{A}, \boldsymbol{\Omega}).
\end{aligned}$$

Krylov subspaces of Krylov subspaces are Krylov subspaces

In general, if $\mathbf{K}$ (and hence $\mathbf{W}$) have sk columns, approximating $\mathbf{X} \approx \mathbf{W}^\top f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W})$ is ostensibly s-times expensive than if $\mathbf{K}$ has k columns.

Theorem. Suppose $\mathbf{Q}_s = [\mathbf{\Omega}\ \mathbf{A\Omega}\ \cdots\ \mathbf{A}^{s-1}\mathbf{\Omega}]$. Then, $\mathcal{K}_{s+r}(\mathbf{A}, \mathbf{\Omega}) = \mathcal{K}_{r+1}(\mathbf{A}, \mathbf{Q}_s)$.

Proof.

$$
\begin{aligned}
\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{Q}_s) &= \operatorname{range}\left(\begin{bmatrix} \mathbf{Q}_s & \mathbf{A}\mathbf{Q}_s & \cdots & \mathbf{A}^r\mathbf{Q}_s \end{bmatrix}\right) \\
&= \operatorname{range}\left(\begin{bmatrix} \mathbf{\Omega} & \mathbf{A\Omega} & \cdots & \mathbf{A}^{s-1}\mathbf{\Omega} \\ \mathbf{A\Omega} & \mathbf{A}^2\mathbf{\Omega} & \cdots & \mathbf{A}^{s}\mathbf{\Omega} \\ \mathbf{A}^r\mathbf{\Omega} & \mathbf{A}^{r+1}\mathbf{\Omega} & \cdots & \mathbf{A}^{s+r-1}\mathbf{\Omega} \end{bmatrix}\right) \\
&= \operatorname{range}\left(\begin{bmatrix} \mathbf{\Omega} & \mathbf{A\Omega} & \cdots & \mathbf{A}^{s+r-1}\mathbf{\Omega} \end{bmatrix}\right) = \mathcal{K}_{s+r}(\mathbf{A}, \mathbf{\Omega}).
\end{aligned}
$$

Krylov subspaces of Krylov subspaces are Krylov subspaces

In general, if $\mathbf{K}$ (and hence $\mathbf{W}$) have sk columns, approximating $\mathbf{X} \approx \mathbf{W}^\top f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W})$ is ostensibly s-times expensive than if $\mathbf{K}$ has k columns.

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Proof.

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&= \operatorname{range}\left(\begin{bmatrix} \boldsymbol{\Omega} & \mathbf{A}\boldsymbol{\Omega} & \cdots & \mathbf{A}^{s+r-1}\boldsymbol{\Omega} \end{bmatrix}\right) = \mathcal{K}_{s+r}(\mathbf{A}, \boldsymbol{\Omega}).
\end{aligned}$$

Krylov-aware low-rank approximation[26]

Algorithm 4 Low-rank approximation for matrix functions

1: Sample a standard Gaussian $n \times k$ matrix $\mathbf{\Omega}$
2: Form $\mathbf{K} \approx f(\mathbf{A})\mathbf{\Omega}$ from $\mathcal{K}_s(\mathbf{A}, \mathbf{\Omega})$ $\triangleright$ $(s-1)k$ matvces with $\mathbf{A}$
3: Compute $\mathbf{W} = \textsc{orth}(\mathbf{K})$
4: Form $\mathbf{X} \approx \mathbf{W}^\mathsf{T} f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W})$ $\triangleright$ rk matvces with $\mathbf{A}$
5: **return** $\mathbf{W}\mathbf{X}\mathbf{W}^\mathsf{T} \approx \mathbf{W}\mathbf{W}^\mathsf{T} f(\mathbf{A})\mathbf{W}\mathbf{W}^\mathsf{T}$

Some effort need worked out to implement this efficiently and stably.

Deeper theoretical analysis[25]

[25] Persson, T. C., and Musco 2023.
[26] T. C. and Hallman 2023.

Krylov-aware low-rank approximation[26]

Algorithm 5 Krylov-aware low-rank approximation

1: Sample a standard Gaussian $n \times k$ matrix $\mathbf{\Omega}$
2: Form basis $\mathbf{K}$ for $\mathcal{K}_s(\mathbf{A}, \mathbf{\Omega})$ $\triangleright$ $(s-1)k$ matvces with $\mathbf{A}$
3: Compute $\mathbf{W} = \textsc{orth}(\mathbf{K})$
4: Form $\mathbf{X} \approx \mathbf{W}^\mathsf{T} f(\mathbf{A})\mathbf{W}$ from $\mathcal{K}_{r+1}(\mathbf{A}, \mathbf{W}) = \mathcal{K}_{s+r}(\mathbf{A}, \mathbf{\Omega})$ $\triangleright$ rk matvces with $\mathbf{A}$
5: **return** $\mathbf{W}\mathbf{X}\mathbf{W}^\mathsf{T} \approx \mathbf{W}\mathbf{W}^\mathsf{T} f(\mathbf{A})\mathbf{W}\mathbf{W}^\mathsf{T}$

Some effort need worked out to implement this efficiently and stably.

Deeper theoretical analysis[25]

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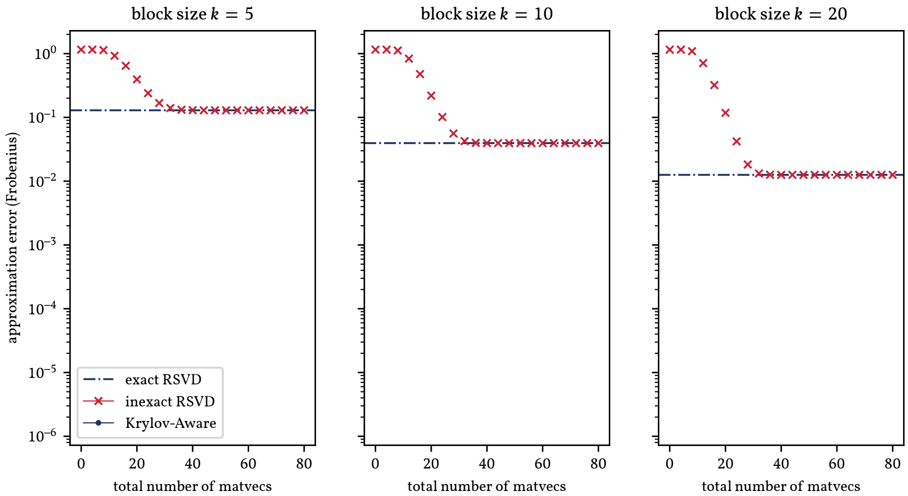
Numerical experiment: exponential function

Setup: $f(x) = \exp(-\beta x)$, $\mathbf{A}$ Hamiltonian of a spin system



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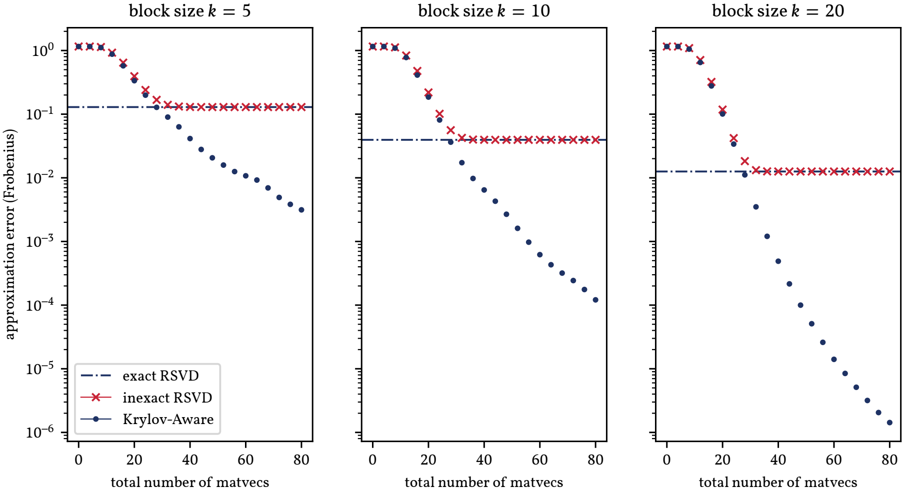


Part III: Advancing basic science

There is a ton of potential for NLA to advance basic science.

- T. C. and Cheng 2022
- T. C. 2023
- T. C., Chen, Li, Nzeuton, Pan, and Wang 2023
- T. C., Trogdon, and Ubaru 2021

Quantum equilibrium thermodynamics

Consider a quantum system consisting of subsystems (s) and (b) with Hamiltonian

$$\mathbf{H} = \bar{\mathbf{H}}_\mathrm{s} + \bar{\mathbf{H}}_\mathrm{b} + \mathbf{H}_\mathrm{sb}, \qquad \bar{\mathbf{H}}_\mathrm{s} = \mathbf{H}_\mathrm{s} \otimes \mathbf{I}_\mathrm{b}, \quad \bar{\mathbf{H}}_\mathrm{b} = \mathbf{I}_\mathrm{s} \otimes \mathbf{H}_\mathrm{b}. \tag{1}$$

In thermal equilibrium at interver temperature β, the state of the system is described by a density matrix

$$\boldsymbol{\rho}_\mathrm{t}(\beta) = \frac{\exp(-\beta\mathbf{H})}{Z_\mathrm{t}(\beta)}, \qquad Z_\mathrm{t}(\beta) = \mathrm{tr}(\exp(-\beta\mathbf{H}); \tag{2}$$

The denisty matrix for subsystem (s) is given by

$$\boldsymbol{\rho}^*(\beta) = \mathrm{tr}_\mathrm{b}(\boldsymbol{\rho}_\mathrm{t}(\beta)) = \frac{\mathrm{tr}_\mathrm{b}(\exp(-\beta\mathbf{H}))}{\mathrm{tr}(\exp(-\beta\mathbf{H}))}, \tag{3}$$

where $\mathrm{tr}_b(\,\cdot\,)$ is the *partial trace* over subsystem (b).[27]

[27] Campisi, Zueco, and Talkner 2010; Ingold, Hänggi, and Talkner 2009; Talkner and Hänggi 2020.

von Neumann entropy of Heisenberg spin chains

The von Neumann entropy $-\mathrm{tr}(\boldsymbol{\rho}^*(\beta)\ln(\boldsymbol{\rho}^*(\beta)))$ is a measure of the entanglement betweeen subsystems (s) and (b).

Understanding the von Neumann entropy for a range of a system with Hamiltonian $\mathbf{H}(\theta)$ at a range of parameter values θ and inverse temperatures β is of interest.

We will consider a special case

$$\mathbf{H} = \sum_{i,j}\left[J^{\mathrm{x}}_{i,j}\boldsymbol{\sigma}^{\mathrm{x}}_i\boldsymbol{\sigma}^{\mathrm{x}}_j + J^{\mathrm{y}}_{i,j}\boldsymbol{\sigma}^{\mathrm{y}}_i\boldsymbol{\sigma}^{\mathrm{y}}_j + J^{\mathrm{z}}_{i,j}\boldsymbol{\sigma}^{\mathrm{z}}_i\boldsymbol{\sigma}^{\mathrm{z}}_j\right] + \frac{h}{2}\sum_{i=1}^{N}\boldsymbol{\sigma}^{\mathrm{z}}_i.$$

where h is the magnetic field strength.

Subsystem (s) corresponds to $i = 1, 2$ and subsystem (b) corresponds to the rest of the spins.

Key question:

How to compute reduced density matrices numerically?

A starting point: stochastic trace estimation

If $\mathbf{b}$ is a standard Gaussian random vector:

$$\mathbb{E}[\mathbf{b}^\mathsf{T} f(\mathbf{A})\mathbf{b}] = \operatorname{tr}(f(\mathbf{A})), \qquad \mathbb{V}[\mathbf{b}^\mathsf{T} f(\mathbf{A})\mathbf{b}] = 2\|f(\mathbf{A})\|_\mathsf{F}^2.$$

It's standard to use a KSM to approximate products $\mathbf{b} \mapsto \mathbf{b}^\mathsf{T} f(\mathbf{A})\mathbf{b}$.

Lots of work balancing the cost of the KSM with the variance of the estimator[28].

[28] Han, Malioutov, Avron, and Shin 2017; Ubaru, Chen, and Saad 2017; T. C., Trogdon, and Ubaru 2021; T. C., Trogdon, and Ubaru 2022; Braverman, Krishnan, and Musco 2022.

Partial traces

Suppose $\mathbf{A}$ is a $d_\mathrm{s} d_\mathrm{b} \times d_\mathrm{s} d_\mathrm{b}$ matrtix partitioned as:

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{1,1} & \mathbf{A}_{1,2} & \cdots & \mathbf{A}_{1,d_\mathrm{s}} \\ \mathbf{A}_{2,1} & \mathbf{A}_{2,2} & \cdots & \mathbf{A}_{2,d_\mathrm{s}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}_{d_\mathrm{s},1} & \mathbf{A}_{d_\mathrm{s},2} & \cdots & \mathbf{A}_{d_\mathrm{s},d_\mathrm{s}} \end{bmatrix},$$

Partial traces

Then the partial trace (wrt. this partitioning) is defined as:

$$\mathrm{tr}_{\mathrm{b}}(\mathbf{A}) = \begin{bmatrix} \mathrm{tr}(\mathbf{A}_{1,1}) & \mathrm{tr}(\mathbf{A}_{1,2}) & \cdots & \mathrm{tr}(\mathbf{A}_{1,d_{\mathrm{s}}}) \\ \mathrm{tr}(\mathbf{A}_{2,1}) & \mathrm{tr}(\mathbf{A}_{2,2}) & \cdots & \mathrm{tr}(\mathbf{A}_{2,d_{\mathrm{s}}}) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{tr}(\mathbf{A}_{d_{\mathrm{s}},1}) & \mathrm{tr}(\mathbf{A}_{d_{\mathrm{s}},2}) & \cdots & \mathrm{tr}(\mathbf{A}_{d_{\mathrm{s}},d_{\mathrm{s}}}) \end{bmatrix}.$$

An algorithm for partial traces[29]

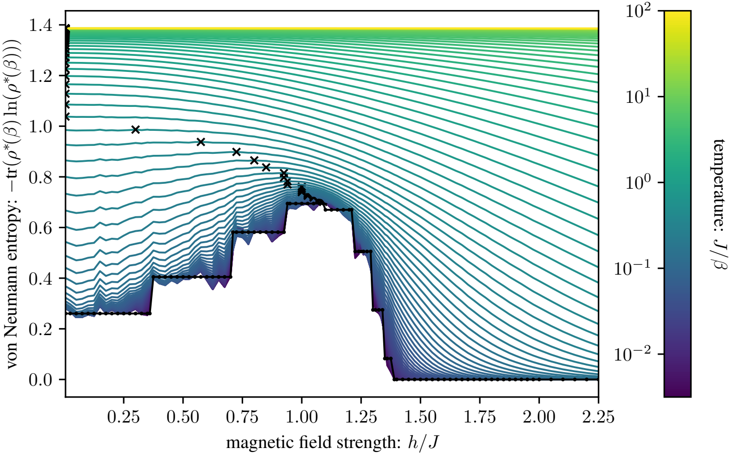
We can use a randomized estimator:

$$(\mathbf{I}_{d_\mathrm{s}} \otimes \mathbf{b})^\top \mathbf{A} (\mathbf{I}_{d_\mathrm{s}} \otimes \mathbf{b}) = \begin{bmatrix} \mathbf{b}^\top \mathbf{A}_{1,1} \mathbf{b} & \mathbf{b}^\top \mathbf{A}_{1,2} \mathbf{b} & \cdots & \mathbf{b}^\top \mathbf{A}_{1,d_\mathrm{s}} \mathbf{b} \\ \mathbf{b}^\top \mathbf{A}_{2,1} \mathbf{b} & \mathbf{b}^\top \mathbf{A}_{2,2} \mathbf{b} & \cdots & \mathbf{b}^\top \mathbf{A}_{2,d_\mathrm{s}} \mathbf{b} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{b}^\top \mathbf{A}_{d_\mathrm{s},1} \mathbf{b} & \mathbf{b}^\top \mathbf{A}_{d_\mathrm{s},2} \mathbf{b} & \cdots & \mathbf{b}^\top \mathbf{A}_{d_\mathrm{s},d_\mathrm{s}} \mathbf{b} \end{bmatrix}.$$

Then use a KSM to approximate products with $\mathbf{A} = f(\mathbf{H})$.

[29] T. C. and Cheng 2022.

von Neumann entropy phase plot[30]



[30] T. C. and Cheng 2022.

Partial trace estimator: variance reduction

For any matrix $\widetilde{\mathbf{A}}$,

$$\mathrm{tr}_b(\mathbf{A}) = \mathrm{tr}_b(\widetilde{\mathbf{A}}) + \mathrm{tr}_b(\mathbf{A} - \widetilde{\mathbf{A}}).$$

So we might try to use the estimator

$$\mathrm{tr}_b(\mathbf{A}) \approx \mathrm{tr}_b(\widetilde{\mathbf{A}}) + \widehat{\mathrm{tr}}_b^{\,m}(\mathbf{A} - \widetilde{\mathbf{A}}).$$

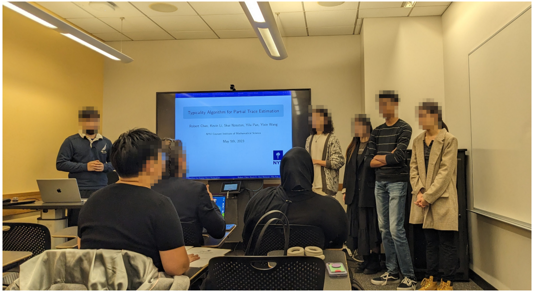
which will have reduced variance if $\|\mathbf{A} - \widetilde{\mathbf{A}}\|_\mathsf{F}^2 \ll \|\mathbf{A}\|_\mathsf{F}^2$.

This residual trick is widely used in regular trace estimation.[31]

But there are a number of numerical issues with generalizing to partial traces of matrix functions.

[31] Girard 1987; Weiße, Wellein, Alvermann, and Fehske 2006; Lin 2016; Morita and Tohyama 2020; Meyer, Musco, Musco, and Woodruff 2021.

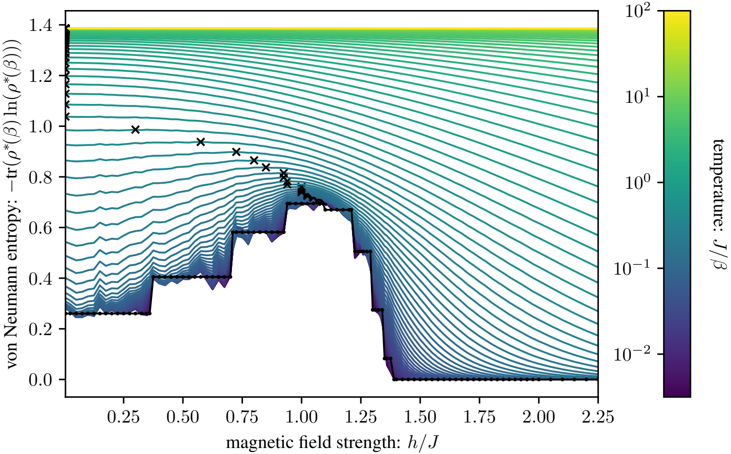
Student involvement



students were a major part of this project, and were able to:

- write and receive grant for research funding
- present at NYU undergrad conference, SIAM NY-NJ-PA annual meeting, Alan Edelman's birthday conference
- perform numerical experiments on NYU's Greene supercomputer

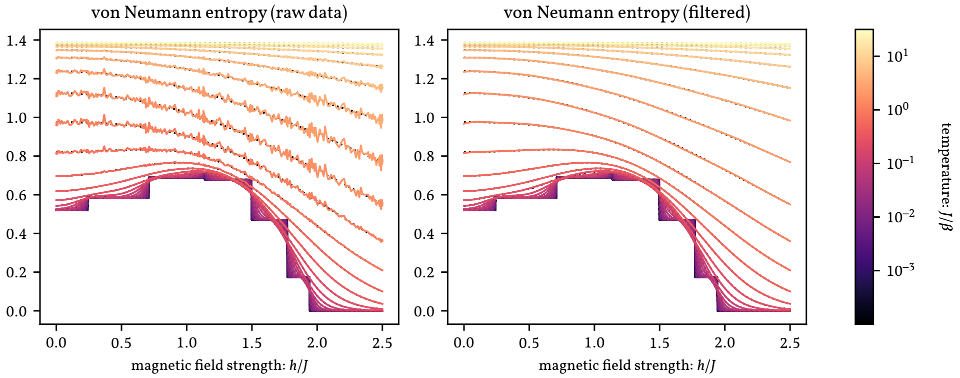
von Neumann entropy phase plot[32]



[32]T. C. and Cheng 2022.

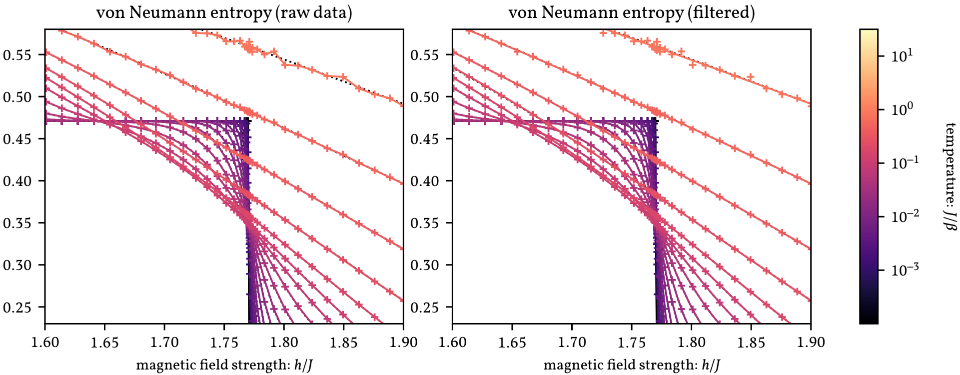
von Neumann entropy phase plot: improved algorithm[33]

We can compute these phase plots, which are more accurate at low temperature, orders of magnitude faster.



[33] T. C., Chen, Li, Nzeuton, Pan, and Wang 2023.

von Neumann entropy phase plot: improved algorithm[34] (cropped)



[34] T. C., Chen, Li, Nzeuton, Pan, and Wang 2023.

My research program

Focus: design and analysis of practically fast and theoretically justified (randomized) algorithms for fundamental linear algebra tasks

Goal: develop tools to support the advancement of knowledge in current scientific applications

Mode: collaboration with a range of fields, and involvement and training of (minority) students

Hope: provide conceptually simple insights into key problems

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