Randomized matrix-free quadrature

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`chen.pw/slides.pdf`

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 $f(\mathbf{A})$ is defined as

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

Trace estimation

We will look at some algorithms for estimating

$$\operatorname{tr}(f(\mathbf{A})) = f(\lambda_1) + \cdots + f(\lambda_n).$$

These algorithms use:

- Stochastic trace estimation
- Krylov subspace methods

A number of widely used algorithms[1] fall into this class, but it's still an active area of algorithm development[2]

[1] Skilling 1989; Silver and Röder 1994; Silver, Roeder, Voter, and Kress 1996; Weiße, Wellein, Alvermann, and Fehske 2006; Bai, Fahey, and Golub 1996.

[2] Lin 2016; Gambhir, Stathopoulos, and Orginos 2017; Saibaba, Alexanderian, and Ipsen 2017; Morita and Tohyama 2020; Meyer, Musco, Musco, and Woodruff 2021; Li and Zhu 2021; Chen and Hallman 2022; Persson and Kressner 2022.

Direct methods

Can compute $f(\mathbf{A})$ via eigendecomposition of $\mathbf{A}$. However,

- this is slow: n^3 computation
- intractable storage costs: even if $\mathbf{A}$ is sparse, $f(\mathbf{A})$ typically is not
  - for $n = 2^{20}$, a $n \times n$ matrix of 64bit numbers requires 8.8 terrabytes

However, matrix products with $\mathbf{A}$ might be tractable.

Integral representation

We can write the trace as an integral

$$\operatorname{tr}(f(\mathbf{A})) = n \int f \mathrm{d}\Phi,$$

where the cumulative empirical spectral measure (CESM) Φ is

$$\Phi(x) := \sum_{i=1}^{n} \frac{1}{n} \mathbb{1}(\lambda_i \leq x) = \operatorname{tr}(\mathbb{1}(\mathbf{A} \leq x)).$$

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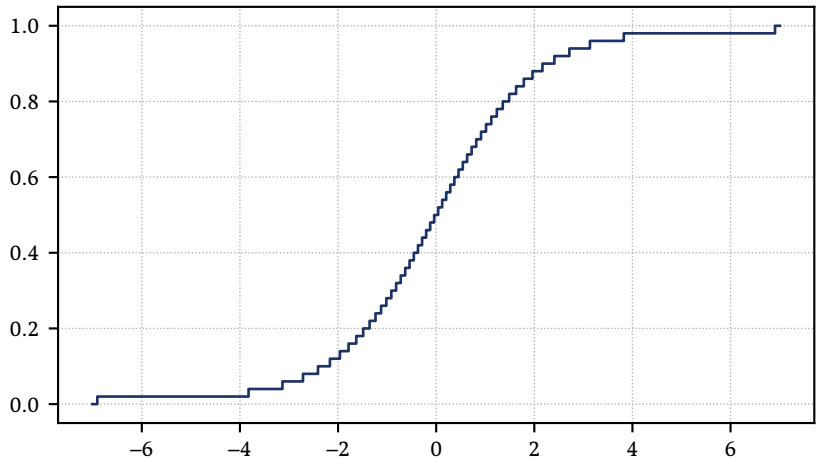
trace approximation $\leftrightarrow$ CESM approximation

Approximating the CESM



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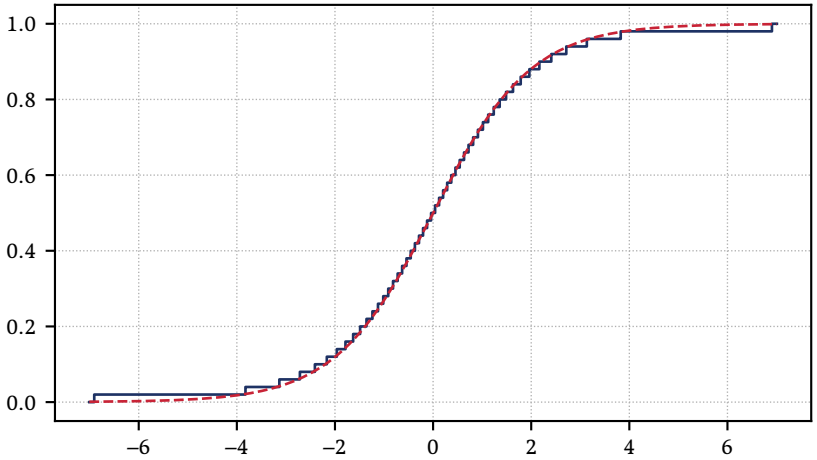

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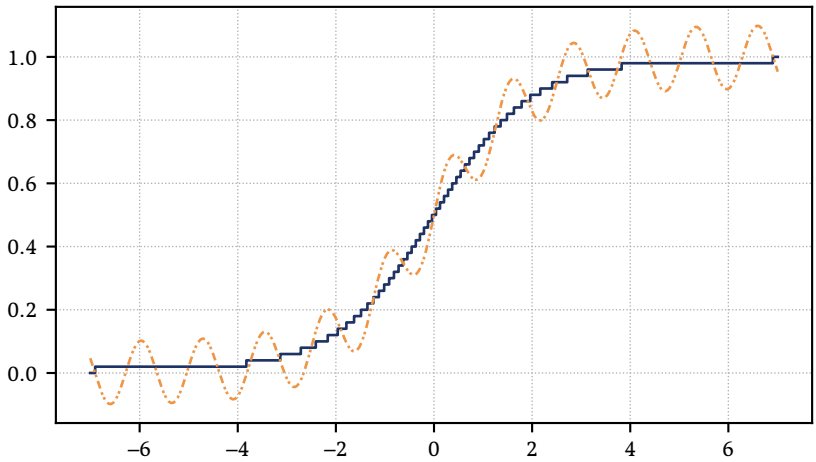

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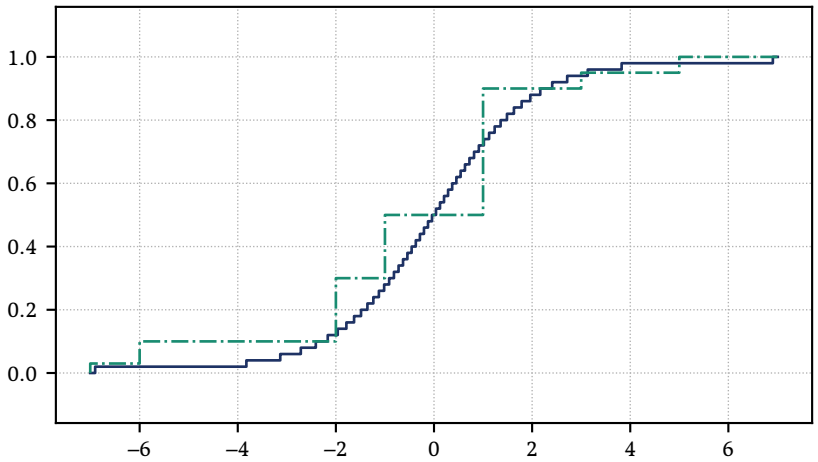

Global approximation to CESM

Goal: Get a coarse approximation to Φ such that integrals are nearly preserved

Idea: Compute quadrature rule for Φ

- $\int x^k \mathrm{d}\Phi = \mathrm{tr}(\mathbf{A}^k)$

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Idea: Compute quadrature rule for Φ

- $\int x^k d\Phi = \mathrm{tr}(\mathbf{A}^k)$

Problem: We can't compute integrals against Φ without computing traces

Idea: stochastic trace estimation

Stochastic trace estimation

It's well known that when $\mathbf{v}$ is such that $\mathbb{E}[\mathbf{v}\mathbf{v}^\mathsf{T}] = n^{-1}\mathbf{I}$, then

$$n\mathbb{E}[\mathbf{v}^\mathsf{T}\mathbf{B}\mathbf{v}] = \operatorname{tr}(\mathbf{B}).$$

We call an estimator $\mathbf{v}^\mathsf{T}\mathbf{B}\mathbf{v}$ a quadratic trace estimator.

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- Often attributed to Hutchinson 1989
- Earlier work by Girard 1987 and Skilling 1989
- Use of random states as algorithmic tool since at least 1970s[3]
- Morally equivalent to quantum typicality from late 1920s[4]

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The weighted CESM

We can write quadratic forms as an integral

$$\mathbf{v}^\top f(\mathbf{A})\mathbf{v} = \int f \mathrm{d}\Psi$$

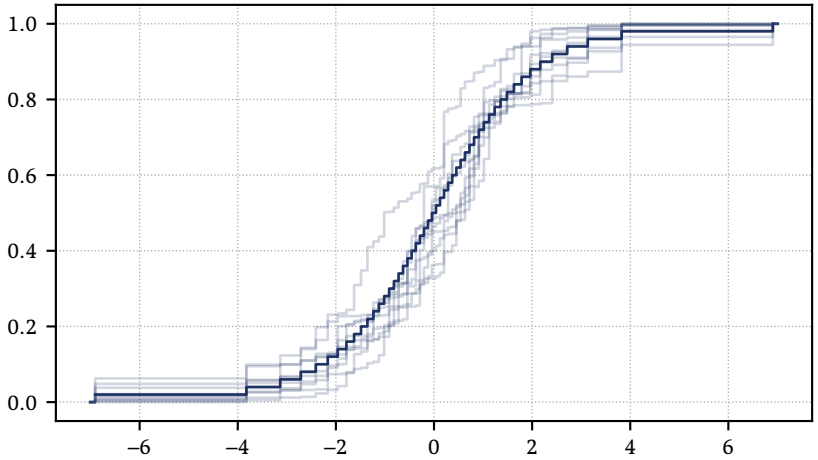
where

$$\Psi(x) := \sum_{i=1}^{n} |\mathbf{v}^\top \mathbf{u}_i|^2 \mathbb{1}(\lambda_i \leq x).$$

If $\mathbf{v}$ is an isotropic random vector,

$$\mathbb{E}[\Psi(x)] = \sum_{i=1}^{n} \mathbb{E}[|\mathbf{v}^\top \mathbf{u}_i|^2] \mathbb{1}(\lambda_i \leq x) = \sum_{i=1}^{n} \frac{1}{n} \mathbb{1}(\lambda_i \leq x) = \Phi(x).$$

The weighted CESM



Polynomial quadrature

Let $[f]_s^{\circ p}$ be a degree s polynomial approximation to f and $[\Psi]_s^{\circ q}$ the induced quadrature approximation to Ψ defined by

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Given a distribution function μ, let $\{p_i\}_{i=0}^{\infty}$ be the (normalized) orthogonal polynomials. Define moments,

$$m_i := \int p_i \mathrm{d}\Psi = \mathbf{v}^{\mathsf{T}} p_i(\mathbf{A})\mathbf{v}.$$

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If $[f]_s^{\circ \mathrm{p}} = c_0 p_0 + \cdots + c_s p_s$, then

$$\int f \mathrm{d}[\Psi]_s^{\circ \mathrm{q}} = \int \sum_{i=0}^{s} c_i p_i \mathrm{d}\Psi = \sum_{i=0}^{s} c_i \int p_i \mathrm{d}\Psi = \sum_{i=0}^{s} c_i m_i.$$

Algorithms

So, we get an algorithm:

$$\operatorname{tr}(f(\mathbf{A})) \approx \int f \mathrm{d}\langle [\Psi_i]_s^{\circ \mathrm{q}} \rangle = \frac{1}{n_{\mathrm{v}}} \sum_{i=1}^{n} \int f \mathrm{d}[\Psi_i]_s^{\circ \mathrm{q}}.$$

Different choices of $[f]_s^{\circ \mathrm{p}}$ correspond to different algorithms:

- Kernel Polynomial Method: damped Chebyshev approximation
- Stochastic Lanczos Quadrature: Interpolation at zeros of orthogonal polynomials of Ψ

Requires construction of Krylov subspaces

$$\operatorname{span}\{\mathbf{v}_i, \mathbf{A}\mathbf{v}_i, \dots, \mathbf{A}^k \mathbf{v}_i\}.$$

A unified framework[5]

Traditionally, algorithms like KPM would be implemented using an explicit Chebyshev recurrence

[5]Chen, Trogdon, and Ubaru 2022.

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A key observation: we could instead use the output of Lanczos

- allows a posteriori choice of hyperparameters
  - more stable implementations
  - can cheaply try different quadrature approximations
- allows simultaneous theoretical analysis of algorithms
- allows tradeoffs between algorithms to be more clearly understood

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Finite precision arithmetic

It's well know that the Lanczos algorithm is unstable, so people are afraid of using it without reorthogonalization[6] (expensive)

[6] Jaklič and Prelovšek 1994; Silver, Roeder, Voter, and Kress 1996; Aichhorn, Daghofer, Evertz, and Linden 2003; Weiße, Wellein, Alvermann, and Fehske 2006; Ubaru, Chen, and Saad 2017; Granziol, Wan, and Garipov 2019.

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However, for certain tasks, the algorithm is actually backwards stable in a certain (useful sense)[7]even without reorthogonalization

- for these problems, "instability" is actually just an ill-conditioned task
- i.e. computing certain quantities is inherently hard, but we don't really need to compute them accurately to get what we want

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Moreover, direct implementations of alternate algorithms like KPM are stable given good hyper-parameter choice, but exponentially unstable otherwise.

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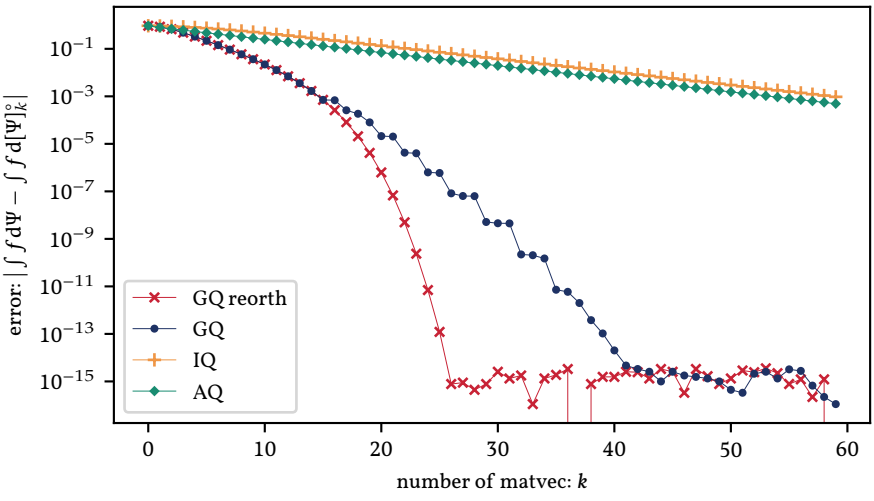
Example: Runge function



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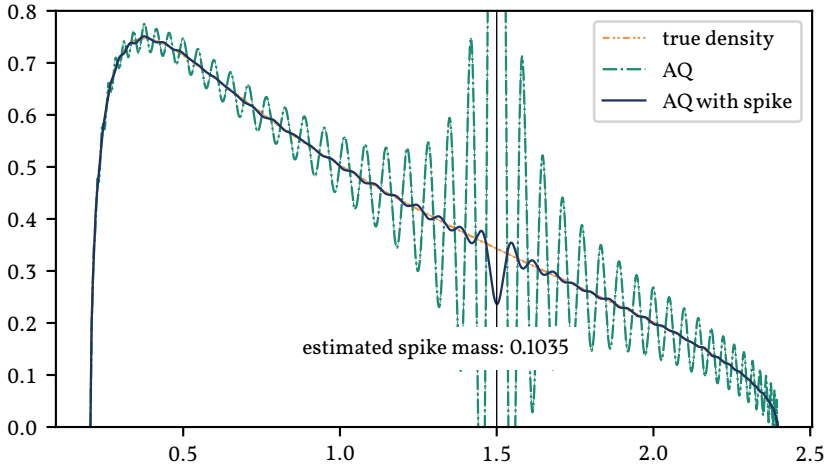

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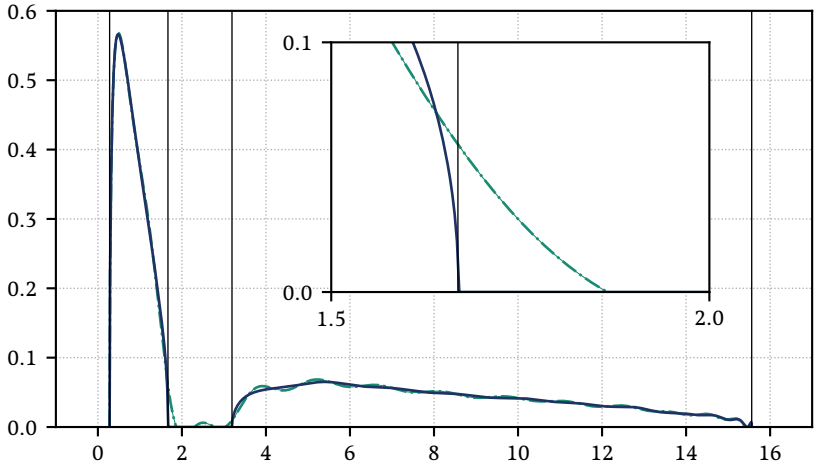

A simple analysis of the variance (for Gaussians) implies

$$|\mathbf{B} - \langle \mathbf{v}_\ell^\mathsf{T} \mathbf{B} \mathbf{v}_\ell \rangle| \sim \|\mathbf{B}\|_\mathsf{F} (n_\mathrm{v})^{-1/2}.$$

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More refined concentration inequalities

$$\mathbb{P}\big[\, |\mathbf{B} - \langle \mathbf{v}_\ell^\top \mathbf{B} \mathbf{v}_\ell \rangle| > \epsilon \,\big] \leq \delta.$$

– Applied Math/CS (iid entries): early analyses[8], refined analyses[9]

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- Applied Math/CS (iid entries): early analyses[8], refined analyses[9]
- Physics (uniform from hypersphere): Chebyshev[10], sub-Gaussian[11](via Lèvy's Lemma), refined bounds for practical dimensions[12]

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Low rank approximation

We can always decompose

$$\operatorname{tr}(\mathbf{B}) = \operatorname{tr}(\widehat{\mathbf{B}}) + \operatorname{tr}(\widetilde{\mathbf{B}}), \qquad \text{where} \qquad \widetilde{\mathbf{B}} := \mathbf{B} - \widehat{\mathbf{B}}.$$

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So, let's output

$$\operatorname{tr}(\mathbf{B}) = \operatorname{tr}(\widehat{\mathbf{B}}) + \langle \boldsymbol{\psi}_\ell^\mathsf{T} \widetilde{\mathbf{B}} \boldsymbol{\psi}_\ell \rangle = \operatorname{tr}(\widehat{\mathbf{B}}) + \frac{1}{m} \operatorname{tr}(\boldsymbol{\Psi}^\mathsf{T} \widetilde{\mathbf{B}} \boldsymbol{\Psi})$$

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This is beneficial if:

- $\operatorname{tr}(\widehat{\mathbf{B}})$ can be computed efficiently, and
- the variance of $\operatorname{tr}(\boldsymbol{\Psi}^\mathsf{T} \widetilde{\mathbf{B}} \boldsymbol{\Psi})$ is reduced compared to $\operatorname{tr}(\boldsymbol{\Psi}^\mathsf{T} \mathbf{B} \boldsymbol{\Psi})$

A lot of recent work[13] uses this idea to varying extent

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Hutch++[14]

Take $\widehat{\mathbf{B}}$ as low rank approximation $\widehat{\mathbf{B}} = \mathbf{Q}\mathbf{Q}^\top\mathbf{B}\mathbf{Q}\mathbf{Q}^\top$

- Compute $\mathbf{Q}$ by sketching: $\mathbf{Q} = \textsc{orth}(\mathbf{B}\mathbf{\Omega})$ where $\mathbf{\Omega}$ is $n \times b$ random matrix

Simplify a bit:

- $\operatorname{tr}(\widehat{\mathbf{B}}) = \operatorname{tr}(\mathbf{Q}\mathbf{Q}^\top\mathbf{B}\mathbf{Q}\mathbf{Q}^\top) = \operatorname{tr}(\mathbf{Q}^\top\mathbf{B}\mathbf{Q})$
- $\operatorname{tr}(\widetilde{\mathbf{B}}) = \operatorname{tr}((\mathbf{I} - \mathbf{Q}\mathbf{Q}^\top)\mathbf{B}(\mathbf{I} - \mathbf{Q}\mathbf{Q}^\top))$
- $\operatorname{tr}(\mathbf{\Psi}^\top\widetilde{\mathbf{B}}\mathbf{\Psi}) = \operatorname{tr}(\mathbf{Y}^\top\mathbf{B}\mathbf{Y})$, where $\mathbf{Y} = (\mathbf{I} - \mathbf{Q}\mathbf{Q}^\top)\mathbf{\Psi}$.

Number of matvecs with $\mathbf{B}$ is: $2b + m$, and if we set $b = m$, can get scaling

$$\text{accuracy} \sim (\#\ \text{matvecs})^{-1}$$

[14] Meyer, Musco, Musco, and Woodruff 2021.

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$$\text{span}\{\mathbf{\Omega}, \mathbf{A\Omega}, \dots, \mathbf{A}^q\mathbf{\Omega}\}$$

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Naive Hutch++ would take $\mathbf{Q} \in \mathbb{R}^{n \times b}$ as a basis for our approximation to $f(\mathbf{A})\mathbf{\Omega}$.

Instead, take $\mathbf{Q} \in \mathbb{R}^{n \times (q+1)b}$ as basis for the whole Krylov subspace

- Same number of matvecs with $\mathbf{A}$, but (much) larger search space..

Efficient approximation of $f(\mathbf{A})\mathbf{Q}$

Regardless of our choice of $\mathbf{Q}$, the next step is approximating $f(\mathbf{A})\mathbf{Q}$.

Suppose we use n iterations of Lanczos. Then we need to construct

$$\text{span}\{\mathbf{Q}, \mathbf{AQ}, \dots, \mathbf{A}^n\mathbf{Q}\}$$

If $\mathbf{Q}$ has $(q+1)b$ instead of b columns, this ostensibly requires $n(q+1)b$ matvecs with $\mathbf{A}$ instead of nb required by a naive implementation.

Efficient approximation of $f(\mathbf{A})\mathbf{Q}$

Recall, $\mathbf{Q}$ is a basis for

$$\text{span}\{\mathbf{\Omega}, \mathbf{A\Omega}, \dots, \mathbf{A}^q\mathbf{\Omega}\}.$$

Thus, the columns of $\mathbf{A}^j\mathbf{Q}$ span

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So actually,

$$\text{span}\{\mathbf{Q}, \mathbf{AQ}, \dots, \mathbf{A}^n\mathbf{Q}\} = \text{span}\{\mathbf{\Omega}, \mathbf{A\Omega}, \dots, \mathbf{A}^{q+n}\mathbf{\Omega}\}.$$

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In other words, to approximate $f(\mathbf{A})\mathbf{Q}$ we only need nb matrix-vector products!

Krylov aware stochastic trace estimation[15]

This "Krylov aware" idea is simple, but provides many benefits.

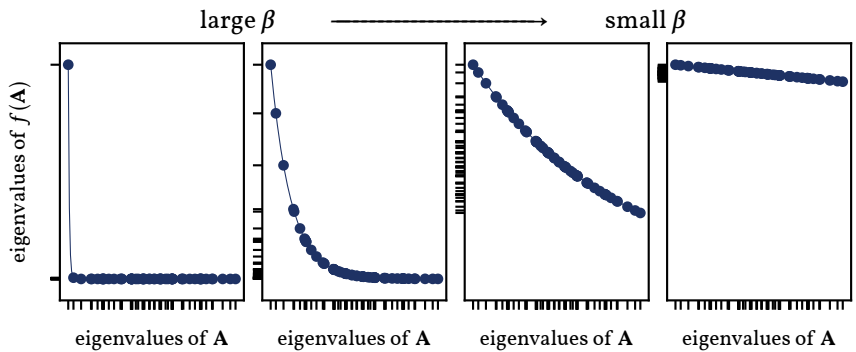
- use a (much) larger projection space "for free"
- algorithm is now agnostic to f
  - we can easily compute approximations to $\operatorname{tr}(f(\mathbf{A}))$ for multiple f without additional matrix products with $\mathbf{A}$.
  - in particular, the approximation we get is a quadrature approximation for Ψ

[15] Chen and Hallman 2022.

Example: equilibrium thermodynamics of quantum spin systems

In quantum physics, we often wish to compute $\mathrm{tr}(f(\mathbf{A})) = \mathrm{tr}(\exp(-\beta\mathbf{A}))$ for all $\beta > 0$.

- if $\beta = \infty$ (zero temperature), then we only need ground state(s)
- if $\beta = 0$ (high temperature), then quadratic trace estimation works very well
- for intermediate beta, we might expect low-rank approaches to work well



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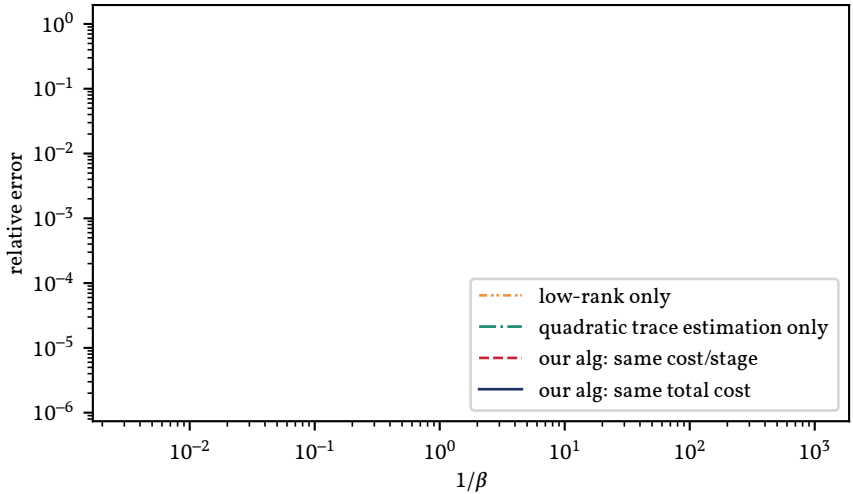
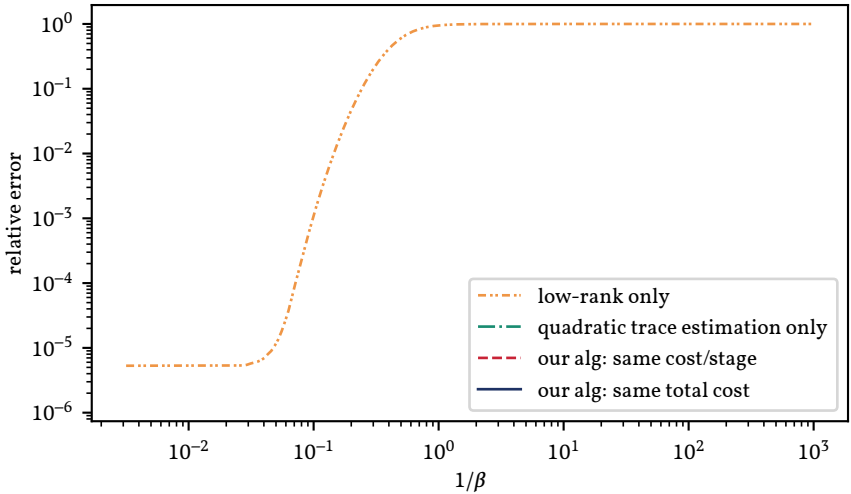
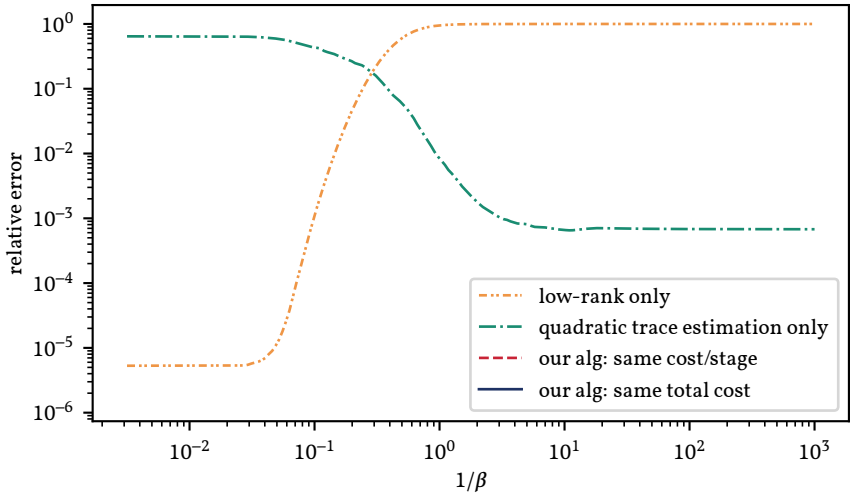


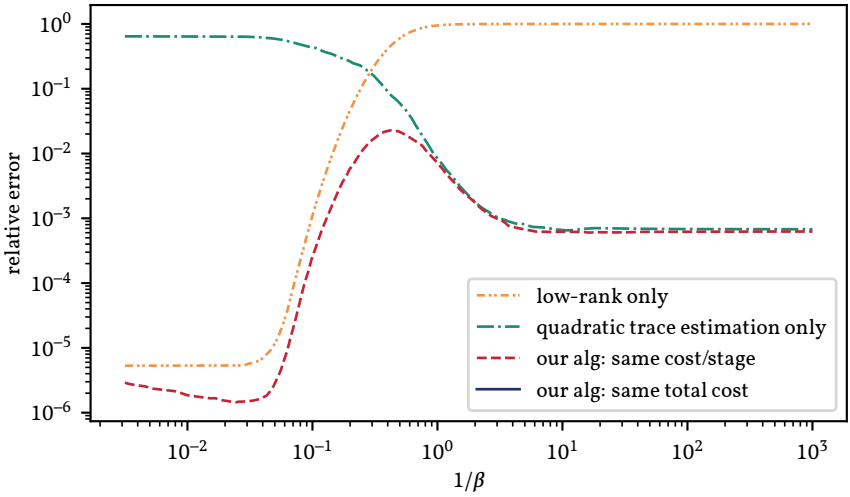
Example: quantum spin systems; $\mathrm{tr}(\exp(-\beta \mathbf{A}))$



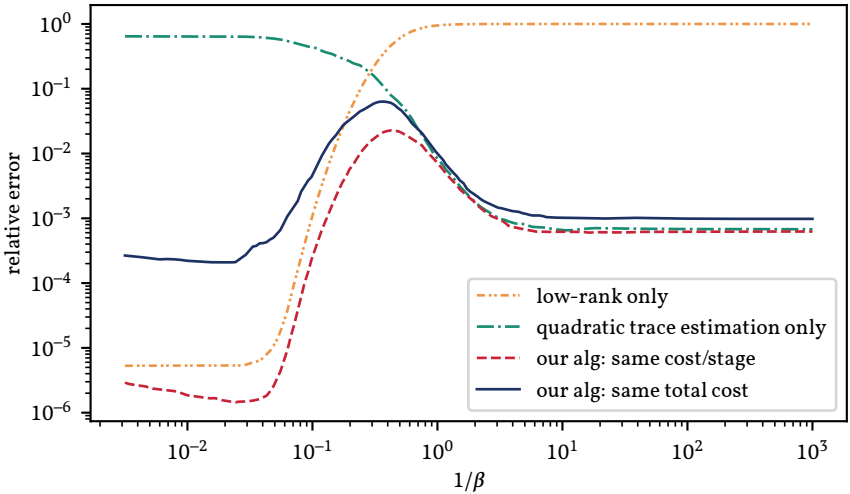
Example: quantum spin systems; $\mathrm{tr}(\exp(-\beta \mathbf{A}))$



Example: quantum spin systems; $\mathrm{tr}(\exp(-\beta \mathbf{A}))$



Example: quantum spin systems; $\mathrm{tr}(\exp(-\beta \mathbf{A}))$



Variants

We also have a number of modifications to make this idea more practical:

- Using the information in the space $\text{span}\{\mathbf{\Omega}, \mathbf{A\Omega}, \dots, \mathbf{A}^{q+n}\mathbf{\Omega}$ we can approximate

$$\|(\mathbf{I} - \mathbf{QQ}^\mathsf{T} f(\mathbf{A})(\mathbf{I} - \mathbf{QQ}^\mathsf{T})\|$$

  in order to determine a good value of q.
- If memory or reorthogonalization costs are an issue, we can use restarting, and pick $\mathbf{Q} \subset \text{span}\{\mathbf{\Omega}, \mathbf{A\Omega}, \dots, \mathbf{A}^{q+1}\mathbf{\Omega}\}$
  - e.g. $\mathbf{Q} = \mathbf{A}^{q+1}\mathbf{\Omega}$

Future work

- $\mathrm{tr}(\exp(-\beta(\mathbf{A} + h\mathbf{B})))$ for all $\beta > 0$, $h \in [-h_0, h_0]$.
- generalize low-rank algorithms to partial traces
- better understanding of stability
- lower bounds in matrix-vector query models
- better relationships between physics, applied math, and CS

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