Concentration in the Lanczos algorithm

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Joint work with Tom Trogdon

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Introduction

We often want to evaluate $\mathbf{v}^\top f(\mathbf{A})\mathbf{v}$ where $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ is a $n \times n$ symmetric matrix, $\mathbf{v}$ is an arbitrary vector and f is a scalar function so that $f(\mathbf{A})$ is

$$f(\mathbf{A}) := \mathbf{U}f(\mathbf{\Lambda})\mathbf{U}^\top.$$

For instance, such expressions might arise in randomized algorithms for spectral sums since whenever $\mathbb{E}[\mathbf{v}\mathbf{v}^\top] = \mathbf{I}$ we have

$$\mathbb{E}[\mathbf{v}^\top f(\mathbf{A})\mathbf{v}] = \mathrm{tr}(f(\mathbf{A})).$$

Approximation via Lanczos

A common approach to approximate $\mathbf{v}^\top f(\mathbf{A})\mathbf{v}$ when $\mathbf{A}$ is symmetric is via the Lanczos algorithm. Lanczos outputs an orthonormal basis $\mathbf{Q}$ for Krylov subspace and a tridiagonal matrix $\mathbf{T}$ giving the polynomial recurrence needed to construct this basis.

The Lanczos approximation is then defined as

$$\mathbf{v}^\top \mathbf{Q} f(\mathbf{T}) \mathbf{Q}^\top \mathbf{v} = \hat{\mathbf{e}}^\top f(\mathbf{T}) \hat{\mathbf{e}}$$

where $\hat{\mathbf{e}} = [1, 0, \dots, 0]^\top$.

Empirical spectral measure/weighted empirical spectral measure

We say $\mu : \mathbb{R} \to [0,1]$ is a probability distribution function if μ is weakly increasing, right continuous, and $\lim_{x\to-\infty} \mu(x) = 0$ and $\lim_{x\to\infty} \mu(x) = 1$.

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Empirical spectral measure (ESM):

$$\Phi[\mathbf{A}](x) = \sum_{i=1}^{n} \frac{1}{n} \mathbb{1}[\lambda_i \leq x]$$

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Weighted ESM:

$$\Psi[\mathbf{A}, \mathbf{v}](x) = \sum_{i=1}^{n} ([\mathbf{U}]_{:,i}^{\mathsf{T}} \mathbf{v})^2 \mathbb{1}[\lambda_i \leq x] = \mathbf{v}^{\mathsf{T}} \mathbb{1}[\mathbf{A} \leq x] \mathbf{v}$$

Gaussian quadrature

Gaussian quadrature for μ defined as

$$[\mu]_k^{\mathrm{gq}}(x) = \sum_{i=1}^{k} \omega_i \mathbb{1}[\theta_i \leq x]$$

where $\{\omega_i\}_{i=1}^k$ and $\{\theta_i\}_{i=1}^k$ are chosen so that μ and $[\mu]_k^{\mathrm{gq}}$ share moments through degree $2k-1$.

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The k-point Gaussian quadrature rule $[\mu]_k^{\mathrm{gq}}$ for Ψ is obtained by constructing an interpolatory quadrature rule at the roots $\{\theta_i\}_{i=1}^k$ of the degree k orthogonal polynomial p_k of μ.

Gaussian quadrature via Lanczos

If $\mu = \Psi[\mathbf{A}, \mathbf{v}]$ then $\mathbf{T}$ from Lanczos gives upper left $k \times k$ block of Jacobi matrix for orthogonal polynomials.[1] Thus,

- Nodes are eigenvalues of $\mathbf{T}$
- Weights are squares of first components of eigenvectors of $\mathbf{T}$

Thus,

$$[\Psi[\mathbf{A}, \mathbf{v}]]_k^{\mathrm{gq}} = \Psi[\mathbf{T}, \hat{\mathbf{e}}]$$

The Lanczos approximation to the weighted CESM is itself a probability distribution function.

[1] Golub and Meurant 2009.

Analysis of algorithms

Given a problem $\mathcal{P} : \mathbb{R}^N \to \mathbb{R}^M$ (e.g. solving a linear system) and an algorithm $\mathcal{A} : \mathbb{R}^N \to \mathbb{R}^M$ to compute a solution to the problem (e.g. Conjugate Gradient), how do we study the performance of the algorithm?

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- Worst case analysis
  - how bad can the algorithm be on the "hardest possible" input?
- Smoothed analysis
  - How "rare" are these hard inputs?
- Average case behavior
  - How does the algorithm behave on a "typical" problem?
- Numerical stability
  - How does our algorithm behave in finite precision arithmetic?

Average case behavior of the Lanczos method

We will run the Lanczos algorithm on $\mathbf{A}, \hat{\mathbf{e}}$ for k iterations to construct a Gaussian quadrature rule for $\Psi[\mathbf{A}, \hat{\mathbf{e}}]$ where $\mathbf{A} \sim \mathrm{GOE}(n)$ and $\hat{\mathbf{e}} = [1, 0, \ldots, 0]^\top$.

To generate $\mathbf{A}$ can generate $\mathbf{X}$ with i.i.d. standard normal entries and then define

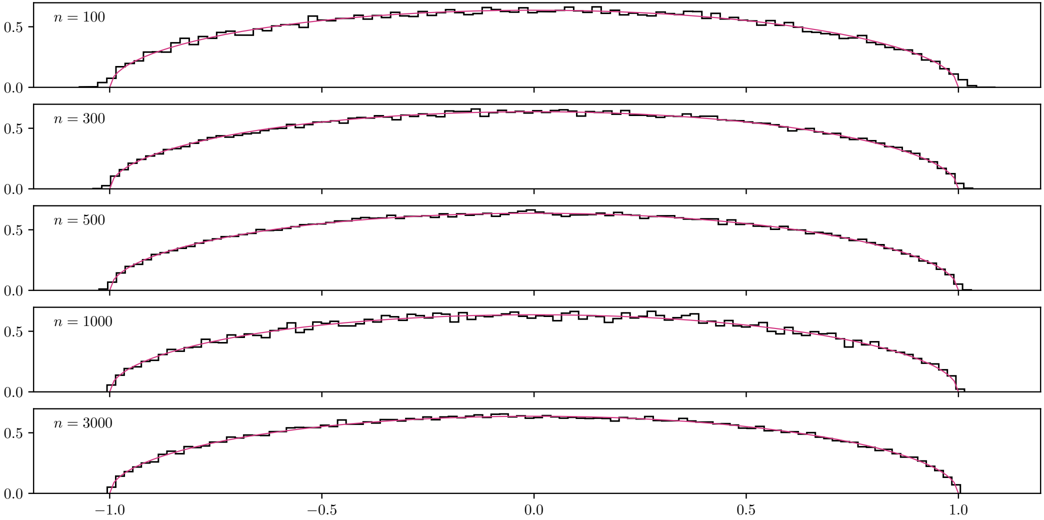
$$\mathbf{A} = \frac{\mathbf{X} + \mathbf{X}^\top}{2\sqrt{2n}}.$$

Equivalently, for $i \leq j$ entries of $\mathbf{A}$ are independent with distribution

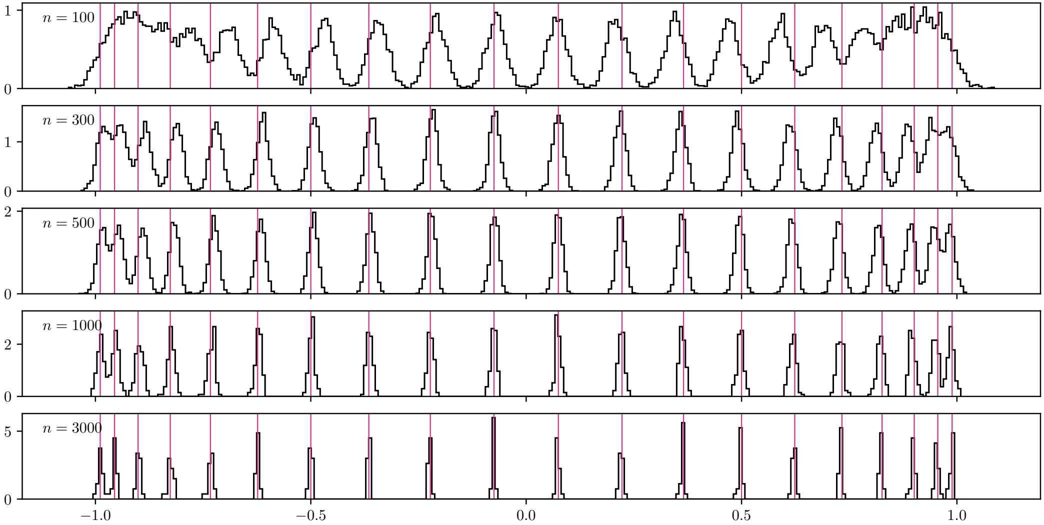
$$2\sqrt{2n}[\mathbf{A}]_{i,i} \sim \mathcal{N}(0, 2), \qquad 2\sqrt{2n}[\mathbf{A}]_{i,j} \sim \mathcal{N}(0, 1)$$

Note that $\mathbf{A}$ is unitarily invariant and the eigenvalues eventually lie between $[-1, 1]$ with high probability.

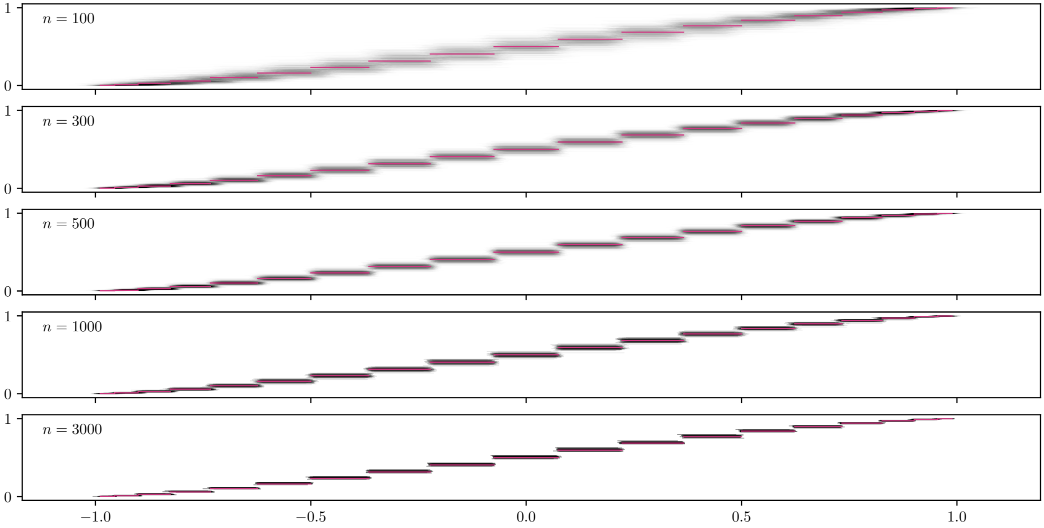
Weighted empirical spectral measure



Gaussian quadrature node (Ritz values)



Gaussian quadrature rule



Remarks

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These examples were computed in finite precision arithmetic without reorthogonalization

- isn't the Lanczos algorithm unstable?

Example: instability of Lanczos method[2]

In finite precision arithmetic, the Lanczos algorithm might behave extremely differently than in exact arithmetic.

$$\mathbf{A} = \begin{bmatrix} 0 & & & & & \\ & 0.00025 & & & & \\ & & 0.0005 & & & \\ & & & 0.00075 & & \\ & & & & 0.001 & \\ & & & & & 10 \end{bmatrix}, \qquad \mathbf{v} = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

[2] Parlet and Scott 1979.

Example: instability of Lanczos

Denote by $\mathbf{T}, \mathbf{Q}$ the exact arithmetic output and $\tilde{\mathbf{T}}, \tilde{\mathbf{Q}}$ the finite precision output. How many digits of accuracy do we have for the following quantities:

$$\tilde{\mathbf{Q}} - \mathbf{Q} \qquad\qquad \tilde{\mathbf{T}} - \mathbf{T} \qquad\qquad \tilde{\mathbf{Q}}^\top \tilde{\mathbf{Q}} - \mathbf{I}$$

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$$\begin{bmatrix} - & - & 12 & 7 & 1 \\ - & - & 12 & 7 & 0 \\ - & 17 & 13 & 11 & 0 \\ - & - & 12 & 7 & 0 \\ - & - & 12 & 7 & 1 \\ - & 17 & 8 & 3 & 0 \end{bmatrix} \quad \begin{bmatrix} - & - & & & & \\ - & - & - & & & \\ & - & - & 19 & & \\ & & 19 & 14 & 10 & \\ & & & 10 & 5 & 2 \\ & & & & 2 & 0 \end{bmatrix} \quad \begin{bmatrix} 16 & 16 & 17 & 8 & 4 & 0 \\ 16 & 16 & 12 & 8 & 3 & 0 \\ 17 & 12 & 16 & 15 & 7 & 4 \\ 8 & 8 & 15 & 15 & 15 & 9 \\ 4 & 3 & 7 & 15 & - & 17 \\ 0 & 0 & 4 & 9 & 17 & - \end{bmatrix}$$

Example: instability of Lanczos

Even for a very small example without any super extreme numbers, the Lanczos algorithm is not at all forward stable.

There is a lot of theory about Lanczos in finite precision (although no real forward analysis)[3]

[3] Paige 1971; Paige 1976; Paige 1980; Grcar 1981; Simon 1982; Greenbaum 1989; Meurant 2006.

Lanczos in the large n limit

Returning to exact arithmetic, let's consider applying Lanczos to $\mathbf{A}, \mathbf{v}$ where $\mathbf{A} \sim \text{GOE}(n)$. Since $\mathbf{A}$ is unitarily invariant, this is equivalent to considering $\mathbf{A}, \hat{\mathbf{e}}$.

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The Lanczos algorithm is also unitarily invariant so it will produce the same tridiagonal matrix if we apply it to $\mathbf{V}^\top \mathbf{A} \mathbf{V}, \mathbf{V}^\top \hat{\mathbf{e}}$ for any unitary matrix $\mathbf{V}$. Moreover, the columns of the basis $\mathbf{Q}$ for Krylov subsubspace are just transformed by $\mathbf{V}$.

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If we can find such a transform $\mathbf{V}$ so that $\mathbf{V}^\mathsf{T}\mathbf{A}\mathbf{V}$ is tridiagonal and $\mathbf{V}^\mathsf{T}\hat{\mathbf{e}} = \hat{\mathbf{e}}$ then we know exactly how Lanczos will behave on $\mathbf{A}, \hat{\mathbf{e}}$ because Lanczos on a tridiagonal matrix with starting vector $\hat{\mathbf{e}}$ produces back the same tridiagonal matrix.

Tridiagonalization of GOE

It is well known[4] that GOE can be tridiagonalized:

$$\frac{1}{2\sqrt{2n}}\begin{bmatrix} G_2 & G_1 & \cdots & \cdots & G_1 \\ G_1 & G_2 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & G_1 \\ G_1 & \cdots & \cdots & G_1 & G_2 \end{bmatrix} \xrightarrow[]{\substack{\text{unitary} \\ \text{tridiagonalization}}} \frac{1}{2\sqrt{2n}}\begin{bmatrix} G_2 & \chi_{n-1} & & & \\ \chi_{n-1} & G_2 & \chi_{n-2} & & \\ & \chi_{n-2} & \ddots & \ddots & \\ & & \ddots & \ddots & \chi_1 \\ & & & \chi_1 & G_2 \end{bmatrix}$$

The transform does not change the first entry of a vector so Lanczos on $\mathbf{A}, \hat{\mathbf{e}}$ will produce this tridiagonal matrix (in distribution).

[4] Trotter 1984; Dumitriu and Edelman 2002.

Tridiagonalization of GOE

Let's look at the top-left $k \times k$ block as $n \to \infty$.

We know as $n \to \infty$, $(\chi_d - \mu_d)/\sigma_d \xrightarrow{\mathrm{d}} \mathcal{N}(0,1)$ where $\mu_d \approx \sqrt{n-1} + O(n^{-1/2})$ and $\sigma_d^2 = d - \mu_d^2 \approx (n-1)/(2n) + O(n^{-1})$.

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$$\lim_{n\to\infty} \frac{1}{2\sqrt{2n}} \begin{bmatrix} G_2 & \chi_{n-1} & & & \\ \chi_{n-1} & G_2 & \chi_{n-2} & & \\ & \chi_{n-2} & \ddots & \ddots & \\ & & \ddots & \ddots & \chi_{n-k} \\ & & & \chi_{n-k} & G_2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{bmatrix}$$

Perturbation analysis

We can then analyze $\hat{\mathbf{e}}^T f(\mathbf{T})\hat{\mathbf{e}}$ using that

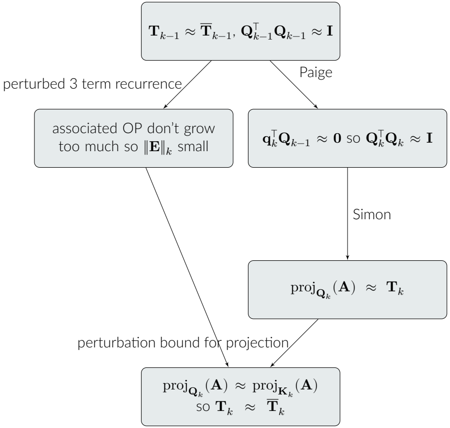
$$\hat{\mathbf{e}}^T f(\mathbf{T})\hat{\mathbf{e}} = \int f(x)\mathrm{d}\Psi[\mathbf{T},\hat{\mathbf{e}}](x).$$

To do this we do a perturbation analysis for this integral based on perturbations of tridiagonal matrices.

Forward stability of Lanczos on GOE (very brief overview)

Notation:

- $\mathbf{T}_k, \mathbf{Q}_k$ output of finite precision Lanczos
- $\overline{\mathbf{T}}_k$ limiting tridiagonal matrix
- $\mathbf{K}_k = [p_0(\mathbf{A})\mathbf{v}, \ldots, p_{k-1}(\mathbf{A})\mathbf{v}]$ (these are polynomials of $\mathbf{T}_k$)
- $\mathbf{E}_k = \mathbf{Q}_k - \mathbf{K}_k$ (can write in terms of associated polynomials of $\mathbf{T}_k$)



Summary

- For fixed k, the tridiagonal matrix output by the Lanczos algorithm run on a GOE matrix of size n concentrates rapidly as $n \to \infty$, and we can study the "average case" behavior of Lanczos as well as the fluctuations of Lanczos about this average case.
  - For any matrix and any ball of nonzero radius centered at this matrix, there is a non-zero probability of sampling a GOE matrix from within that ball
- We observe that Lanczos is (whp) forward stable for sufficiently large matrices[5]
  - We think we can prove this rigorously (probably need $\epsilon = O(1/n)$)
  - This would give (maybe first true) forward analysis result on Lanczos

[5] testing very big dense matrices is prohibitively expensive so we haven't done super big tests yet

Final remark

Quote from Edelman and Rao[6]:

> *It is a mistake to link psychologically a random matrix with the intuitive notion of a 'typical' matrix or the vague concept of 'any old matrix'.*

[6] Edelman and Rao 2005.

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