Convergence of the Arnoldi process for unitary matrices

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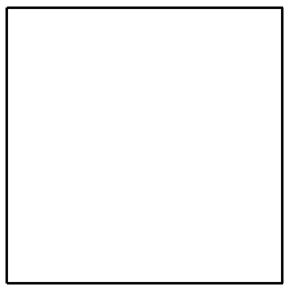
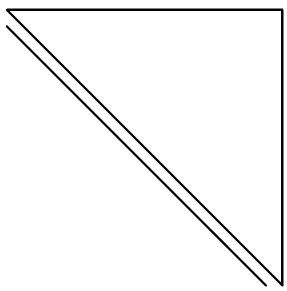
1. The IAP



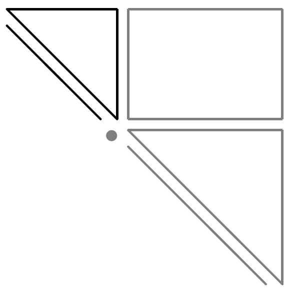
full unitary matrix

↓



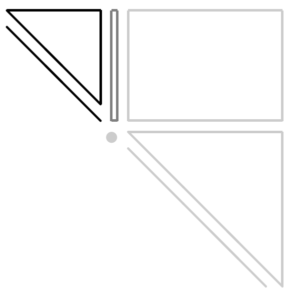
reduction to Hessenberg form;
the subdiagonal contains strictly positive numbers

↓



taking a principal left upper block;
this is not unitary anymore

↓



renormalizing the last column to obtain a unitary matrix

2. Orthogonal Polynomials

- Unitary matrix $U \in \mathbb{C}^{N\times N}$
- Simple eigenvalues $\lambda_1, \ldots, \lambda_N$, eigenvectors $v_1, \ldots, v_N$
- Unit starting vector b
- $\mu := \sum |\langle b, v_j\rangle|^2 \delta_{\lambda_j}$ $\quad (\to \int \mathrm{d}\mu = 1)$

Lemma 1 *For every function $f : \mathbb{T} \to \mathbb{C}$, we have $\|f(U)b\|^2 = \int |f|^2 \,\mathrm{d}\mu$.*

- IAP transforms U into an upper Hessenberg matrix H
- $\phi_n(z) := \det(zI_n - H_n)$

Lemma 2 *The polynomial ϕ_n is the monic polynomial of degree n that is orthogonal with respect to μ.*

Arnoldi minimization problem:

Minimize $\|p_n(U)b\|$ among all monic polynomials p_n of degree n.

3. Unitary Hessenberg Matrices

- $H = G_1(\gamma_1) \cdots G_{N-1}(\gamma_{N-1}) \tilde{G}_N(\gamma_N)$
- $|\gamma_j| < 1$ for $j = 1, \ldots, N-1$ and $|\gamma_N| = 1$
- $G_j(\alpha) =$
$$\begin{bmatrix} I_{j-1} & & & \\ & -\alpha & \sqrt{1-|\alpha|^2} & \\ & \sqrt{1-|\alpha|^2} & \bar{\alpha} & \\ & & & I_{N-j-1} \end{bmatrix}$$
- $\tilde{G}_N(\alpha) = \begin{bmatrix} I_{N-1} & \\ & -\alpha \end{bmatrix}.$
- notation $H = H(\gamma_1, \ldots, \gamma_N)$
- $H_n = H(\gamma_1, \ldots, \gamma_n)$
- $\phi_n(0) = \gamma_n$
- $H_n \rightsquigarrow \tilde{H}_n$ (unitary)
- $\tilde{H}_n = H(\gamma_n, \ldots, \gamma_{n-1}, \rho_n)$ with $|\rho_n| = 1$

4. Para-Orthogonal Polynomials

- reciprocal polynomial $p^*(z) = z^n \overline{p(1/\bar{z})}$
- para-orthogonal polynomials $\psi_n(z) := \frac{\phi_n(z)+\omega_n\phi_n^*(z)}{1+\omega_n\bar{\gamma}_n}$, with $|\omega_n| = 1$
- if $\omega_n = \rho_n\left(\frac{1-\bar{\rho}_n\gamma_n}{1-\rho_n\bar{\gamma}_n}\right)$, then $\psi_n = \det(zI_n - \tilde{H}_n)$

Isometric Arnoldi minimization problem:

Minimize $\|p_n(U)b\|$ among all monic polynomials p_n of degree n satisfying $p_n(0) = \rho_n$, where $\rho_n \in \mathbb{T}$ is given.

Theorem 3 *The minimizer of the Isometric Arnoldi minimization problem is unique and it is given by the monic para-orthogonal polynomial $\psi_n(z)$ where ω_n is related to ρ_n as above.*

Proposition 4 *Let $n < N$. Then the zeroes of ψ_n are separated by the eigenvalues of U.*

5. Theoretical Setting

- A *sequence* of unitary matrices $(U_N)_N$, each of dimension $N \times N$.
- The eigenvalues $\{\lambda_{k,N}\}_k$ and orthonormal eigenvectors $\{v_{k,N}\}_k$.
- A unit starting vector $b_N \in \mathbb{C}^N$ for every N.
- The $n \times n$ unitary Hessenberg matrix $\tilde{H}_{n,N}$ created by n steps of the IAP, with $n < N$.
- The characteristic polynomials $\psi_{n,N}$ of $\tilde{H}_{n,N}$.
- The eigenvalues $\{\theta_{k,n,N}\}_k$ of $\tilde{H}_{n,N}$, which are called the isometric Ritz values.

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6. Potential Theory

$$U^{\mu}(z) = \int \log \frac{1}{|z - z'|} \, \mathrm{d}\mu(z'),$$

$$I(\mu) = \iint \log \frac{1}{|z - z'|} \, \mathrm{d}\mu(z) \mathrm{d}\mu(z').$$

7. Conditions

1. There exists a probability measure σ with U^σ real valued and continuous such that

$$\lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \delta_{\lambda_{j,N}} = \sigma.$$

2. For all $\varepsilon > 0$ there exists a $\delta \in (0,1)$ and an $N_0 \in \mathbb{N}$ so that for all $N > N_0$ and for all $k \leqslant N$

$$\prod_{\substack{j=1 \\ 0<|\lambda_{j,N}-\lambda_{k,N}|<\delta}}^{N} |\lambda_{j,N} - \lambda_{k,N}| > \mathrm{e}^{-N\varepsilon}.$$

3. For every N, we have that $\|b_N\| = 1$ and

$$\lim_{N\to\infty} \Big(\min_{1\leqslant k\leqslant N} |\langle b_N, v_{k,N}\rangle| \Big)^{1/N} = 1.$$

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limits: We let N and n go to ∞ in such fashion that $n/N \to t \in (0,1)$. notation: $\lim_{\substack{n,N\to\infty \\ n/N\to t}}$

8. Results

Theorem 5 *There exists a probability measure μ_t, depending only on t and σ, such that*

$$\lim_{\substack{n,N\to\infty\\ n/N\to t}} \frac{1}{n}\sum_{j=1}^{n} \delta_{\theta_{j,n,N}} = \mu_t,$$

$$0 \leqslant t\mu_t \leqslant \sigma, \qquad \int \mathrm{d}\mu_t = 1.$$

μ_t minimizes the logarithmic energy $I(\mu)$ among all measures μ satisfying $0 \leqslant t\mu \leqslant \sigma$ and $\int \mathrm{d}\mu = 1$. Moreover the logarithmic potential U^{μ_t} of μ_t is a continuous function on $\mathbb{C}$. There also exists a real constant F_t such that

$$\lim_{\substack{n,N\to\infty\\ n/N\to t}} \|\psi_{n,N}(U_N)b_N\|^{1/n} = \exp(-F_t)$$

and

$$\begin{cases} U^{\mu_t}(z) = F_t & \text{for } z \in \operatorname{supp}(\sigma - t\mu_t), \\ U^{\mu_t}(z) \leqslant F_t & \text{for } z \in \mathbb{C}. \end{cases}$$

8. Results (2)

Theorem 6 *For every* $(\lambda_{k_N,N})_N$ *converging to* $\lambda \in \mathbb{T}$ *and for every* $t \in (0,1)$

$$\limsup_{\substack{n,N\to\infty \\ n/N\to t}} \min_j |\lambda_{k_N,N} - \theta_{j,n,N}|^{1/n} \leqslant \exp\bigl(U^{\mu_t}(\lambda) - F_t\bigr).$$

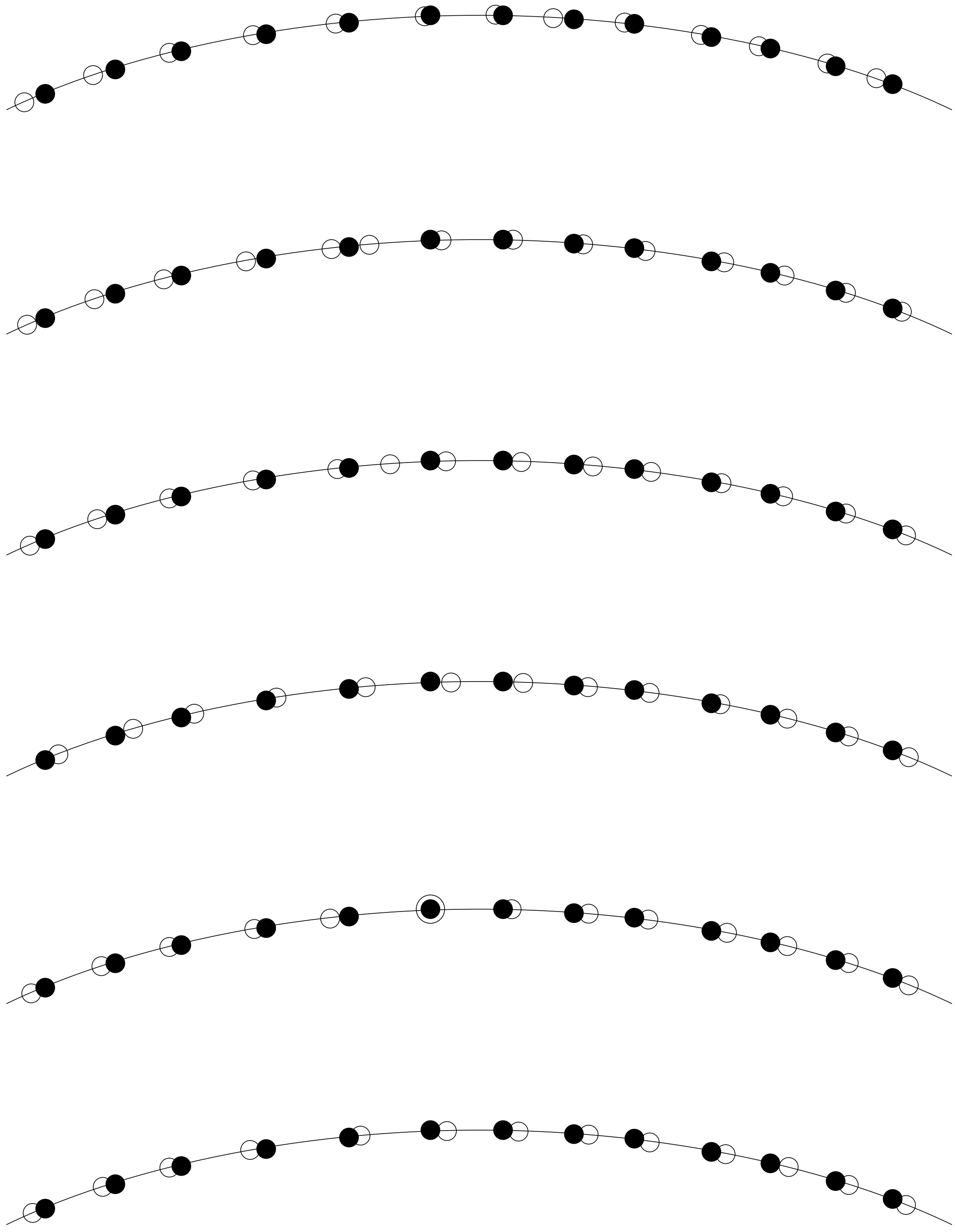
We define the set

$$\Lambda(t,\sigma) := \{z \in \mathbb{T} \mid U^{\mu_t}(z) < F_t\}.$$

Theorem 7 *For* nearly *every* $(\lambda_{k_N,N})_N$ *converging to* $\lambda \in \Lambda(t,\sigma)$ *and for every* $t \in (0,1)$

$$\lim_{\substack{n,N\to\infty \\ n/N\to t}} \min_j |\lambda_{k_N,N} - \theta_{j,n,N}|^{1/n} = \exp\Bigl(2\bigl(U^{\mu_t}(\lambda) - F_t\bigr)\Bigr).$$

9. Position i.R.v.



10. Numerical Setting

- We fix a matrix U, hence also N.
- We let n go from 1 to N, hence t goes from 0 to 1.

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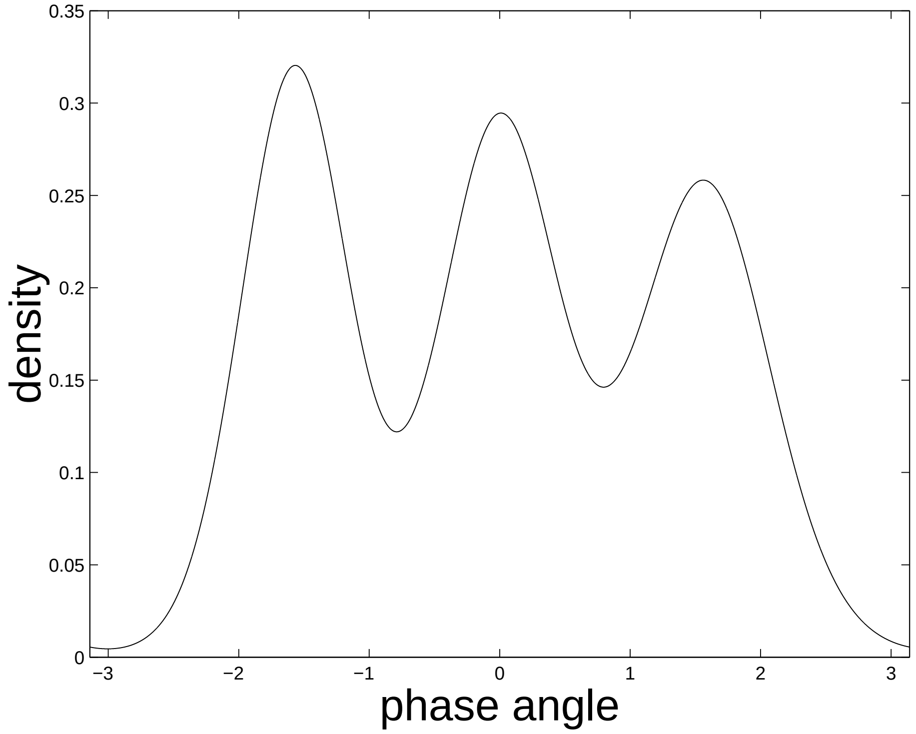
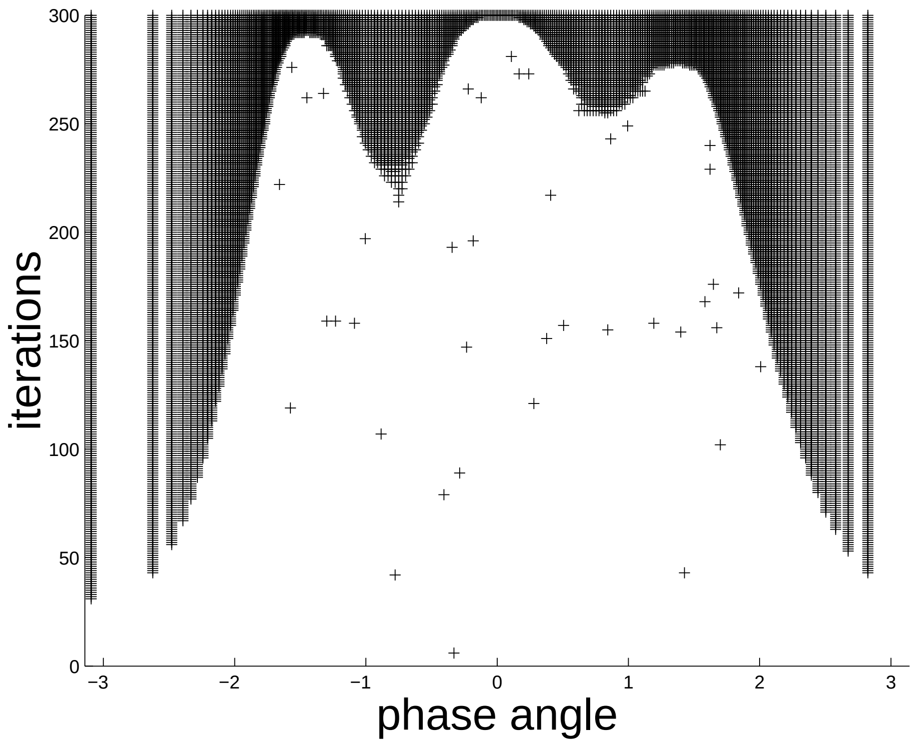
11. Equilibrium measure

- Remember μ_t minimizes $I(\mu)$ among all measures μ satisfying $0 \leqslant t\mu \leqslant \sigma$.
- If we minimize without constraint, we get *the equilibrium measure* $\mu_{\mathbb{T}}$.
- $\mu_{\mathbb{T}}$ is equal to the Lebesgue measure.
- So if $t\mu_{\mathbb{T}} \leqslant \sigma$, $\mu_t = \mu_{\mathbb{T}}$ and we can not expect any convergence.
- One can show that in the region where $t\mu_{\mathbb{T}} > \sigma$, $t\mu_t = \sigma$.

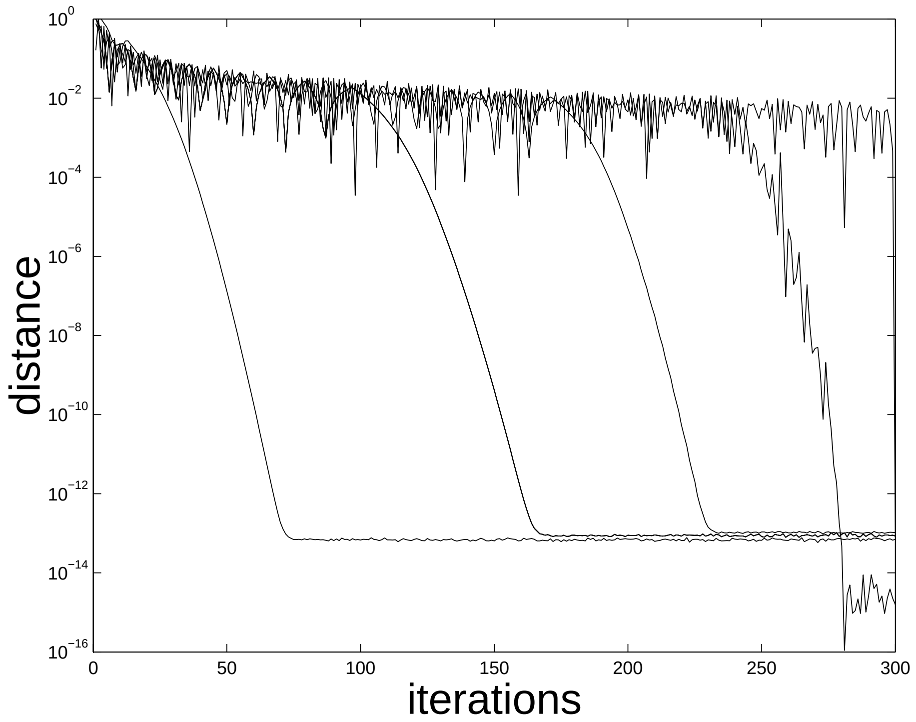
- At first no eigenvalues are found.
- Then $t\mu_{\mathbb{T}}$ hits σ.
- So in the region with the lowest eigenvalue density, eigenvalues are found first!

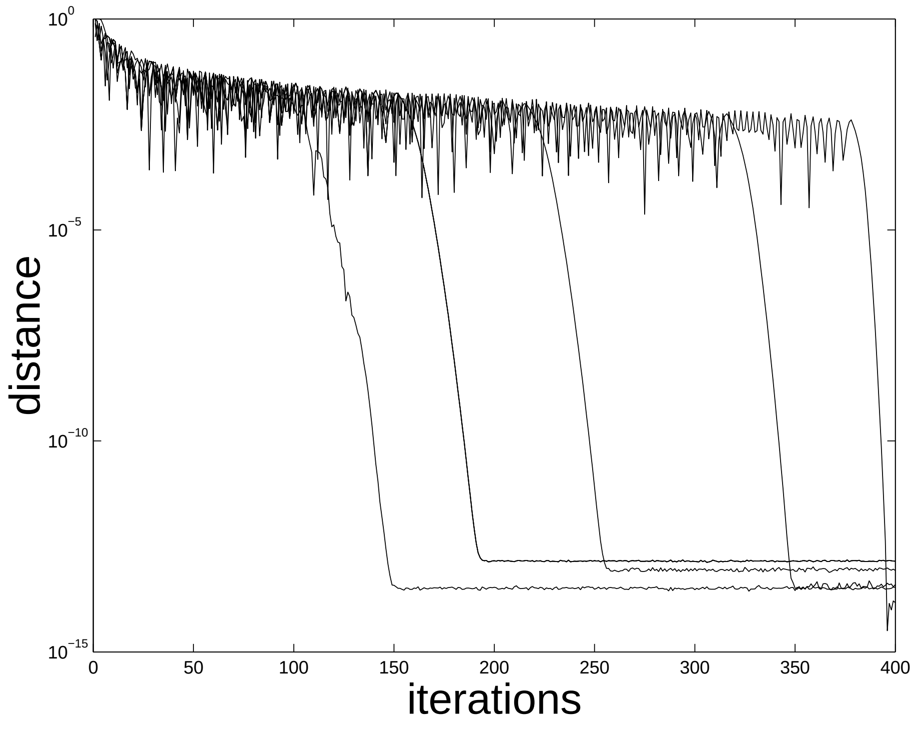
12. Numerical Experiments





12. Numerical Experiments (2)





12. Numerical Experiments