Refined decay bounds on the entries of spectral projectors associated with sparse Hermitian matrices

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Overview

Introduction

- Decaying matrices
- Spectral projectors
- Previous results

Refined decay bounds

- Exploiting an integral representation of sign(x)
- Asymptotically optimal bound
- Bound related with the eigenvalue distribution

Introduction

Decaying matrices

Exponential off-diagonal decay: $\{A_n\}_n$, $A_n \in \mathbb{C}^{n\times n}$,

$$|[A_n]_{ij}| \leq C\rho^{|i-j|}, \quad \text{for all } i, j,$$

$C > 0$ and $0 < \rho < 1$ are independent of n.

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$C > 0$ and $0 < \rho < 1$ are independent of n.

For all m define the m-banded truncation of A_n as

$$[A_n^{(m)}]_{ij} = \begin{cases} [A_n]_{ij} & \text{if } |i-j| \le m, \\ 0 & \text{otherwise.} \end{cases}$$

For all $\varepsilon > 0$ there is m independent of n s.t. $\|A_n - A_n^{(m)}\|_p \le \varepsilon$ for all n, where $p = 1, 2, \infty$ [Benzi-Razouk, 2007].

$A_n^{(m)}$ is m-banded $\Longrightarrow$ has $\mathcal{O}(n)$ non-zero entries.

Decay for matrix functions

Matrix functions: $A \in \mathbb{C}^{n\times n}$ Hermitian, $A = U\Lambda U^*$ spectral decomposition, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Then $f(A)$ is defined by

$$f(A) = Uf(\Lambda)U^*, \quad f(\Lambda) = \mathrm{diag}(f(\lambda_1), \ldots, f(\lambda_n)).$$

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Given a set $\mathcal{S}$, define $E_k(f, \mathcal{S}) = \inf_{p_k \in \mathcal{P}_k} \sup_{x \in \mathcal{S}} |f(x) - p_k(x)|$, where $\mathcal{P}_k$ is the set of polynomials with degree at most k.

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- $A \in \mathbb{C}^{n\times n}$ Hermitian and m-banded, $\sigma(A) \subset \mathcal{S}$, $E_k(f, \mathcal{S}) \leq C\rho^k$ for all $k \geq 0$. Then

  $$|[f(A)]_{ij}| \leq C\rho^{\frac{|i-j|}{m} - 1} \quad \text{for all } i \neq j.$$

  The bound depends only on $\mathcal{S}$ and on m, not on n.
  If $\{A_n\}_n$ is s.t. $\sigma(A_n) \subset \mathcal{S}$ and A_n is m-banded for all n, then $\{f(A_n)\}_n$ has an exponential off-diagonal decay.

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- $A \in \mathbb{C}^{n\times n}$ Hermitian and m-banded, $\sigma(A) \subset \mathcal{S}$, $E_k(f, \mathcal{S}) \le C\rho^k$ for all $k \ge 0$. Then

  $$|[f(A)]_{ij}| \le C\rho^{\frac{|i-j|}{m}-1} \quad \text{for all } i \ne j.$$

  The bound depends only on $\mathcal{S}$ and on m, not on n.
  If $\{A_n\}_n$ is s.t. $\sigma(A_n) \subset \mathcal{S}$ and A_n is m-banded for all n, then $\{f(A_n)\}_n$ has an exponential off-diagonal decay.
- If A is not m-banded, it still holds that $|[f(A)]_{ij}| \le C\rho^{d(i,j)}$ for all $i \ne j$, where $d(i,j)$ is the geodesic distance on $\mathcal{G}(A)$.
  Under suitable hypotheses on $\mathcal{G}(A)$ [Frommer-Schimmel-Schweitzer, 2021], $f(A)$ is close to a sparse matrix.

Spectral projector

$H \in \mathbb{C}^{n\times n}$ Hermitian, $\sigma(H) \subset [b_1, a_1] \cup [a_2, b_2]$, $b_1 < a_1 < a_2 < b_2$.

The spectral projector associated with $[b_1, a_1]$ is given by:

$$P = h_\mu(H), \quad h_\mu(x) = \begin{cases} 1 & \text{if } x < \mu, \\ 1/2 & \text{if } x = \mu, \\ 0 & \text{if } x > \mu, \end{cases}$$

where μ is arbitrary between a_1 and a_2.

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where μ is arbitrary between a_1 and a_2.

- The function $h_\mu(x)$ is not continuous over $[b_1, b_2]$.
- **Invariance for linear transformations**: if $\tilde{H} = cH + d$, then $P = \tilde{P} = h_{\tilde{\mu}}(\tilde{H})$, where $\tilde{\mu} = c\mu + d$. Note that $\sigma(\tilde{H}) = c\,\sigma(H) + d$.
- We can assume $\sigma(H) \subset [-b, -a] \cup [a, b]$, $0 < a < b$, so $\mu = 0$ and $h_0(x) =: h(x)$.
- $h(x) = (1 - \operatorname{sign}(x))/2$, so $|[P]_{ij}| = |[\operatorname{sign}(H)]_{ij}|/2$ for $i \neq j$.

Previous result

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Idea: $\mathrm{sign}(x) = x(x^2)^{-1/2}$.
$q_k(y) \approx y^{-1/2}$, $y \in [a^2, b^2] \implies xq_k(x^2) \approx \mathrm{sign}(x)$, $x \in [-b, -a] \cup [a, b]$.

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Theorem [Benzi-Boito-Razouk, 2013]

Let H be Hermitian and m-banded with $\sigma(H) \subset [-b, -a] \cup [a, b]$.
Then, for $1 < \chi < \bar{\chi} := \frac{b+a}{b-a}$,

$$2|[P]_{ij}| = |[\operatorname{sign}(H)]_{ij}| \leq \frac{2bM(\chi)}{\chi - 1} \left(\frac{1}{\chi}\right)^{\frac{|i-j|}{2m} - \frac{1}{2}} \quad \text{for all } i \neq j,$$

where $M(\chi) = \frac{1}{\sqrt{z_0}}$, $z_0 = \left[\frac{b^2+a^2}{b^2-a^2} - \frac{\chi^2+1}{2\chi}\right] \frac{b^2-a^2}{2}$.

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For i, j fixed, we can minimize in χ.

The optimized bound numerically behaves as $\left(\frac{b-a}{b+a}\right)^{\frac{|i-j|}{2m}}$.

Refined decay bounds

Exploiting an integral representation of $\mathrm{sign}(x)$

$$\mathrm{sign}(H) = \frac{2}{\pi}\int_0^\infty H(H^2 + t^2 I)^{-1}\,\mathrm{d}t,$$
$$|[\mathrm{sign}(H)]_{ij}| \le \frac{2}{\pi}\int_0^\infty |[H(H^2 + t^2 I)^{-1}]_{ij}|\,\mathrm{d}t.$$

Idea: Bound $|[H(H^2+t^2)^{-1}]_{ij}|$ and integrate [Benzi-Simoncini, 2015].

$q_k(y) \approx (y+t^2)^{-1} \implies xq_k(x^2) \approx x(x^2+t^2)^{-1}$, and the best polynomial approximation of the inverse gives a single bound.

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Theorem [Benzi-R., 2021]

Let H be Hermitian, m-banded, $\sigma(H) \subset [-b,-a] \cup [a,b]$. Then

$$|[P]_{ij}| \le \frac{(1+\sqrt{b/a})^2}{4}\left(\frac{b-a}{b+a}\right)^{\frac{|i-j|}{2m}-\frac{1}{2}} \quad \text{for all } i,j. \tag{1}$$

We get the previous behaviour without optimization.

Asymptotically optimal bound

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It is shown (see [Eremenko-Yuditskii, 2007]) that

$$E_k(\mathrm{sign}(x), [-b, -a] \cup [a, b]) = \mathcal{O}\left(\frac{1}{\sqrt{k}} \left(\frac{b-a}{b+a} \right)^{\frac{k}{2}} \right) \quad \text{as } k \to \infty.$$

If $H = H^*$ is Hermitian and m-banded, $\sigma(H) \subset [-b, -a] \cup [a, b]$, then

$$|[\mathrm{sign}(H)]_{ij}| \leq \frac{C}{\sqrt{\frac{|i-j|}{m} - 1}} \left(\frac{b-a}{b+a} \right)^{\frac{|i-j|}{2m} - \frac{1}{2}},$$

for some $C > 0$.

However, such C is still unknown.

Asymptotically optimal bound

Theorem [Benzi-R., 2021]

Let H be Hermitian, m-banded, $\sigma(H) \subset [-b,-a] \cup [a,b]$. Let $C_1 = \frac{1}{2ab}$, $C_2 = \frac{a^2+ab+b^2}{8a^3b^3}$, and $0 < \tau < \bar{\tau} := \sqrt{\frac{C_1}{C_2}}$. Then

$$|[P]_{ij}| \le \frac{K_1(\tau)}{\sqrt{\frac{|i-j|}{m} - 1}} \left(\frac{b-a}{b+a}\right)^{\frac{|i-j|}{2m}-\frac{1}{2}} + K_2\, q(\tau)^{\frac{|i-j|}{2m}-\frac{1}{2}} \tag{2}$$

for $|i-j| \ge m$, where $q(\tau) = \frac{\sqrt{b^2+\tau^2}-\sqrt{a^2+\tau^2}}{\sqrt{b^2+\tau^2}+\sqrt{a^2+\tau^2}}$ and

$K_1(\tau) = \frac{(1+b/a)^2}{2\sqrt{2\pi(C_1-\tau^2 C_2)}}, \quad K_2 = \frac{1}{4}\left(1+\sqrt{b/a}\right)^2.$

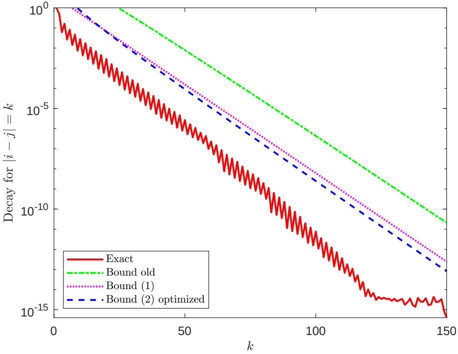
$q(\tau) < q(0) = \frac{b-a}{b+a} \implies$ optimal asymptotic behaviour for all $\tau > 0$.

We can also optimize to get the best possible bound.

Comparison between the bounds

$H \in \mathbb{C}^{150\times 150}$ Hermitian and tridiagonal.

$\sigma(H) \subset [-1, -0.2] \cup [0.2, 1]$ uniformly distributed.



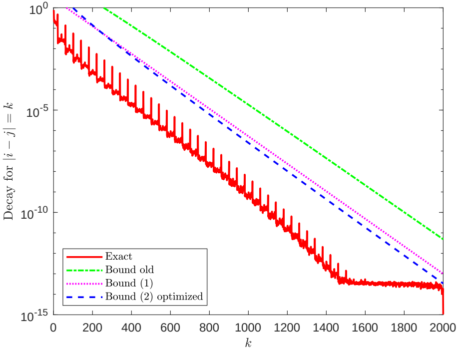
Solid line: $d_P(k) = \max_{|i-j|=k} |P_{ij}|$. **Other lines**: bounds for $|i-j| = k$.

Remark: The bounds are independent of the size.

Comparison between the bounds

$H \in \mathbb{C}^{2000\times 2000}$ Hermitian, 20-banded.

$\sigma(H) \subset [-1,-0.3] \cup [0.3,1]$ uniformly distributed.



Solid line: $d_P(k) = \max_{|i-j|=k} |P_{ij}|$. **Other lines**: bounds for $|i-j|=k$.

Remark: The bounds are independent of the size.

Bounds related with the eigenvalue distribution

The decay of the entries of A^{-1} benefits from certain eigenvalue distributions [Frommer-Schimmel-Schweitzer, 2018].

Does a similar property hold for spectral projectors?

Bounds related with the eigenvalue distribution

Theorem **[Benzi-R., 2021]**

Let $H = H^*$ be m-banded with $\sigma(H) \subset [-b, -a] \cup [a, b]$. Let $b = b_0 > b_1 > \ldots, > b_\nu = a$, with $\nu \leq n$, be the distinct values of $|\lambda|$ for $\lambda \in \sigma(H)$. Then

$$|[P_{ij}]| \leq C_\ell q_\ell^{\frac{|i-j|}{2m} - \frac{1}{2} - \ell} \quad \text{for } \ell = 0, 1, \ldots, \left\lceil \frac{|i-j|}{2m} - \frac{1}{2} \right\rceil, \tag{3}$$

where $C_\ell = \frac{1}{4}\left(1 + \sqrt{\frac{b_\ell}{a}}\right)^2$, $q_\ell = \frac{b_\ell - a}{b_\ell + a}$.

Bounds related with the eigenvalue distribution

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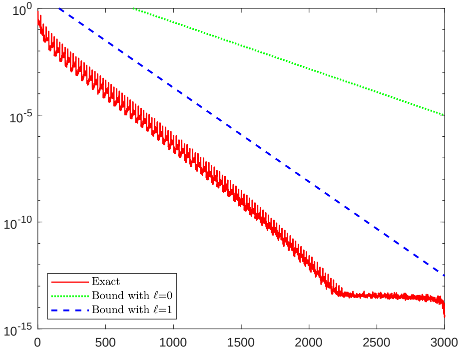
where $C_\ell = \frac{1}{4}\left(1 + \sqrt{\frac{b_\ell}{a}}\right)^2, q_\ell = \frac{b_\ell - a}{b_\ell + a}$.

For fixed i, j, when ℓ increases:

- $q_\ell << q_{\ell-1}$ when $b_\ell << b_{\ell-1}$.
- Smaller exponent: trade-off with the geometric rate.
- One or few isolated eigenvalue of maximum modulus do not contribute to the decay.
- Certain eigenvalue distributions lead to superexponential decay.

One isolated eigenvalue

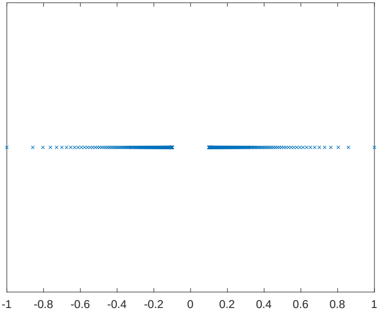
$H \in \mathbb{C}^{3000\times3000}$, Hermitian, 20-banded,
$\sigma(H) \subset \{-1\} \cup [-0.5, -0.1] \cup [0.1, 0.5]$, and -1 has multiplicity 10.

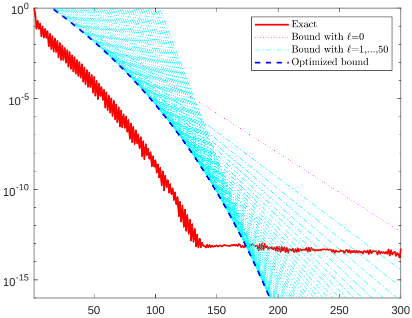


Bound (3) with $\ell = 1$ catches the behaviour.

Superexponential decay

$H \in \mathbb{C}^{300\times 300}$, Hermitian, tridiagonal, $\sigma(H) \subset [-1,-0.1] \cup [0.1,1]$.





Left: $\sigma(H)$, symmetric with respect to the origin. There are several isolated eigenvalues at the extremes. They cluster near the spectral gap.

Right: Exact decay compared with the bounds.

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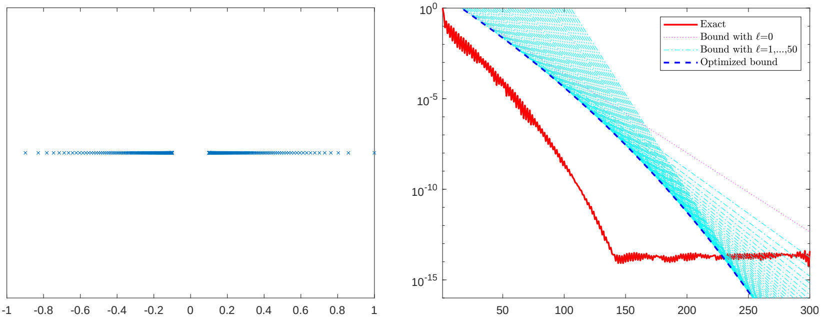

Left: $\sigma(H)$, no symmetry is present. There are several isolated eigenvalues at the extremes. They cluster near the spectral gap.
Right: Exact decay compared with the bounds.

Conclusions

We developed three new decay bounds for the entries of spectral projectors.

- The first is a single bound that describes well the decay.
- The second is optimal in the sense of polynomial approximation.
- The third catches the behaviour in presence of extremal isolated eigenvalues.

Some open problems are:

- Find an appropriate bound for the case of nonsymmetric intervals.
- Try new strategies to obtain smaller constant factors.
- Establish connections with more complicated eigenvalue distributions.

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Thank you for the attention!

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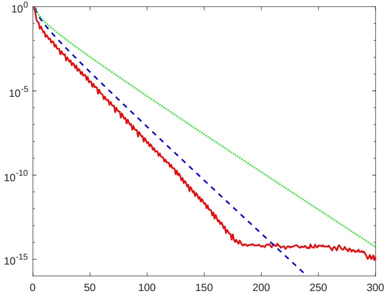
Non-symmetric intervals

$$E_k(\mathrm{sign}(x), [-b_1, -a] \cup [a, b_2]) = \mathcal{O}(k^{-\frac{1}{2}} e^{-\eta k}),$$

$$\eta = \int_{-1}^{K} \frac{K-x}{\sqrt{(1-x^2)(x+b_1/a)(x-b_2/a)}}\,\mathrm{d}x \left(= \log\left(\frac{b+a}{b-a}\right) \text{ if } b_1 = b_2 = b \right), \text{ where}$$

$$K = \frac{\int_{-1}^{1} x((1-x^2)(x+b_1/a)(x-b_2/a))^{-1/2}\,\mathrm{d}x}{\int_{-1}^{1}((1-x^2)(x+b_1/a)(x-b_2/a))^{-1/2}\,\mathrm{d}x}.$$



$H \in \mathbb{C}^{300\times 300}$, tridiagonal, $\sigma(H) \subset [-0.5, -0.1] \cup [0.1, 1]$. Rate with $C = 1$.
Dashed line: $b_1 = 0.5, b_2 = 1$. **Dotted line**: $b_1 = b_2 = 1$.

Inverse function and general analytic functions

- $f(A) = A^{-1}$, $\sigma(A) \subset [a, b]$, $0 < a < b$. In this case $E_k(x^{-1}, [a, b]) = Cq^{k+1}$ [Meinardus, 1967], where

$$C = (1 + \sqrt{b/a})^2/2b, \quad q = (\sqrt{b} - \sqrt{a})/(\sqrt{b} + \sqrt{a}).$$

  A is m-banded $\Longrightarrow$ $|[A^{-1}]_{ij}| \leq Cq^{\frac{|i-j|}{m}}$, $i \neq j$ [Demko-Moss-Smith, 1984].
  Remark: $q = (\sqrt{b/a} - 1)/(\sqrt{b/a} + 1) \Longrightarrow$ connection with CG.

- $\sigma(A) \subset [-1, 1]$, f analytic over the ellipse $\mathcal{E}_\chi$ with foci in ± 1 and sum of semiaxes $\chi > 1$. From Bernstein's Theorem [Meinardus, 1967]

$$E_k(f, [-1, 1]) \leq \frac{2M(\chi)}{\chi - 1}\left(\frac{1}{\chi}\right)^k, \quad M(\chi) = \max_{z \in \mathcal{E}_\chi} |f(z)|.$$

  A is m-banded $\Longrightarrow$ $|[f(A)]_{ij}| \leq \frac{2M(\chi)}{\chi-1}\left(\frac{1}{\chi}\right)^{\frac{|i-j|}{m}-1}$ [Benzi-Golub, 1999].
  Remark: We can shift and scale any A to have $\sigma(A) \subset [-1, 1]$.

Insights on bound (1)

- $|[\mathrm{sign}(H)]_{ij}| \leq \frac{2}{\pi} \int_0^\infty |[H(H^2 + t^2 I)^{-1}]_{ij}| \, \mathrm{d}t.$
- $q_k(y) \approx (y + t^2)^{-1}$ of best approximation, $y \in [a^2, b^2]$. Then

  $$E_{2k+1}(x(x^2 + t^2)^{-1}, [-b, -a] \cup [a, b]) \leq \|x(x^2 + t^2)^{-1} - xq_k(x^2)\|_\infty$$
  $$\leq b \, \|(y + t^2)^{-1} - q_k(y)\| = b \, E_k((y + t^2)^{-1}, [a^2, b^2]).$$
  $$= b \, C(t) q(t)^{k+1},$$

  where $C(t) = (1 + \sqrt{\frac{b^2+t^2}{a^2+t^2}})^2 / 2(b^2 + t^2)$, $q(t) = \frac{\sqrt{b^2+t^2} - \sqrt{a^2+t^2}}{\sqrt{b^2+t^2} + \sqrt{a^2+t^2}}$.
- $|[H(H^2 + t^2)^{-1}]_{ij}| \leq b \, C(t) q(t)^{\frac{|i-j|}{2m} - \frac{1}{2}}$.
- $\int_0^\infty |[H(H^2 + t^2 I)^{-1}]_{ij}| \, \mathrm{d}t \leq \int_0^\infty C(t) q(t) \, \mathrm{d}t \leq \int_0^\infty b \, C(t) \, \mathrm{d}t \cdot q(0).$
- $\int_0^\infty C(t) \, \mathrm{d}t = \int_0^\infty \frac{1}{2(b^2+t^2)} \, \mathrm{d}t + \int_0^\infty \frac{1}{2(a^2+t^2)} \, \mathrm{d}t + \int_0^\infty \frac{1}{\sqrt{b^2+t^2}\sqrt{a^2+t^2}} \, \mathrm{d}t.$
  First$= \pi/4b$; Second$= \pi/4a$; Third$\leq \pi/2\sqrt{ab}$.
- $|[\mathrm{sign}(H)]_{ij}| \leq \frac{1}{2} \left(1 + 2\sqrt{b/a} + b/a\right) q(0) = \frac{1}{2} \left(1 + \sqrt{\frac{b}{a}}\right)^2 \left(\frac{b-a}{b+a}\right)$

Insights on bound (2)

Idea: $\alpha = \frac{|i-j|}{2m} - \frac{1}{2}$, $C_1 = \frac{1}{2ab}$, $C_2 = \frac{a^2+ab+b^2}{8a^3b^3}$, $0 < \tau < \bar{\tau} := \sqrt{\frac{C_1}{C_2}}$,
$\int_0^\infty C(t)q(t)^\alpha \, dt = \int_0^\tau C(t)q(t)^\alpha \, dt + \int_\tau^\infty C(t)q(t)^\alpha \, dt$

- $q(t)^\alpha \leq q(0)^\alpha e^{-(C_1 - \tau^2 C_2)\alpha t^2}$ for $0 \leq t \leq \tau$. Then
  $\int_0^\tau C(t)q(t)^\alpha \, dt \leq C(0) \int_0^\tau q(t) \, \mathrm{d}t \leq C(0)q(0) \int_0^\infty e^{-(C_1-\tau^2 C_2)\alpha t^2} \, \mathrm{d}t$
  $\approx C(0)q(0)^\alpha / \sqrt{\frac{|i-j|}{m} - 1}$.
- $\int_\tau^\infty C(t)q(t)^\alpha \, \mathrm{d}t \leq \int_0^\infty C(t) \, \mathrm{d}t \cdot q(\tau)^\alpha$.

Insights on bound (3)

Bound for $|[H(H^2+t^2I)^{-1}]_{ij}|$.

$b = b_0 > b_1 > \cdots > b_\nu = a$ moduli of eigenvalues of H.

$$R_\ell(x) = \prod_{i=0}^{\ell-1}\left(1 - \frac{x}{b_i^2+t^2}\right)$$

$R_\ell(b_i^2+t^2) = 0$ for $i = 0,\dots,\ell-1$, $|R_\ell(b_i^2+t^2)| < 1$ for $i = \ell,\dots,\nu$ and $R_\ell(0) = 1$.

$p_k(x) = \frac{1-R_\ell(x)}{x} - q_{k-\ell}(x)$, $q_{k-\ell}(x) \approx 1/x$ best, $x \in [a^2+t^2, b_\ell^2+t^2]$, so

$$\frac{x}{x^2+t^2} - xp_k(x^2+t^2) = xR_\ell(x^2+t^2)\left(\frac{1}{x^2+t^2} - q_{k-\ell}(x^2+t^2)\right)$$

$$\begin{aligned}
&\max_{x=b_0,\dots,b_\nu}\left|\frac{x}{x^2+t^2} - xp_k(x^2+t^2)\right| \\
\le\, & b_\ell \max_{x=b_\ell,\dots,b_\nu}\left|\frac{1}{x^2+t^2} - q_{k-\ell}(x^2+t^2)\right| \\
\le\, & b_\ell C_\ell(t) q_\ell(t)^{k+1}.
\end{aligned}$$

Spectra used for the experiments

Symmetric:

$$\lambda_i^{(j)} = (-1)^j \left[1 + 0.9\left(1 - \frac{i-1}{149} - 2\sqrt{1 - \frac{i-1}{149}}\right)\right] \in [-1, -0.1] \cup [0.1, 1],$$

for $i = 1, \ldots, 150$ and $j = 0, 1$.

Non symmetric:

$$\lambda_i = (-1)^i \left[1 + 0.9\left(1 - \frac{i-1}{299} - 2\sqrt{1 - \frac{i-1}{299}}\right)\right] \in [-1, -0.1] \cup [0.1, 1],$$

for $i = 1, \ldots, 300$.