Pseudospectra, Nearest Matrices with Multiple Eigenvalues and Optimization of Symmetric Eigenvalues

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Outline

Pseudospectra

Definition (ϵ-pseudospectrum)

$$\Lambda_\epsilon(A) = \bigcup_{\|E\|_2 \le \epsilon} \Lambda(A+E)$$

$$= \left\{ \lambda \in \mathbb{C} : \|(A-\lambda I)^{-1}\|_2 \ge \frac{1}{\epsilon} \right\}$$

$$= \{ \lambda \in \mathbb{C} : \sigma_n(A-\lambda I) \le \epsilon \}$$

($\sigma_j(\cdot)$: jth largest singular value)

Properties

- $\Lambda_\epsilon(A)$ is compact.
- It has at most n disconnected components (one component around each eigenvalue).

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Wilkinson Distance

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$$\mathcal{W}(A) = \inf\{\|\delta A\|_2 : \exists\lambda \ \ (A + \delta A) \text{ has } \lambda \text{ as a multiple eigenvalue}\}$$

Note: Above definition is equivalent to the distance to the nearest defective matrix.

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Wilkinson distance measures the sensitivity of the worst-conditioned eigenvalue to perturbations.

- Any matrix close to being defective has an ill-conditioned eigenvalue.
- Conversely, Ruhe (1970) and Wilkinson (1971) showed that any matrix with an ill-conditioned eigenval. is close to being defective

Wilkinson's bound

$$\mathcal{W}(A) \leq \|A\|_2 / \sqrt{\kappa(\lambda)^2 - 1}$$

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Geometric View of Wilkinson Distance

$$\mathcal{C}(A) := \inf\{\epsilon : \#comp\,(\Lambda_\epsilon(A)) \leq n-1\}$$

- It was conjectured by Demmel (1983), and later proven by Alam and Bora (2005) that
  - $\mathcal{W}(A) = \mathcal{C}(A)$.
  - Furthermore two components of $\Lambda_\epsilon(A)$ for $\epsilon = \mathcal{C}(A)$ coalesce at λ_* iff a nearest matrix at a distance of $\mathcal{W}(A)$ has λ_* as a multiple eigenvalue.

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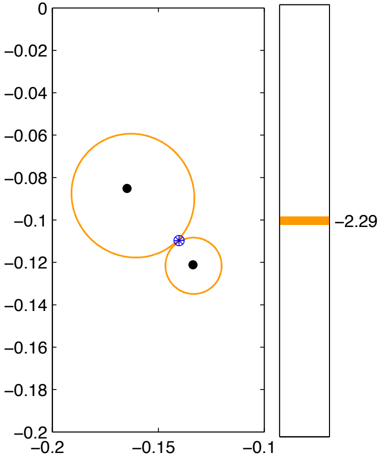
Geometric View of Wilkinson Distance

Orr-Sommerfeld matrix

- $\mathcal{W}(A) = \mathcal{C}(A) = 10^{-2.29}$
- $\lambda_* = -0.1402 - 0.1097i$ (point of coalescence marked with asterisk) is the multiple eigenvalue of a nearest matrix



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$\mathcal{W}_r(A) = \inf\{\|\delta A\|_2 : \exists\lambda \;\; (A+\delta A)$ has λ as an eigenvalue of algebraic mult $\geq r\}$

The singular value characterization (M. 2011)

$$\mathcal{W}_r(A) = \inf_{\lambda\in\mathbb{C}} \sup_{\gamma} \sigma_{nr-r+1}\left(\begin{bmatrix} A-\lambda I & \gamma_{1,2} I & \gamma_{1,3} I & \cdots & \gamma_{1,r} I \\ 0 & A-\lambda I & \gamma_{2,3} I & & \vdots \\ 0 & 0 & \ddots & & \\ & & & A-\lambda I & \gamma_{r-1,r} I \\ & & & 0 & A-\lambda I \end{bmatrix}\right)$$

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1. Geometric interpretation of $\mathcal{W}_r(A)$ in terms of pseudospectra
2. Optimizing symmetric eigenvalues numerically (e.g. computation of $\mathcal{W}_r(A)$)

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$$\mathcal{C}_r(A) := \inf\{\epsilon : \#comp\,(\Lambda_\epsilon(A)) \leq n - r + 1\}$$

- $\mathcal{W}_2(A) = \mathcal{C}_2(A)$
- Is $\mathcal{W}_r(A) = \mathcal{C}_r(A)$ for $r > 2$? Turns out not true in general.

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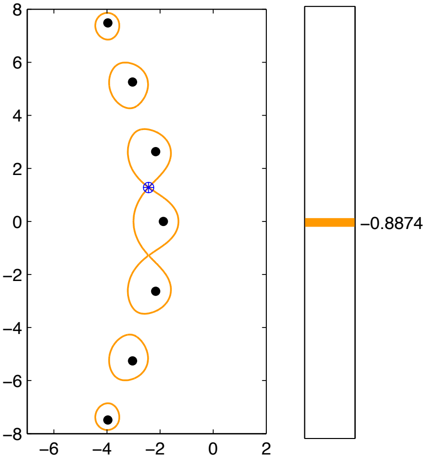
Guess in terms of Pseudospectra

Matrix resulting from a discretization of the convection-diffusion operator

- $\mathcal{W}_2(A) = \mathcal{C}_2(A) = 10^{-0.887}$
- $\lambda_* = -2.4326 + 1.2803i$ (point of coalescence marked with asterisk) is the multiple eigenvalue of a nearest matrix



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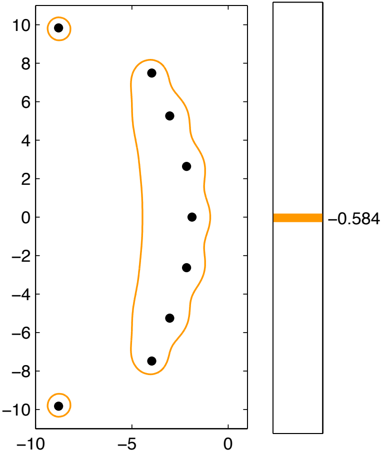
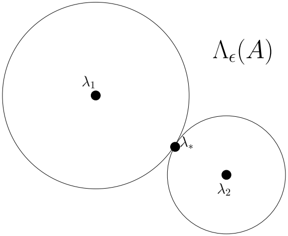
- $\Lambda_\epsilon(A)$ is illustrated for $\epsilon = 10^{-0.584}$.



Guess in terms of Pseudospectra

$\mathcal{W}_2(A) \leq \mathcal{C}_2(A)$



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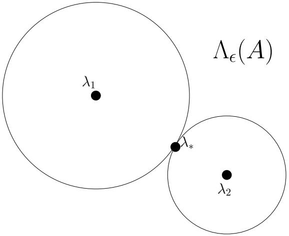

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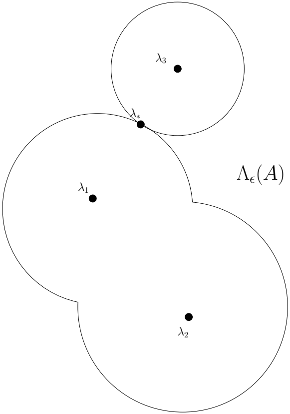
$\mathcal{W}_r(A) \not\leq \mathcal{C}_r(A)$ for $r > 2$



There doesn't exist a perturbation ΔA_* of norm ϵ s.t. $\lambda_1(A + \Delta A_*) = \lambda_2(A + \Delta A_*) = \lambda_3(A + \Delta A_*) = \lambda_*$

Outline

A Special Singular Value Function

A special singular value function

For $r > 2$ the function

$$g_{(r)}(\lambda) := \sup_{\gamma} \sigma_{nr-r+1}\Bigg(\underbrace{\begin{bmatrix} A-\lambda I & \gamma_{1,2} I & \gamma_{1,3} I & \dots & \gamma_{1,r} I \\ 0 & A-\lambda I & \gamma_{2,3} I & & \vdots \\ 0 & 0 & \ddots & & \\ & & & A-\lambda I & \gamma_{r-1,r} I \\ & & & 0 & A-\lambda I \end{bmatrix}}_{\mathcal{A}(\lambda,\gamma)\in\mathbb{C}^{rn\times rn} \;:=}\Bigg)$$

takes the role of $g(\lambda) = \sigma_n(A - \lambda I)$.

Note : $g_{(r)}(\lambda)$ is the distance from A to the nearest matrix with λ as an eigenvalue with algebraic multiplicity $\geq r$.

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A Special Singular Value Function

Theorem (Alam and Bora)

Let $\lambda_* \in \mathbb{C}$ be a critical point of $g(\lambda) = \sigma_n(A - \lambda I)$ such that

(i) $g(\lambda_*) = \epsilon > 0$, *and*

(ii) *the multiplicity of $\sigma_n(A - \lambda_* I)$ is one.*

There exists a rank one perturbation δA with norm ϵ such that $A + \delta A$ has λ_* as a (defective) multiple eigenvalue.

A Special Singular Value Function

Theorem

Let $\lambda_* \in \mathbb{C}$ be a critical point of $g_{(r-1)}(\lambda)$ such that

(i) $g_{(r-1)}(\lambda_*) = \epsilon > 0$*, and*

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There exists a rank $(r-1)$ perturbation δA with norm ϵ such that $A + \delta A$ has λ_* as a (defective) eigenvalue with algebraic multiplicity $\geq r$.

Generalized Pseudospectra

Definition (Generalized (ϵ, r)-pseudospectrum)

$$\Lambda_{\epsilon,r}(A) = \bigcup_{\|E\|_2 \leq \epsilon} \{\lambda \in \mathbb{C} : \mathrm{rank}(A + E - \lambda I)^r \leq n - r\}$$

$$= \{\lambda \in \mathbb{C} : g_{(r)}(\lambda) \leq \epsilon\}$$

Examples

- $\Lambda_{\epsilon,1}(A) = \Lambda_\epsilon(A) = \{\lambda \in \mathbb{C} : \sigma_n(A - \lambda I) \leq \epsilon\}$
- $\Lambda_{\epsilon,2}(A) = \left\{\lambda \in \mathbb{C} : \sup_\gamma \sigma_{2n-1}\left(\begin{bmatrix} A - \lambda I & \gamma I \\ 0 & A - \lambda I \end{bmatrix}\right) \leq \epsilon\right\}$

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Generalized Pseudospectra Characterization

$$\mathcal{G}_r(A) := \inf\{\epsilon : \text{ two components of } \Lambda_{\epsilon,r-1}(A) \text{ coalesce}\}.$$

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Conjecture

$\mathcal{W}_r(A) = \mathcal{G}_r(A)$

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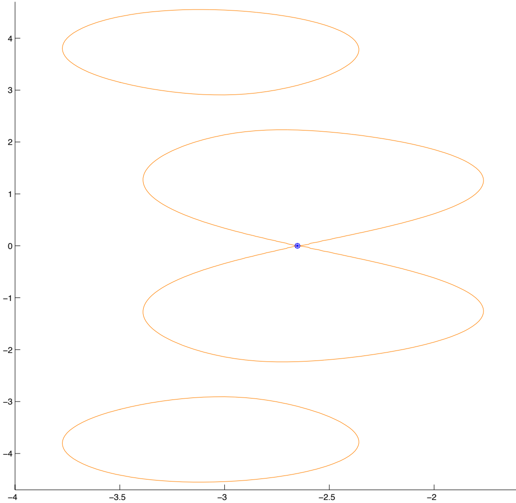
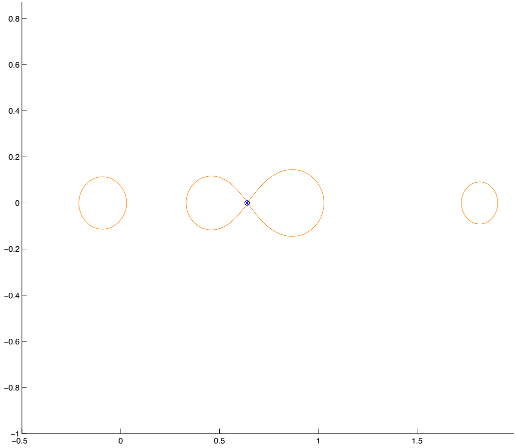
- $\mathcal{W}_3(A) = 10^{-0.584} = \mathcal{G}_3(A)$
- $\Lambda_{\epsilon,2}(A)$ is illustrated for $\epsilon = 10^{-0.584}$.
- $\lambda_* = -2.6520$ (point of coalescence marked with asterisk) is the triple eigenvalue of a nearest matrix



Generalized Pseudospectra Characterization

Hatano matrix

- $\mathcal{W}_3(A) = 10^{-1.1973} = \mathcal{G}_3(A)$
- $\Lambda_{\epsilon,2}(A)$ is illustrated for $\epsilon = 10^{-1.1973}$.
- $\lambda_* = 0.6421$ (point of coalescence marked with asterisk) is the triple eigenvalue of a nearest matrix



Proof of $\mathcal{W}_r(A) \leq \mathcal{G}_r(A)$

Theorem

Let $\lambda_* \in \mathbb{C}$ be a critical point of $g_{(r-1)}(\lambda)$ such that

(i) $g_{(r-1)}(\lambda_*) = \epsilon > 0$, *and*

(ii) *the multiplicity of the singular value $g_{(r-1)}(\lambda_*)$ is one.*

There exists a rank $(r-1)$ perturbation δA with norm ϵ such that $A + \delta A$ has λ_* as a (defective) eigenvalue with algebraic multiplicity $\geq r$.

Suppose two components of $\Lambda_{\epsilon,r-1}(A)$ coalesce at λ_* for $\epsilon = \mathcal{G}_r(A)$.

- Then $g_{(r-1)}(\lambda_*) = \mathcal{G}_r(A)$ and λ_* is a critical point of $g_{(r-1)}(\lambda)$.
- If the multiplicity of $g_{(r-1)}(\lambda_*) = \mathcal{G}_r(A)$ is one, the theorem above implies the existence of a perturbation ΔA_* of norm $\mathcal{G}_r(A)$ such that $(A + \Delta A_*)$ has λ_* as an eigenvalue with algebraic multiplicity $\geq r$.

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Analyticity Result

Theorem (Rellich)

Let $\mathcal{A}(\omega) : \mathbb{R} \rightarrow \mathbb{C}^{n \times n}$ be a Hermitian matrix function that depends on ω analytically. Each root of the characteristic polynomial of $\mathcal{A}(\omega)$ is an analytic function of ω.

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Derivatives of Eigenvalues

Let $\tilde{\lambda}(\omega)$ be one of the unordered eigenvalues with the assoc. unit eigenvector $\tilde{v}(\omega)$ (which also varies analytically w.r.t ω).

First Derivative

$$\tilde{\lambda}'(\omega) = \tilde{v}^*(\omega)\frac{d\mathcal{A}(\omega)}{d\omega}\tilde{v}(\omega)$$

Second Derivative

$$\tilde{\lambda}''(\omega) = \tilde{v}^*(\omega)\frac{d^2\mathcal{A}(\omega)}{d\omega^2}\tilde{v}(\omega) + 2\tilde{v}^*(\omega)\frac{d\mathcal{A}(\omega)}{d\omega}\left[\tilde{\lambda}(\omega)I - \mathcal{A}(\omega)\right]^+\frac{d\mathcal{A}(\omega)}{d\omega}\tilde{v}(\omega)$$

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Derivatives of Eigenvalues

Some observations helpful algorithmically

- Analyticity implies the boundedness of derivatives. In particular we will exploit the existence of a γ such that

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Outline

Quadratic Models

Some notation

- Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a piece-wise analytic function defined in terms of analytic functions $f_1, \dots, f_n : \mathbb{R} \rightarrow \mathbb{R}$,
- γ be an upper bound on the second derivatives (in absolute value) of f_j for $j = 1, \dots, n$,
- $x_k, x \in \mathbb{R}$ and $x_{k,1}, \dots, x_{k,m}$ be points in (x_k, x) where f is not analytic, and
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Quadratic Models

$$f(x) = f(x_k) + \sum_{\ell=0}^{m} \int_{x_{k,\ell}}^{x_{k,\ell+1}} f'(t)dt$$

Note: $x_{k,0} = x_k$ and $x_{k,m+1} = x$

Quadratic Model Function about x_k

$$q_k(x) := f(x_k) + \underline{f}'(x_k)(x - x_k) - \frac{\gamma}{2}(x - x_k)^2$$

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The Algorithm

Suppose that the global minimizer of f is in $[a, b]$.

1. Initially $x_0 = a$, $x_1 = b$ and $s = 1$. Evaluate $f(x_0)$, $f(x_1)$, $f'(x_0)$, and $f'(x_1)$.
2. Find the global minimizer of x_* of $q(x)$ where

$$q(x) = \max_{k=0,s} q_k(x).$$

3. Set $x_{s+1} = x_*$, evaluate $f(x_{s+1})$, $f'(x_{s+1})$.
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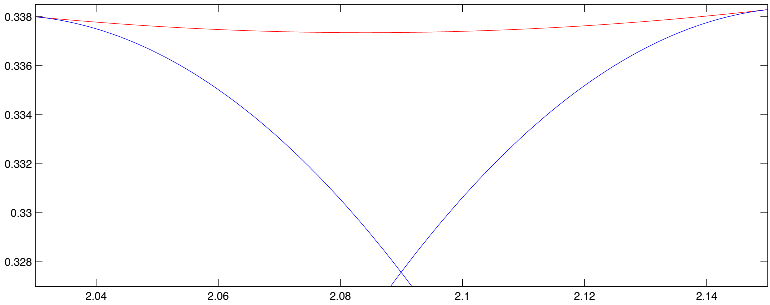
Illustration of the algorithm on $\sigma_n(A - \omega i I)$ where σ_n denotes the smallest singular value.



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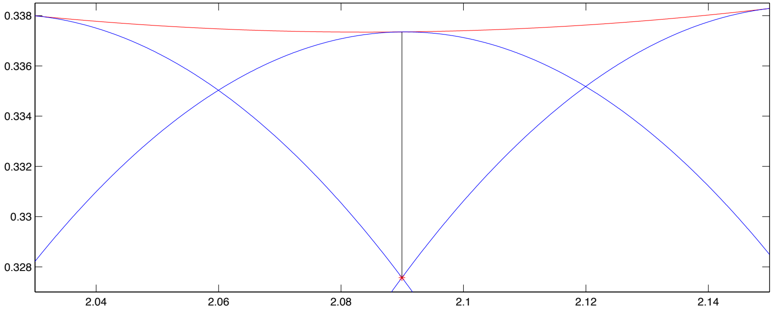

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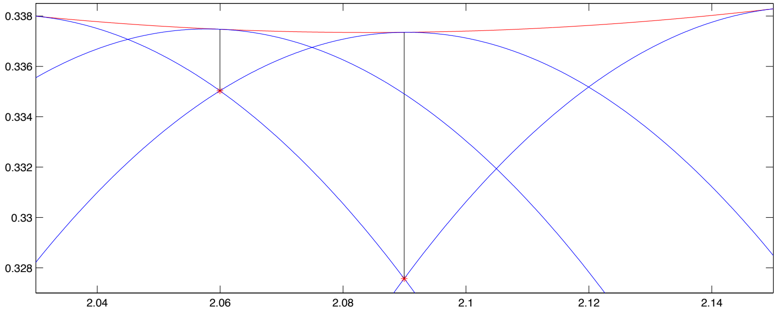

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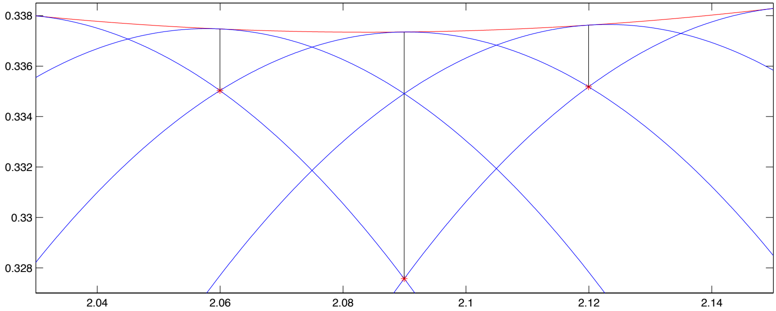

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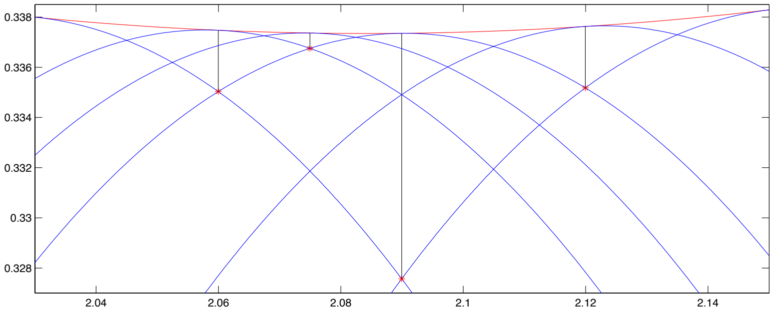

Case Study

Distance to Instability

$$\begin{aligned}\beta(A) &:= \inf\{\|\Delta A\|_2 : x'(t) = (A+\Delta A)x(t) \text{ is unstable}\} \\ &= \inf_{\omega\in\mathbb{R}} \sigma_n(A - \omega i I)\end{aligned}$$

Matrices result from a discretization of the Airy operator

# of function evaluations

n / ϵ	10^{-3}	10^{-5}	10^{-7}	10^{-9}	10^{-11}
25	40	48	56	62	68
100	46	54	65	74	82
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Matrices result from a discretization of the Airy operator

cpu-times

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25	0.06	0.09	0.09	0.10	0.12
100	0.87	0.96	1.13	1.27	1.41
400	13.53	15.73	18.82	21.02	23.26
1600	362	409	474	505	506

Outline

Non-analyticity Result

- For a multivariate Hermitian function $\mathcal{A}(\omega) : \mathbb{R}^n \rightarrow \mathbb{C}^{n \times n}$ that depend on ω analytically an unordered eigenvalue $\tilde{\lambda}(\omega)$ is not analytic in general.

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Model Functions

- Let $f : \mathbb{R}^n \to \mathbb{R}$ be analytic over any line in $\mathbb{R}^n$, and
- γ be an upper bound on the second derivative (on any line in $\mathbb{R}^n$) of f.

Quadratic Model Function about x_k

$$q_k(x) := f(x_k) + \nabla f(x_k)^T (x - x_k) - \frac{\gamma}{2}(x - x_k)^T (x - x_k)$$

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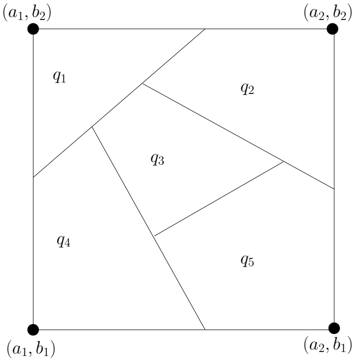

- Split the region where a global minimizer is known to lie into subregions.
- In subregion q_k the quadratic function $q_k(x) \geq q_j(x) \;\; \forall j \neq k$.

The Algorithm

Finding a global minimizer of $q(x) = \max_{k=0,s} q_k(x)$

Solve the quadratic program (QP) for $k = 0, \ldots, s$.

$$\begin{array}{ll} \text{minimize}_{x \in \mathbb{R}^n} & q_k(x) \\ \text{subject to} & q_k(x) \geq q_j(x), \quad j \neq k \\ & x_\ell \in [a_\ell, b_\ell] \quad \ell = 1, \ldots, n \end{array}$$

The Algorithm

Notes on the quadratic program

- The constraints $q_k(x) \geq q_j(x)$ are linear.
- The fact that $q_k(x)$ is negative definite makes the QP NP-hard.
- The solution will be attained at a vertex. There are at most $\binom{s}{n}$ vertices.
- In practice number of vertices is much smaller; for $n = 2$ typically each QP has 5-6 vertices regardless of s.
- For small n each QP can be solved efficiently.

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The Algorithm

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Case Study

Wilkinson Distance

$$\mathcal{W}(A) := \inf\{\|\delta A\|_2 : \exists\lambda \;\; (A+\delta A) \text{ has } \lambda \text{ a multiple eigenvalue}\}$$
$$= \inf_{\lambda\in\mathbb{C}} \sup_{\gamma\in\mathbb{C}} \sigma_{2n-1}\left(\begin{bmatrix} A-\lambda I & \gamma I \\ 0 & A-\lambda I \end{bmatrix}\right)$$

Random matrices

# of function evaluations

n / ϵ	10^{-2}	10^{-3}	10^{-4}	10^{-5}
10	74	80	84	89
20	102	111	114	115
40	101	135	148	155

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Random matrices

cpu-times

n / ϵ	10^{-2}	10^{-3}	10^{-4}	10^{-5}
10	4.90	6.09	6.99	9.22
20	24.5	30.1	34.0	34.3
40	32.8	69.7	90.4	103.6

Summary

- A conjecture has been made relating the the psedospectra and generalized Wilkinson distance.
- In particular it is shown that $\mathcal{W}_r(A) \leq \mathcal{G}_r(A)$.
- A generic algorithm is introduced for the optimization of symmetric eigenvalues based on their analyticity.
- Future work
  - The direction $\mathcal{W}_r(A) \geq \mathcal{G}_r(A)$ remains open.
  - Improvements on the algorithm for the optimization of eigenvalues in the multivariate-case

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