### Numerical Optimization of Eigenvalues of Hermitian Matrix Functions

#### Emre Mengi

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joint with Daniel Kressner (EPF-Lausanne), Ivica Nakić (Univ of Zagreb), Ninoslav Truhar (Univ of Osijek), Mustafa Kılıç (Koç) and E. Alper Yıldırım (Koç)

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### Outline



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Introduction

- Perturbation Results
- One Dimensional Algorithm
- Multi-dimensional Algorithm
- Pencils with Specified Eigenvalues
  - Definition and Motivation

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Numerical Optimization of Eigenvalues of Matrix Functions Pencils with Specified Eigenvalues Summary

Motivation

### Wilkinson Distance

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \hookrightarrow \begin{bmatrix} 0 & 1 \\ \epsilon & 0 \end{bmatrix}$$
$$\lambda_{\pm}(\epsilon) = \pm \sqrt{\epsilon}$$
$$\frac{\lambda_{\pm}(\epsilon) - \lambda(0)}{\epsilon} = \pm \frac{1}{\sqrt{\epsilon}}$$

Eigenvalues associated with a Jordan block are very sensitive to perturbations.

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$$\begin{bmatrix} 0 & 1 \\ 0 & \beta \end{bmatrix} \hookrightarrow \begin{bmatrix} 0 & 1 \\ \epsilon & \beta \end{bmatrix}$$
$$\lambda_{\pm}(\epsilon) = \frac{\beta \pm \sqrt{\beta^2 + 4\epsilon}}{2}$$
$$\frac{\lambda_{-}(\epsilon) - \lambda_{-}(0)}{\epsilon} = \frac{1}{\beta} + O(\epsilon)$$

Matrices close to defective matrices have also very sensitive eigenvalues.

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### Wilkinson Distance

#### Absolute condition number of an eigenvalue $\lambda$

$$\kappa(\lambda) = \lim_{\delta \to 0^+} \sup_{\|\delta A\| \le \delta} \frac{|\lambda(\delta A) - \lambda|}{\|\delta A\|} = \frac{1}{y^* x}$$

where

 $y, x \in \mathbb{C}^n$ : unit left and right eigenvectors associated with  $\lambda$ .

- Jordan blocks:  $y^*x = 0$
- Best conditioned Normal matrices:  $y = x \iff y^* x = 1$

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Numerical Optimization of Eigenvalues of Matrix Functions Pencils with Specified Eigenvalues Summary

### Wilkinson Distance

#### J.H. Wilkinson, The Algebraic Eigenvalue Problem

The eigenvalues corresponding to non-linear elementary divisors must, in general, be regarded as ill-conditioned ... However, we must not be misled into thinking that this is the main form of ill-conditioning. Even if the eigenvalues are distinct and well separated they may still be very ill-conditioned.

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Numerical Optimization of Eigenvalues of Matrix Functions Pencils with Specified Eigenvalues Summary

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### Wilkinson Distance



- Condition numbers for W(0),  $\kappa(\lambda) = \frac{20^{19}}{10! \ 9!}$  for  $\lambda = 10, 11$
- $W(\epsilon)$  has  $\lambda = 10.5$  as a multiple eigenvalue for  $\epsilon \approx 8 \times 10^{-14}$ .

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### Wilkinson Distance



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### Wilkinson Distance



• Condition numbers for W(0),

$$\kappa(\lambda) = \frac{20^{19}}{10! \ 9!}$$
 for  $\lambda = 10, 11$ 

W(ε) has λ = 10.5 as a multiple eigenvalue for ε ≈ 8 × 10<sup>-14</sup>.

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Numerical Optimization of Eigenvalues of Matrix Functions Pencils with Specified Eigenvalues Summary

### Wilkinson Distance

#### Definition (Wilkinson Distance)

The distance in 2-norm from  $A \in \mathbb{C}^{n \times n}$  to the nearest matrix with a multiple eigenvalue

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

is called the Wilkinson distance of A.

Wilkinson's bound

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

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Motivation

## Wilkinson Distance

Singular Value Characterization

#### Define also

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

# Theorem (Malyshev, 1999) (i) Then for all $\lambda \in \mathbb{C}$ $\mathcal{W}(A, \lambda) = \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \left( \begin{bmatrix} A - \lambda I & \gamma I \\ 0 & A - \lambda I \end{bmatrix} \right).$ (ii) Consequently $\mathcal{W}(A) = \inf_{\lambda \in \mathbb{C}} \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \left( \begin{bmatrix} A - \lambda I & \gamma I \\ 0 & A - \lambda I \end{bmatrix} \right)$

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## Wilkinson Distance

Singular Value Characterization

For a matrix pencil  $L(\mu) := A + \mu B$  with  $A, B \in \mathbb{C}^{n \times n}$ 

 $\mathcal{W}(L,\lambda) := \inf\{\|\delta A\|_2 : (A + \delta A) + \mu B \text{ has } \lambda \text{ as a multiple eigenvalue}\}.$ 

Theorem (Kressner, M, Nakic, Truhar 2011) (I) For all  $\lambda \in \mathbb{C}$   $\mathcal{W}(L, \lambda) = \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \left( \begin{bmatrix} A + \lambda B & \gamma B \\ 0 & A + \lambda B \end{bmatrix} \right)$ . (II) Consequently  $\mathcal{W}(L) = \inf_{\lambda \in \mathbb{C}} \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \left( \begin{bmatrix} A + \lambda B & \gamma B \\ 0 & A + \lambda B \end{bmatrix} \right)$ .

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## Wilkinson Distance

Singular Value Characterization

For a matrix polynomial 
$$P(\mu) := \sum_{j=0}^{k} \mu^{j} A_{j}$$
 with  $A_{j} \in \mathbb{C}^{n \times n}$ 

$$\mathcal{W}(\boldsymbol{P},\lambda) := \inf\{\|\delta\boldsymbol{A}\|_{2} : \sum_{j=0}^{k} \mu^{j} \boldsymbol{A}_{j} + \delta\boldsymbol{A} \text{ has } \lambda \text{ as a multiple eigenvalue}\}.$$

eorem (Karow, M, Pelen 2012) For all  $\lambda \in \mathbb{C}$  $\mathcal{W}(P, \lambda) = \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \begin{pmatrix} P(\lambda) & \gamma P'(\lambda) \\ 0 & P(\lambda) \end{bmatrix}$ 

 $\mathcal{W}(P) = \inf_{\lambda \in \mathbb{C}} \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1}$ 

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Theorem (Karow, M, Pelen 2012)

(i) For all  $\lambda \in \mathbb{C}$   $\mathcal{W}(P,\lambda) = \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \left( \begin{bmatrix} P(\lambda) & \gamma P'(\lambda) \\ 0 & P(\lambda) \end{bmatrix} \right).$ (ii) Consequently  $\mathcal{W}(P) = \inf_{\lambda \in \mathbb{C}} \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \left( \begin{bmatrix} P(\lambda) & \gamma P'(\lambda) \\ 0 & P(\lambda) \end{bmatrix} \right).$ 

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Theorem (Karow, M, Pelen 2012)

(i) For all 
$$\lambda \in \mathbb{C}$$

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(ii) Consequently

$$\mathcal{W}(\boldsymbol{P}) = \inf_{\lambda \in \mathbb{C}} \sup_{\gamma \in \mathbb{R}^+} \sigma_{2n-1} \left( \begin{bmatrix} \boldsymbol{P}(\lambda) & \gamma \boldsymbol{P}'(\lambda) \\ \boldsymbol{0} & \boldsymbol{P}(\lambda) \end{bmatrix} \right)$$

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### Wilkinson Distance

Numerical Computation

Inner maximization (Secant or Quasi-Newton)

Any stationary point  $\gamma_* \in \mathbb{R}^+$  of the inner function

$$f(\lambda,\gamma) = \sigma_{2n-1} \left( \begin{bmatrix} A - \lambda I & \gamma I \\ 0 & A - \lambda I \end{bmatrix} \right)$$

is a global maximizer.



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## Wilkinson Distance

Numerical Computation

Outer minimization (Lipschitzness and Analyticity)

 $f(\lambda, \gamma)$  is Lipschitz continuous w.r.t.  $\lambda$  and  $\gamma$  (from the Weyl's theorem).

#### Theorem (Weyl

Let A and E be Hermitian  $n \times n$  matrices and  $\lambda_j(\cdot)$  denote the jth largest eigenvalue of its matrix argument. Then  $|\lambda_j(A) - \lambda_j(A + E)| \le ||E||_2$ .

- W(A, λ) = sup<sub>γ</sub> f(λ, γ) is Lipschitz continuous w.r.t. λ. Lipschitzness solely yields slow-converging algorithms.
- W(A, λ) = sup<sub>γ</sub> f(λ, γ) is also piece-wise analytic w.r.t. λ. Analyticity may yield faster algorithms.

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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### Analyticity Result

#### Theorem (Rellich)

# Let $\mathcal{A}(\omega) : \mathbb{R} \to \mathbb{C}^{n \times n}$ be a Hermitian matrix function that depends on $\omega$ analytically.

- (i) The n roots of the characteristic polynomial of A(ω) can be arranged so that each root λ̃<sub>j</sub>(ω) for j = 1,..., n is an analytic function of ω.
- (ii) There exists an eigenvector  $v_j(\omega)$  associated with  $\tilde{\lambda}_j(\omega)$  for j = 1, ..., n satisfying

(1) 
$$\left( \widetilde{\lambda}_j(\omega) I - \mathcal{A}(\omega) \right) v_j(\omega) = 0 \quad \forall \omega \in \mathbb{R},$$

(2) 
$$\|v_j(\omega)\|_2 = 1 \quad \forall \omega \in \mathbb{R},$$

(3) 
$$v_j^*(\omega)v_k(\omega)=0 \ orall \omega\in\mathbb{R}$$
 for  $k
eq j$ , and

(4)  $\vec{v}_i(\omega)$  is an analytic function of  $\omega$ .

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(ii) There exists an eigenvector v<sub>j</sub>(ω) associated with λ<sub>j</sub>(ω) for j = 1,..., n satisfying
(1) (λ<sub>j</sub>(ω)*I* - A(ω)) v<sub>j</sub>(ω) = 0 ∀ω ∈ ℝ,
(2) ||v<sub>j</sub>(ω)||<sub>2</sub> = 1 ∀ω ∈ ℝ,
(3) v<sub>j</sub><sup>\*</sup>(ω)v<sub>k</sub>(ω) = 0 ∀ω ∈ ℝ for k ≠ j, and
(4) v<sub>j</sub>(ω) is an analytic function of ω.

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# Analyticity Result

The eigenvalues  $\lambda_1(\omega), \ldots, \lambda_n(\omega)$  ordered from largest to smallest of  $\mathcal{A}(\omega)$  are continuous and piece-wise analytic.

e.g.  
Let 
$$\mathcal{A}(\omega) = \begin{bmatrix} 0 & \omega \\ \omega & 0 \end{bmatrix}$$
 with analytic eigenvalues  
 $\tilde{\lambda}_1(\omega) = \omega$  and  $\tilde{\lambda}_2(\omega) = -\omega$ 

Sorted continuous and piece-wise analytic eigenvalues

$$\lambda_1(\omega) = |\omega|$$
 and  $\lambda_2(\omega) = -|\omega|$ 

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# Analyticity Result

The eigenvalues  $\lambda_1(\omega), \ldots, \lambda_n(\omega)$  ordered from largest to smallest of  $\mathcal{A}(\omega)$  are continuous and piece-wise analytic.

e.g.  
Let 
$$\mathcal{A}(\omega) = \begin{bmatrix} 0 & \omega \\ \omega & 0 \end{bmatrix}$$
 with analytic eigenvalue  
 $\tilde{\lambda}_1(\omega) = \omega$  and  $\tilde{\lambda}_2(\omega) = -\omega$ 

Sorted continuous and piece-wise analytic eigenvalues

$$\lambda_1(\omega) = |\omega|$$
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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### Analyticity Result

# The analyticity result does not extend to non-Hermitian functions.

e.g. the roots of the characteristic polynomial of

$$\mathcal{A}(\omega) = \left[ \begin{array}{cc} \mathbf{0} & \mathbf{1} \\ \omega & \mathbf{0} \end{array} \right]$$

are given by  $\pm \sqrt{\omega}$  and not analytic.

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# **Derivatives of Eigenvalues**

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

**First Derivative** 

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

Second Derivative

$$\tilde{\lambda}''(\omega) = v^*(\omega) \frac{d^2 \mathcal{A}(\omega)}{d\omega^2} v(\omega) + 2 \sum_{j, \tilde{\lambda}_j(\omega) \neq \tilde{\lambda}(\omega)} \frac{1}{\tilde{\lambda}(\omega) - \tilde{\lambda}_j(\omega)} \left| v^*(\omega) \frac{d \mathcal{A}(\omega)}{d\omega} v_j(\omega) \right|^2$$

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# **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

$$\left| \widetilde{\lambda}''(\omega) \right| \leq \gamma \quad \forall \omega.$$

• Once  $\tilde{\lambda}(\omega)$  is computed,  $\tilde{\lambda}'(\omega)$  is available for free.

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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#### **Derivatives of Eigenvalues**



Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

#### Outline



- Pencils with Specified Eigenvalues
  - Definition and Motivation

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

#### **Quadratic Models**

#### The algorithm is based on quadratic models.

- Let *f* : ℝ → ℝ be a piece-wise analytic and continuous function in terms of analytic functions *f*<sub>1</sub>,..., *f<sub>n</sub>* : ℝ → ℝ.
- The quadratic model  $q_k(x)$  about  $x_k \in \mathbb{R}$  satisfies  $q_k(x_k) = f(x_k)$  and  $q'_k(x_k) = \underline{f}'(x_k) := \min_{j=1,n} f'_j(x_k)$ .
- Furthermore for all  $x \in \mathbb{R}$  the quadratic model satisfies  $f(x) \ge q_k(x)$

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#### **Quadratic Models**

Let  $\gamma$  be an upper bound on second derivatives (in abs value) of  $f_j$  and  $x_{k,1}, \ldots, x_{k,m}$  be points in  $(x_k, x)$  where f is not analytic

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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

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

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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

Note:  $f'(t) \geq \underline{f}'(x_k) - \gamma(t - x_k) \quad \forall t \in (x_k, x) \setminus \{x_{k,1}, \dots, x_{k,m}\}$ 

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

#### **Quadratic Models**

#### Quadratic Model about $x_k$

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

satisfies  $f(x) \ge q_k(x)$  for all  $x \in \mathbb{R}$ .

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# The Algorithm

#### Task : locate a global minimizer of f on a given interval [a, b].

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

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

- 3 Set  $x_{s+1} = x_*$ , evaluate  $f(x_{s+1}), f'(x_{s+1})$ .
- Let  $\ell = q(x_*)$  and  $u = max_{k=0,s+1}f(x_k)$ .
- **(**) While  $u l > \epsilon$ , increment *s* and repeat steps 2-4.

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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#### The Algorithm

Illustration of the algorithm on  $\sigma_n(A - \omega iI)$  where  $\sigma_n$  denotes the smallest singular value.



Emre Mengi Optimization of Eigenvalues of Hermitian Matrix Functions

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One Dimensional Algorithm

#### **Generic Analyticity**

Many eigenvalue functions of interest are generically analytic on a dense subset.

e.g. 
$$f(\omega) := \lambda_1 \left( \frac{A e^{i\theta} + A^* e^{-i\theta}}{2} \right)$$
 is generically *analytic at all*  $\theta$ .



Optimization of Eigenvalues of Hermitian Matrix Functions
Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### Modulus of the outermost point in the field of values

$$F(A) = \{z^*Az \mid z \in \mathbb{C}^n \text{ s.t. } \|z\|_2 = 1\}$$

is called the numerical radius.

Case Study

# Numerical Radius $r(A) := \max_{[0,2\pi)} \lambda_1 \left( \frac{A \cdot e^{i\theta} + A^* e^{-i\theta}}{2} \right)$

- Field of values is a convex set.
- Contains the eigenvalues.
- Numerical radius is used to analyze the convergence of the classical iterative algorithms for linear systems.

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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# Case Study



Dotted-lines represent the boundary of the field of values, red circle marks the outermost point in the field of values

Optimization of Eigenvalues of Hermitian Matrix Functions



One Dimensional Algorithm

### Computation of numerical radius for matrices resulting from Poisson equation

# of function evaluations					
$n/\epsilon$	10 <sup>-4</sup>	10 <sup>-6</sup>	10 <sup>-8</sup>	10 <sup>-10</sup>	10 <sup>-12</sup>
100	45	54	64	73	81
400	44	54	65	74	83
900	67	77	88	99	119

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### Computation of numerical radius for matrices resulting from Poisson equation

cpu-times					
$n/\epsilon$	10 <sup>-4</sup>	10 <sup>-6</sup>	10 <sup>-8</sup>	10 <sup>-10</sup>	$10^{-12}$
100	1.0	1.2	1.4	1.6	1.9
400	9.0	10.9	12.9	14.6	17.5
900	156	177	201	225	267

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# Case Study

 $H_{\infty}$  norm

The transfer function for the linear system

$$x'(t) = Ax(t) + Bu(t), y(t) = Cx(t) + Du(t)$$

is given by  $H(s) = C(sI - A)^{-1}B + D$ .

# $\sup_{\omega\in\mathbb{R}} \sigma_1\left(C(\omega i l - A)^{-1}B + D\right)$

Matrices result from a discretization of the heat equation

### # of function evaluations

$n/\epsilon$	$10^{-4}$	$10^{-6}$	$10^{-8}$	$10^{-10}$
100	23	32	39	47
200	22	29		44
400	18	24	29	34
	16	19	22	27

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Emre Mengi Optimization of Eigenvalues of Hermitian Matrix Functions

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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### Matrices result from a discretization of the heat equation

### cpu-times

$n/\epsilon$	10 <sup>-4</sup>	10 <sup>-6</sup>	10 <sup>-8</sup>	$10^{-10}$
100	0.3	0.5	0.5	0.6
200	1.5	1.9	2.3	2.8
400	8.3	10.8	12.9	17.6
800	53	63	73	92

Emre Mengi Optimization of Eigenvalues of Hermitian Matrix Functions

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### Outline



Pencils with Specified Eigenvalues
 Definition and Motivation

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# Non-analyticity Result

 For a multivariate Hermitian function A(ω) : ℝ<sup>n</sup> → C<sup>n×n</sup> that depends on ω the eigenvalues λ̃<sub>j</sub>(ω) are not analytic in general no matter how they are ordered.

e.g. The roots of the characteristic polynomial of

$$\mathcal{A}(\omega) = \begin{bmatrix} \omega_1 & \frac{\omega_1 + \omega_2}{2} \\ \frac{\omega_1 + \omega_2}{2} & \omega_2 \end{bmatrix}$$

are given by  $\omega_1 + \omega_2 \pm \sqrt{2}\sqrt{\omega_1^2 + \omega_2^2}$  and not analytic.

But there is an ordering such that λ
<sub>j</sub>(ω) for j = 1,..., n is analytic over any line in ℝ<sup>n</sup> (Rellich's result).

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### Model Functions

### • Let $f : \mathbb{R}^n \to \mathbb{R}$ be analytic over any line in $\mathbb{R}^n$ , and

• The quadratic model  $q_k(x)$  about  $x_k \in \mathbb{R}^n$  satisfies  $q_k(x_k) = f(x_k)$  and  $\nabla q_k(x_k) = \nabla f(x_k)$ .

• Furthermore for all  $x \in \mathbb{R}^n$  the quadratic model satisfies  $f(x) \ge q_k(x).$ 

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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- Let  $f : \mathbb{R}^n \to \mathbb{R}$  be analytic over any line in  $\mathbb{R}^n$ , and
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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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### **Quadratic Models**

Let  $\phi(\alpha) := f(x_k + \alpha p)$  where  $p := (x - x_k)/||x - x_k||$  and  $\gamma$  be an upper bound on the second derivative (on any line in  $\mathbb{R}^n$ ) of  $\phi$ . Denote also points in the interval  $[0, ||x - x_k||]$  where  $\phi(\alpha)$  is not differentiable by  $\alpha^{(1)}, \ldots, \alpha^{(m)}$ .

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### **Quadratic Models**

Let  $\phi(\alpha) := f(x_k + \alpha p)$  where  $p := (x - x_k)/||x - x_k||$  and  $\gamma$  be an upper bound on the second derivative (on any line in  $\mathbb{R}^n$ ) of  $\phi$ . Denote also points in the interval  $[0, ||x - x_k||]$  where  $\phi(\alpha)$  is not differentiable by  $\alpha^{(1)}, \ldots, \alpha^{(m)}$ .

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

Note:  $\alpha^{(0)} := 0$  and  $\alpha^{(m+1)} := \|x - x_k\|$ .

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### **Quadratic Models**

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

$$\geq f(x_k) + \sum_{\ell=0}^m \int_{\alpha^{(\ell)}}^{\alpha^{(\ell+1)}} \phi'(0) - \gamma t dt$$

Note:  $\phi'(t) = \phi'(0) - \gamma t = \nabla f(x_k)^T \rho - \gamma t$ 

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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

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### **Model Functions**

### Quadratic Model about $x_k$

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

satisfies  $f(x) \ge q_k(x)$  for all  $x \in \mathbb{R}^n$ .

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# The Algorithm

Task : locate a global minimizer of  $f : \mathbb{R}^n \to \mathbb{R}$  on a given box

$$\mathcal{B} := \{ x \in \mathbb{R}^n \mid x_\ell \in [a_\ell, b_\ell] \text{ for } \ell = 1, \dots, n \}$$

- Initially let  $x_0$  be the midpoint of the box and s = 0. Evaluate  $f(x_0)$  and  $f'(x_0)$ .
- ② Find the global minimizer  $x_*$  of q(x) on  $\mathcal{B}$  where

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

- 3 Set  $x_{s+1} = x_*$ , evaluate  $f(x_{s+1}), f'(x_{s+1})$ .
- Let  $\ell = q(x_*)$  and  $u = max_{k=0,s+1}f(x_k)$ .
- **(**) While  $u l > \epsilon$ , increment *s* and repeat steps 2-4.

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Initially let x<sub>0</sub> be the midpoint of the box and s = 0.
 Evaluate f(x<sub>0</sub>) and f'(x<sub>0</sub>).

<sup>(2)</sup> Find the global minimizer  $x_*$  of q(x) on  $\mathcal{B}$  where  $q(x) = \max_{k=0.5} q_k(x)$ .

- 3 Set  $x_{s+1} = x_*$ , evaluate  $f(x_{s+1}), f'(x_{s+1})$ .
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- Let  $\ell = q(x_*)$  and  $u = max_{k=0,s+1}f(x_k)$ .
- Solution While  $u l > \epsilon$ , increment *s* and repeat steps 2-4.

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# The Algorithm

Task : locate a global minimizer of  $f : \mathbb{R}^n \to \mathbb{R}$  on a given box

$$\mathcal{B} := \{ x \in \mathbb{R}^n \mid x_\ell \in [a_\ell, b_\ell] \text{ for } \ell = 1, \dots, n \}$$

- Initially let x<sub>0</sub> be the midpoint of the box and s = 0.
   Evaluate f(x<sub>0</sub>) and f'(x<sub>0</sub>).
- ② Find the global minimizer  $x_*$  of q(x) on  $\mathcal{B}$  where

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

- Set  $x_{s+1} = x_*$ , evaluate  $f(x_{s+1}), f'(x_{s+1})$ .
- Let  $\ell = q(x_*)$  and  $u = max_{k=0,s+1}f(x_k)$ .
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- Initially let  $x_0$  be the midpoint of the box and s = 0. Evaluate  $f(x_0)$  and  $f'(x_0)$ .
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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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The calculation of a global minimizer of

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

on the box  $\ensuremath{\mathcal{B}}$  appears to be difficult computationally.

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# The Algorithm

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

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

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Emre Mengi Optimization of Eigenvalues of Hermitian Matrix Functions

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

## The Algorithm

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

# Solve the quadratic program (QP) for k = 0, ..., s.minimize\_{x \in \mathbb{R}^n} q\_k(x)subject to $q_k(x) \ge q_j(x), j \ne k$ $x_\ell \in [a_\ell, b_\ell] \ \ell = 1, ..., n$

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

# The Algorithm

### Notes on the quadratic program

- The constraints  $q_k(x) \ge q_j(x)$  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  $\begin{pmatrix} s+1 \\ n \end{pmatrix}$  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.

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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### Convergence

#### Theorem (Convergence)

Let  $f : \mathbb{R}^n \to \mathbb{R}$  be an analytic function. Then every limit point of the sequence of iterates generated by the multi-dimensional algorithm is a global minimizer of f over the box

$$\mathcal{B} := \{ x \in \mathbb{R}^n : x_\ell \in [a_\ell, b_\ell] \text{ for } \ell = 1, \dots, n \}$$

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Multi-dimensional Algorithm

Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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 $\mathcal{B} := \{x \in \mathbb{R}^n : x_\ell \in [a_\ell, b_\ell] \text{ for } \ell = 1, \dots, n\}$ 

In practice the rate of convergence appears *linear* due to the fact that when the estimates are close to global minimizers, the algorithm essentially becomes a steepest descent algorithm.

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### Case Study

#### Distance to Uncontrollability

$$\mathcal{U}(A,B) := \inf\{ \left\| \begin{bmatrix} \Delta A & \Delta B \end{bmatrix} \right\|_{2} | x'(t) = (A + \Delta A)x(t) + (B + \Delta B)u(t)$$
  
is uncontrollable}
$$= \min_{z \in \mathbb{C}} \sigma_n \left( \begin{bmatrix} A - zI & B \end{bmatrix} \right)$$

#### Matrices resulting from heat equation

#### # of function evaluations

$n/\epsilon$	$10^{-2}$	$10^{-4}$	$10^{-6}$	$10^{-8}$
100	345	548	747	
200	456	569	767	1066
400	615	734	849	1047

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Multi-dimensional Algorithm

### **Case Study**

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Multi-dimensional Algorithm

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cpu-times					
n/ε	10 <sup>-2</sup>	10 <sup>-4</sup>	10 <sup>-6</sup>	10 <sup>-8</sup>	
100	38	56	73	82	
200	53	65	84	113	
400	315	374	427	521	

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Multi-dimensional Algorithm

Optimization of Eigenvalues of Hermitian Matrix Functions

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

### Case Study

Level sets of the function  $g(z) = \sigma_n \begin{pmatrix} A - zI & B \end{bmatrix}$  on the complex plane.



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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

#### Wilkinson Distance

Case Study

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

#### Random matrices

#### # of function evaluations

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

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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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$n/\epsilon$	10 <sup>-2</sup>	10 <sup>-3</sup>	$10^{-4}$	10 <sup>-5</sup>
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Perturbation Results One Dimensional Algorithm Multi-dimensional Algorithm

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#### cpu-times

$n/\epsilon$	10 <sup>-2</sup>	10 <sup>-3</sup>	10 <sup>-4</sup>	10 <sup>-5</sup>
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

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Definition and Motivation

### Outline



2 Numerical Optimization of Eigenvalues of Matrix Functions

- Perturbation Results
- One Dimensional Algorithm
- Multi-dimensional Algorithm
- Pencils with Specified Eigenvalues
  - Definition and Motivation

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Definition and Motivation

### **Problem Definition**

•  $\lambda_1, \ldots, \lambda_k \in \mathbb{C}$  be given scalars, and  $\mathcal{S} = \{\lambda_1, \ldots, \lambda_k\}$ 

- r be a given positive integer
- $m_i(A, B)$ : Algebraic multip of  $\lambda_i$  as an eigenvalue of  $A \lambda B$

Definition (Distance to Pencils with Specified Eigenvalues)

$$\tau_r(A, B, S) = \inf \left\{ \|\delta A\|_2 : \sum_{j=1}^k m_j(A + \delta A, B) \ge r \right\}$$

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Definition and Motivation

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$$\tau_r(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{\mathcal{S}}) = \inf\left\{ \|\delta\boldsymbol{A}\|_2 : \sum_{j=1}^k m_j(\boldsymbol{A} + \delta\boldsymbol{A}, \boldsymbol{B}) \ge r \right\}$$

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Definition and Motivation

### Shape Estimation from Moments

# Estimating a polygon from moments (Elad, Milanfar, Golub; 2004)



Given moments

$$\mathcal{M}_k = \int \int_P z^k \, dx \, dy$$

for k = 1, ..., m.

Estimate the vertices  $z_j \in \mathbb{C}$  for j = 1, ..., n of P.

Definition and Motivation

### Shape Estimation from Moments

- The vertices z<sub>j</sub> are the eigenvalues of a pencil T<sub>0</sub> − λT<sub>1</sub> where T<sub>0</sub>, T<sub>1</sub> ∈ C<sup>m×n</sup> (with m > n) are Hankel matrices defined in terms of M<sub>k</sub>.
- Because of measurement errors the perturbed pencil  $\widetilde{T}_0 \lambda \widetilde{T}_1$  has generically no eigenvalues.
- Find a nearby pencil with the full set of eigenvalues inf<sub>S∈C<sup>n</sup></sub> τ<sub>n</sub>(τ̃<sub>0</sub>, τ̃<sub>1</sub>, S).

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Definition and Motivation

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Summary

Definition and Motivation

### **Rank Characterization**

$$C(\mu, \Gamma) := \begin{bmatrix} \mu_1 & -\gamma_{21} & \dots & -\gamma_{r1} \\ 0 & \mu_2 & \dots & -\gamma_{r2} \\ & & \ddots & \\ 0 & & & \mu_r \end{bmatrix}$$

#### Theorem (Sylvester Characterization)

Let  $A - \lambda B$  be a pencil with  $A, B \in \mathbb{C}^{m \times n}$  such that  $m \ge n$  and  $\operatorname{rank}(B) = n$ ,  $S = \{\lambda_1, \ldots, \lambda_k\}$  be a set consisting of distinct complex scalars and  $r \in \mathbb{Z}^+$ . Then the following two statements are equivalent.

$$\bigcirc \sum_{j=1}^k m_j(A,B) \ge r$$

) There exists a 
$$\mu\in\mathcal{S}^r$$
 such tha

 $\dim\{X \in \mathbb{C}^{n \times r} : AX - BXC(\mu, \Gamma) = 0\} \ge r$ 

for all  $\Gamma \in \mathcal{G}(\mu) := \{\Gamma : C(\mu, \Gamma) \text{ has Jordan blocks of maximal size.} \}$ .

Summary

Definition and Motivation

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 $1) \sum_{j=1}^{k} m_j(A,B) \ge r$ 

) There exists a  $\mu\in \mathcal{S}^r$  such that

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Definition and Motivation

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Summary

Definition and Motivation

Rank Characterization Kroneckerization of the Sylvester Equation

Recall the Identity

$$\operatorname{vec}(FXG) = (G^T \otimes F)\operatorname{vec}(X)$$
where  $X = \begin{bmatrix} x_1 & \dots & x_r \end{bmatrix} \in \mathbb{C}^{n \times r}$  and  $\operatorname{vec}(X) = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} \in \mathbb{C}^{nr}$ .

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Definition and Motivation

Rank Characterization Kroneckerization of the Sylvester Equation

In particular

$$AX - BXC(\mu, \Gamma) = 0 \Leftrightarrow ((I \otimes A) - (C^{T}(\mu, \Gamma) \otimes B)) \operatorname{vec}(X) = 0.$$

• Consequently  $\dim\{X \in \mathbb{C}^{n \times r} : AX - BXC(\mu, \Gamma) = 0\} \ge r$   $\Leftrightarrow$   $\operatorname{rank}\left(\left((I \otimes A) - (C^{T}(\mu, \Gamma) \otimes B)\right)\right) \le nr - r$ 

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Definition and Motivation

Rank Characterization Kroneckerization of the Sylvester Equation

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$$AX - BXC(\mu, \Gamma) = 0 \Leftrightarrow ((I \otimes A) - (C^{T}(\mu, \Gamma) \otimes B)) \operatorname{vec}(X) = 0.$$

Consequently

$$\dim\{X \in \mathbb{C}^{n \times r} : AX - BXC(\mu, \Gamma) = 0\} \ge r$$
$$\Leftrightarrow$$
$$\operatorname{rank}\left(\left((I \otimes A) - (C^{T}(\mu, \Gamma) \otimes B)\right)\right) \le nr - r$$

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Summary

Definition and Motivation

## Rank Characterization

Kroneckerization of the Sylvester Equation

$$\mathcal{L}(\mu, \Gamma, A, B) := \begin{pmatrix} ((I \otimes A) - (C^{T}(\mu, \Gamma) \otimes B)) \\ \gamma_{21}B & A - \mu_{2}B & 0 \\ & \ddots & \\ & & A - \mu_{r-1}B & 0 \\ \gamma_{r1}B & \gamma_{r2}B & \gamma_{r(r-1)}B & A - \mu_{r}B \end{bmatrix}$$

#### Theorem (Rank Characterization)

Given a pencil  $A - \lambda B$  with  $A, B \in \mathbb{C}^{m \times n}$  such that  $m \ge n$  and  $\operatorname{rank}(B) = n$ , a set  $S = \{\lambda_1, \ldots, \lambda_k\}$  consisting of distinct complex scalars and  $r \in \mathbb{Z}^+$ . Then the following two statements are equivalent.

2) There exists a 
$$\mu\in \mathcal{S}^{\mathsf{r}}$$
 such that

 $\operatorname{rank}\left(\mathcal{L}(\mu, \Gamma, A, B)\right) \leq nr - r$ 

for all  $\Gamma \in \mathcal{G}(\mu)$ .

Summary

Definition and Motivation

### Rank Characterization

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Kroneckerization of the Sylvester Equation

$$C(\mu, \Gamma, A, B) := \left( \left( (I \otimes A) - (C^{T}(\mu, \Gamma) \otimes B) \right) \right)$$
  
= 
$$\left[ \begin{array}{ccc} A - \mu_{1}B & 0 & & 0 \\ \gamma_{21}B & A - \mu_{2}B & & 0 \\ & \ddots & & \\ & & A - \mu_{r-1}B & 0 \\ \gamma_{r1}B & \gamma_{r2}B & & \gamma_{r(r-1)}B & A - \mu_{r}B \end{array} \right]$$

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Summary

Definition and Motivation

### Rank Characterization

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Kroneckerization of the Sylvester Equation

$$C(\mu, \Gamma, A, B) := \left( \left( (I \otimes A) - (C^{T}(\mu, \Gamma) \otimes B) \right) \right)$$
  
= 
$$\left[ \begin{array}{ccc} A - \mu_{1}B & 0 & & 0 \\ \gamma_{21}B & A - \mu_{2}B & & 0 \\ & \ddots & & \\ & & A - \mu_{r-1}B & 0 \\ \gamma_{r1}B & \gamma_{r2}B & & \gamma_{r(r-1)}B & A - \mu_{r}B \end{array} \right]$$

#### Theorem (Rank Characterization)

Given a pencil  $A - \lambda B$  with  $A, B \in \mathbb{C}^{m \times n}$  such that  $m \ge n$  and  $\operatorname{rank}(B) = n$ , a set  $S = \{\lambda_1, \ldots, \lambda_k\}$  consisting of distinct complex scalars and  $r \in \mathbb{Z}^+$ . Then the following two statements are equivalent.

$$\bigcirc \sum_{j=1}^{k} m_j(A, B) \ge r$$

) There exists a  $\mu\in \mathcal{S}^r$  such that

 $\operatorname{rank}(\mathcal{L}(\mu, \Gamma, A, B)) \leq nr - r$ 

for all  $\Gamma \in \mathcal{G}(\mu)$ .

Summary

Definition and Motivation

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#### Theorem (Nearest Pencils with Specified Eigenvalues)

Let  $A - \lambda B$  be an  $m \times n$  pencil with  $m \ge n$ ,  $r \in \mathbb{Z}^+$  and  $S = \{\lambda_1, \dots, \lambda_k\}$  be a set of distinct complex scalars. Then the equality

$$\tau_r(A, B, \mathcal{S}) = \inf_{\mu \in \mathcal{S}^r} \sup_{\Gamma} \sigma_{nr-r+1} \left( \mathcal{L} \left( \mu, \Gamma, A, B \right) \right)$$

holds provided that the optimization problem on the right is attained at a  $(\mu_*, \Gamma_*)$  where the multiplicity and linear independence qualifications hold.

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### Summary

- A generic algorithm is introduced for the optimization of symmetric eigenvalues based on their analyticity.
- The algorithm is globally convergent and the rate of convergence is linear in practice.
- Software eigopt at http://home.ku.edu.tr/~emengi/software.html
- A singular value characterization for  $\tau_r(A, B, S)$

- Future
  - Improvements on the algorithm for the optimization of eigenvalues in the multivariate-case
  - A singular value charac for  $\tau_r(A, B, S)$  when both A and B are perturbed.

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