Investigation of Crouzeix's Conjecture via Variational Analysis and Nonsmooth Optimization

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Joint work with
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Limoges, 18 May 2015

Terry Rockafellar

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Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Concluding Remarks

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1987: Our first correspondence and my first invitation to UW

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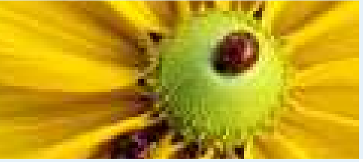

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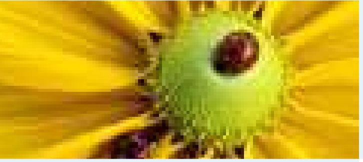

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Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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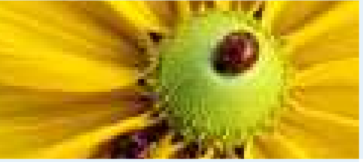
Just a matter of units: he may be 80 in Fahrenheit but in Celsius he is only 27!



Crouzeix's Conjecture

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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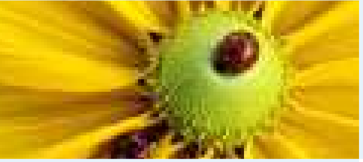
The Field of Values

For $A \in \mathbb{C}^{n \times n}$, the field of values (or numerical range) of A is

$$W(A) = \{v^* A v : v \in \mathbb{C}^n, \|v\|_2 = 1\} \subset \mathbb{C}.$$



The Field of Values

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
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Clearly

$$W(A) \supseteq \sigma(A)$$

where σ denotes spectrum.

The Field of Values

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

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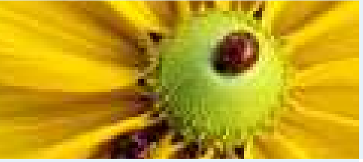
If $AA^* = A^*A$, then

$$W(A) = \operatorname{conv} \sigma(A).$$



The Field of Values

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Concluding Remarks

For $A \in \mathbb{C}^{n\times n}$, the field of values (or numerical range) of A is

$$W(A) = \{v^*Av : v \in \mathbb{C}^n, \|v\|_2 = 1\} \subset \mathbb{C}.$$

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If $AA^* = A^*A$, then

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Toeplitz-Haussdorf Theorem: $W(A)$ is convex for all $A \in \mathbb{C}^{n\times n}$.

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks

Examples

Let

$$J = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} : \quad W(J) \text{ is a disk of radius } 0.5$$

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks

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$$B = \begin{bmatrix} 1 & 2 \\ -3 & 4 \end{bmatrix}: \quad W(B) \text{ is an ``elliptical disk''}$$

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks

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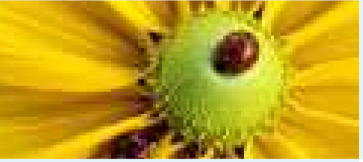
$$D = \begin{bmatrix} 5+i & 0 \\ 0 & 5-i \end{bmatrix} : \quad W(D) \text{ is a line segment}$$



Examples

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

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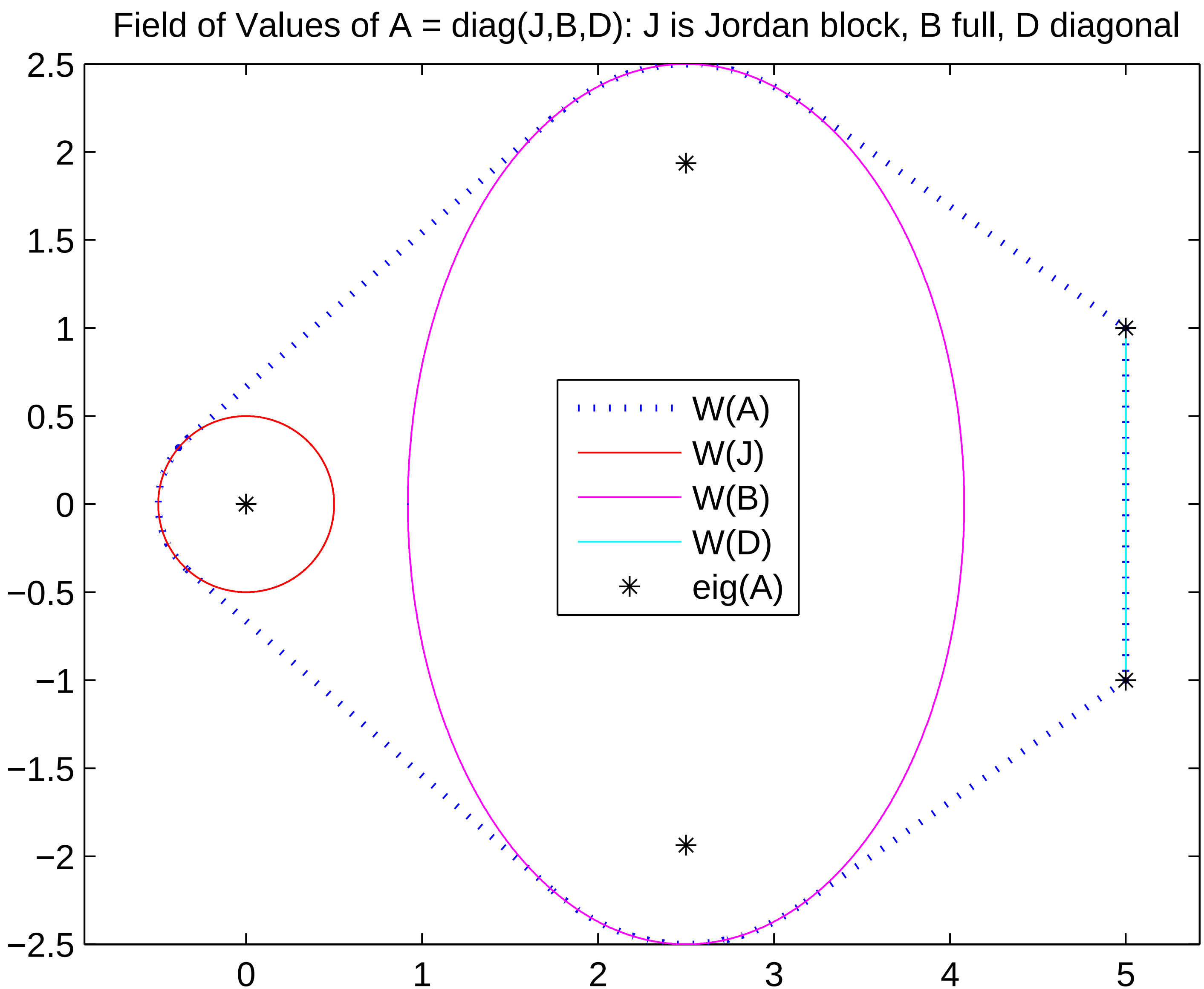
$$A = \mathrm{diag}(J, B, D) : \quad W(A) = \mathrm{conv}\left(W(J), W(B), W(D)\right)$$

Example, continued

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks



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Let $p = p(z)$ be a polynomial and let A be a square matrix.

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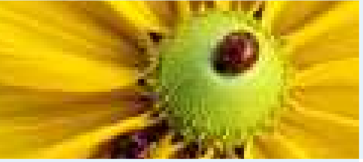
Crouzeix's Conjecture

The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Concluding Remarks



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Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Concluding Remarks

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M. Crouzeix conjectured in "Bounds for analytical functions of matrices", *Int. Eq. Oper. Theory 48* (2004), that for *all* p and A,

$$\|p(A)\|_2 \leq 2\,\|p\|_{W(A)}.$$

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks

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The left-hand side is the 2-norm (spectral norm, maximum singular value) of the matrix $p(A)$.

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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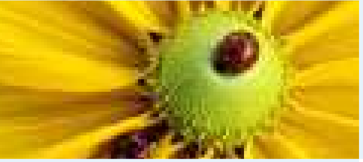
If $p(z) = z$ and A is a 2×2 Jordan block with 0 on the diagonal, then $\|p(A)\|_2 = 1$ and $W(A)$ is a disk centered at 0 with radius 0.5, so the left and right-hand sides are equal.



Crouzeix's Theorem

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Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Concluding Remarks

$$\|p(A)\|_2 \leq 11.08\,\|p\|_{W(A)}$$

i.e., the conjecture is true if we replace 2 by 11.08.

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks

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> "The estimate 11.08 is not optimal. There is no doubt that refinements are possible which would decrease this bound. We are convinced that our estimate is very pessimistic, but to improve it drastically (recall that our conjecture is that 11.08 can be replaced by 2), it is clear that we have to find a completely different method."
>
> - Michel Crouzeix, "Numerical range and functional calculus in Hilbert space", *J. Funct. Anal.* 244 (2007).

Special Cases

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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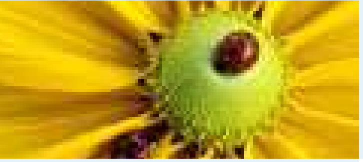

Special Cases

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

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Special Cases

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Concluding Remarks

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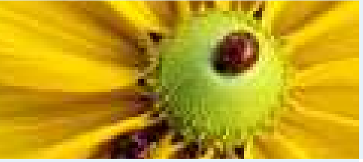

Special Cases

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

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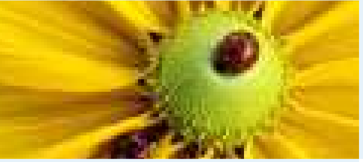

Special Cases

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

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Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks

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- $AA^* = A^*A$ (then the constant 2 can be improved to 1).

The Extreme Points of the Field of Values

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Concluding Remarks

The Extreme Points of the Field of Values

Terry Rockafellar

Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

Crouzeix's Conjecture

Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

Johnson's Algorithm Finds the Extreme Points

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

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Based on R. Kippenhahn (1951), C.R. Johnson (1978) observed that the extreme points of W(A) can be characterized as

$$\text{ext } W(A) = \{z_\theta = v_\theta^* A v_\theta : \theta \in [0, 2\pi)\}$$

where v_θ is a normalized eigenvector corresponding to the largest eigenvalue of the Hermitian matrix

$$H_\theta = \frac{1}{2}\left(e^{i\theta}A + e^{-i\theta}A^*\right).$$

The Extreme Points of the Field of Values

Terry Rockafellar
Crouzeix's Conjecture
The Field of Values
Examples
Example, continued
Crouzeix's Conjecture
Crouzeix's Theorem
Special Cases
The Extreme Points of the Field of Values
Johnson's Algorithm Finds the Extreme Points
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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Crouzeix's Conjecture

The Field of Values

Examples

Example, continued

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Crouzeix's Theorem

Special Cases

The Extreme Points of the Field of Values

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Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

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Thus, we can compute as many extreme points as we like. Continuing with the previous example...

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Crouzeix's Conjecture
The Field of Values
Examples
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Crouzeix's Conjecture
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Special Cases
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Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
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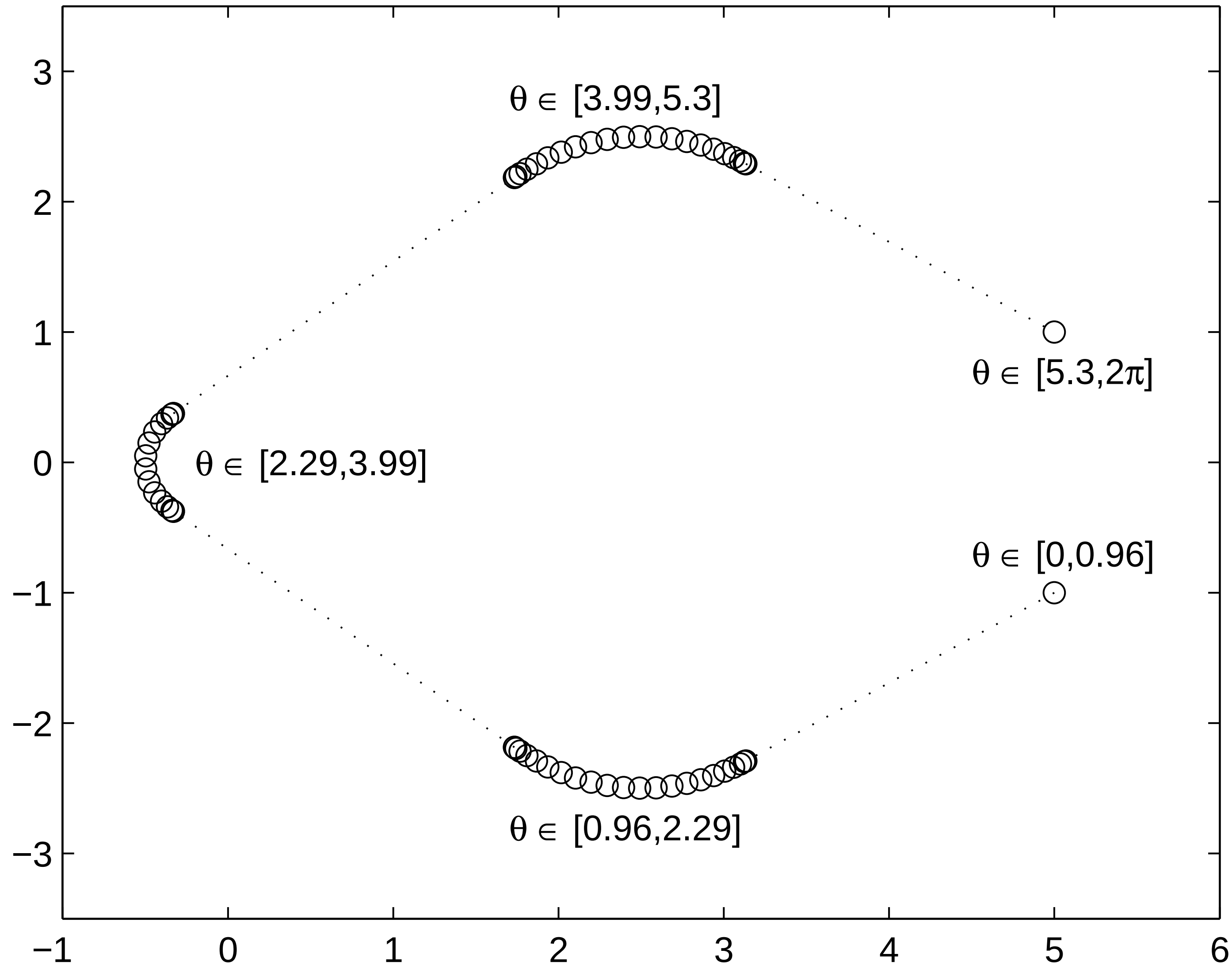


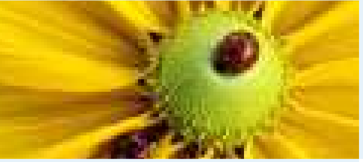
The extreme points of W(A) lie in the union of 5 connected sets

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio

Define the Crouzeix ratio

$$f(p, A) = \frac{\|p\|_{W(A)}}{\|p(A)\|_2}.$$



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Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio

The Gradient and Subgradients of the Crouzeix Ratio

Three Possible Sources of Nonsmoothness in f

Simplest Interesting Case

$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f

Partly Smooth Functions

Partial Smoothness of the Crouzeix Ratio

Varying (c, A) along V_1 Direction

Varying (c, A) along V_2 Direction

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Varying (c, A) along U_2 Direction

Varying (c, A)

The Crouzeix Ratio

Define the Crouzeix ratio

$$f(p, A) = \frac{\|p\|_{W(A)}}{\|p(A)\|_2}.$$

The conjecture states that $f(p, A)$ is bounded below by 0.5 independently of the polynomial degree m and the matrix order n.

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The Crouzeix ratio f is

- A mapping from pairs (p, A) to the reals.

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio

The Gradient and Subgradients of the Crouzeix Ratio

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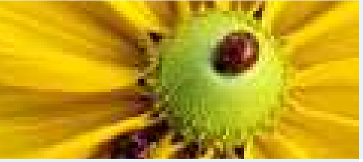

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio

The Gradient and Subgradients of the Crouzeix Ratio

Three Possible Sources of Nonsmoothness in f

Simplest Interesting Case

$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f

Partly Smooth Functions

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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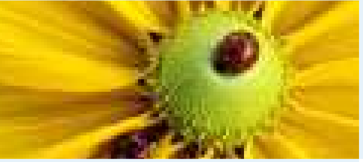

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio

The Gradient and Subgradients of the Crouzeix Ratio

Three Possible Sources of Nonsmoothness in f

Simplest Interesting Case

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Partly Smooth Functions

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Varying (c, A) along V_1 Direction

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- A mapping from pairs (p, A) to the reals.
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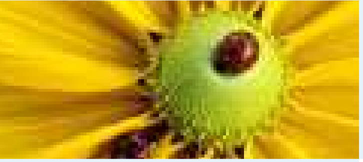
- Not defined if $p(A) = 0$
- Lipschitz continuous at all other points, but not necessarily differentiable



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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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- Semialgebraic

The Gradient and Subgradients of the Crouzeix Ratio

"The chain rule on steroids".

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
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For the numerator, combine:

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(recall its argument is $p(z_\theta(A)) \in \mathbb{C}$)

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio

The Gradient and Subgradients of the Crouzeix Ratio

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Partly Smooth Functions

Partial Smoothness of the Crouzeix Ratio

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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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For the denominator, combine:

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For the denominator, combine:

- the gradient or subgradients of the 2-norm (maximum singular value) of a matrix (well known)

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• the gradient of the matrix polynomial $p(A)$ w.r.t. A (involves differentiating monomial terms A^k w.r.t. A, resulting in Kronecker products).

Three Possible Sources of Nonsmoothness in f

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The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
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Varying (c, A) along V_1 Direction
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- Ties for the max value of $|p(z)|$ on $\mathrm{bd}\, W(A)$ (the most important)

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
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- Ties for the max value of $|p(z)|$ on $\mathrm{bd}\, W(A)$ (the most important)
- A multiple eigenvalue

$$\lambda_{\max}(H_\theta) = \lambda_{\max}\left(\frac{1}{2}\left(e^{i\theta}A + e^{-i\theta}A^*\right)\right).$$

This can be excluded by assuming that $\mathrm{bd}\, W(A)$ does not contain any line segment.

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Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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  This can be excluded by assuming that $\mathrm{bd}\, W(A)$ does not contain any line segment.
- A multiple singular value $\sigma_{\max}(p(A))$.

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Simplest Interesting Case

Optimize over real monic linear polynomials $p(z) \equiv z + c$ and real matrices with order $n = 2$. Let $f(p, A) \equiv f(c, A)$, where now $f : \mathbb{R} \times \mathbb{R}^{2\times 2} \to \mathbb{R}$.

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The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Let $\hat{c} = 0$ and $\hat{A} = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix}$, so $W(\hat{A}) = \mathcal{D}$, the unit disk, and hence $f(\hat{c}, \hat{A}) = 1/2$.

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The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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Let $\hat{c} = 0$ and $\hat{A} = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix}$, so $W(\hat{A}) = \mathcal{D}$, the unit disk, and hence $f(\hat{c}, \hat{A}) = 1/2$.

Theorem The Crouzeix ratio f is regular at $(\hat{c}, \hat{A})$, with

$$\partial f(\hat{c}, \hat{A}) = \mathrm{conv}_{\theta\in[0,2\pi)} \left\{ \left(\frac{1}{2}\cos(\theta), \frac{1}{4} \begin{bmatrix} \cos(\theta) & 0 \\ \cos(2\theta) & \cos(\theta) \end{bmatrix} \right) \right\}$$

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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Sketch of proof: we have $\mathrm{bd}\, W(\hat{A}) = \{\hat{z}_\theta \equiv e^{i\theta} : \theta \in [0, 2\pi)\}$, with $|\hat{z}_\theta + \hat{c}| = 1$ for all θ.

Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
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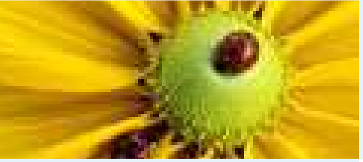

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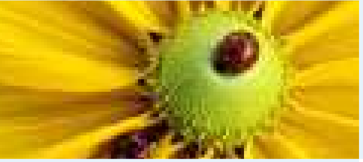

Simplest Interesting Case

Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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Corollary.

$$0 \in \partial f(\hat{c}, \hat{A})$$

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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Proof: the vectors inside the convex hull defined by $\theta = 0, \pi/2, \pi$ and $3\pi/2$ sum to zero.

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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Proof: the vectors inside the convex hull defined by $\theta = 0, \pi/2, \pi$ and $3\pi/2$ sum to zero.

Actually, we knew this must be true as Crouzeix's conjecture is known to hold for $n = 2$, and hence $(\hat{c}, \hat{A})$ is a global minimizer of f, but we expect that this derivation can be extended to larger values of m, n, for which we don't know whether the conjecture holds.

Partly Smooth Functions

Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
Varying (c, A)

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
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For $y \neq 0$ in the V-space, the mapping $t \mapsto h(x + ty)$ is necessarily nonsmooth at $t = 0$, while for $y \neq 0$ in the U-space, $t \mapsto h(x + ty)$ is differentiable at $t = 0$ as long as h is locally Lipschitz.

Partly Smooth Functions

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
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When h is convex, this is consistent with the usage of V-space and U-space in Lemaréchal-Oustry-Sagastizábal (2000).

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
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Partial Smoothness of the Crouzeix Ratio

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Partial Smoothness of the Crouzeix Ratio

Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio

The Gradient and Subgradients of the Crouzeix Ratio

Three Possible Sources of Nonsmoothness in f

Simplest Interesting Case

$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f

Partly Smooth Functions

Partial Smoothness of the Crouzeix Ratio

Varying (c, A) along V_1 Direction

Varying (c, A) along V_2 Direction

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In the example just given, the affine hull of $\partial f(\hat{c}, \hat{A})$ (the V-space) has dimension 2, with basis vectors

$$V_1 = \left(0, \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \right) \text{ and } V_2 = \left(2, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right).$$

Partial Smoothness of the Crouzeix Ratio

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
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Its orthogonal complement, the U-space, is spanned by

$$U_1 = \left(0, \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\right), U_2 = \left(0, \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}\right) \text{ and } U_3 = \left(-1, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right).$$

Partial Smoothness of the Crouzeix Ratio

Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

The Crouzeix Ratio
The Gradient and Subgradients of the Crouzeix Ratio
Three Possible Sources of Nonsmoothness in f
Simplest Interesting Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary Point of f
Partly Smooth Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
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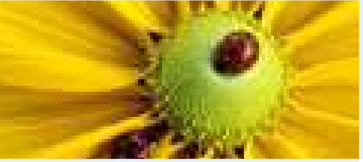
Let's look at $W(\hat{A} + t\Delta A)$ and the Crouzeix ratio $f(\hat{c} + \Delta c, \hat{A} + \Delta A)$ for $t \in [-1, 1]$ where $(\Delta c, \Delta A)$ are given by V_1, V_2, U_1, U_2 and U_3.



Varying (c, A) along V_1 Direction

Terry Rocka
Crouzeix's Conjecture
Variational A of the Crouz Ratio
The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possib Sources of Nonsmoothn
Simplest Int Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary P f
Partly Smoo Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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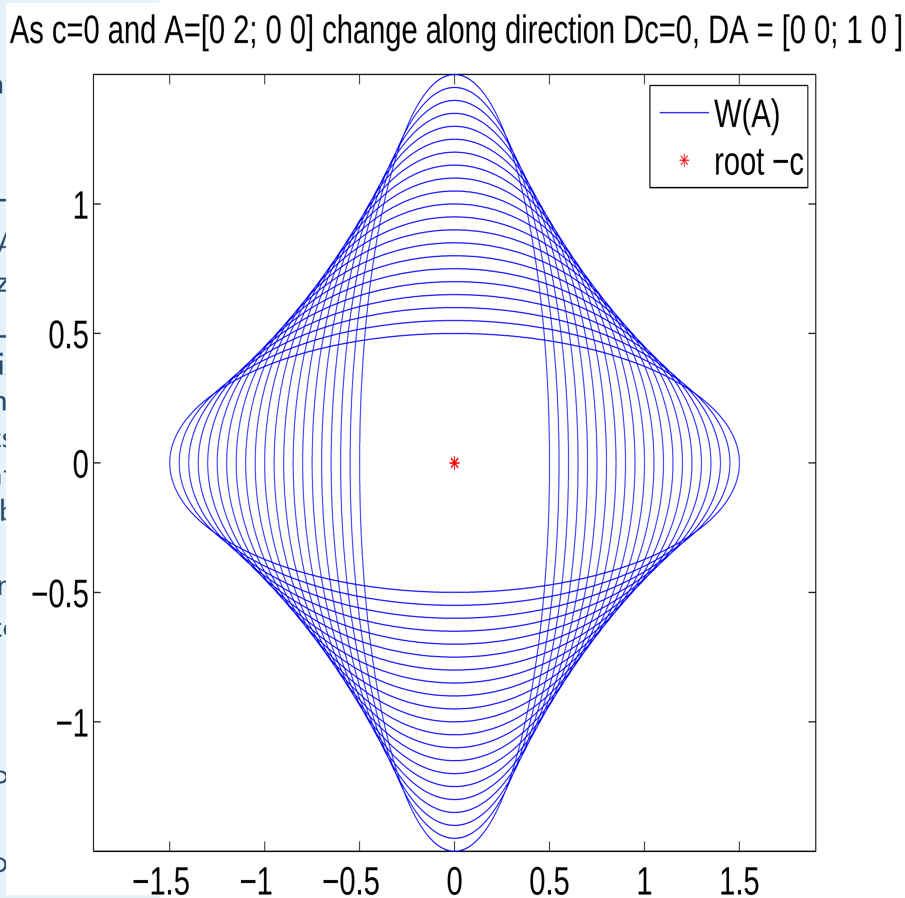
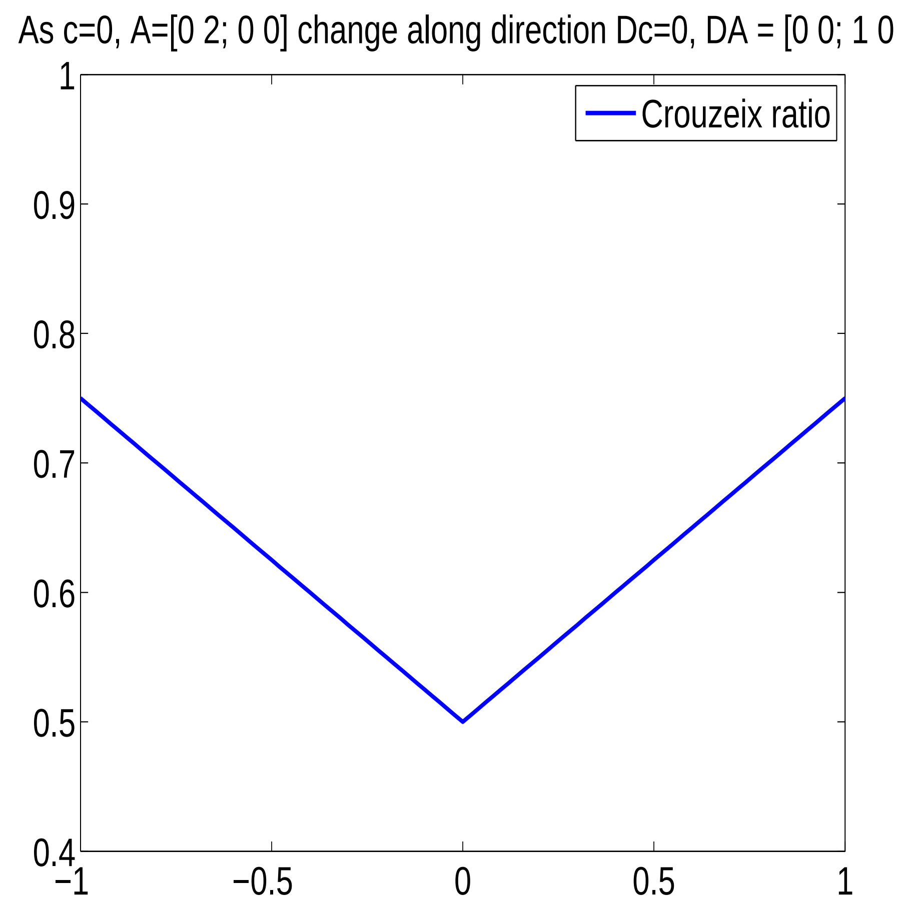
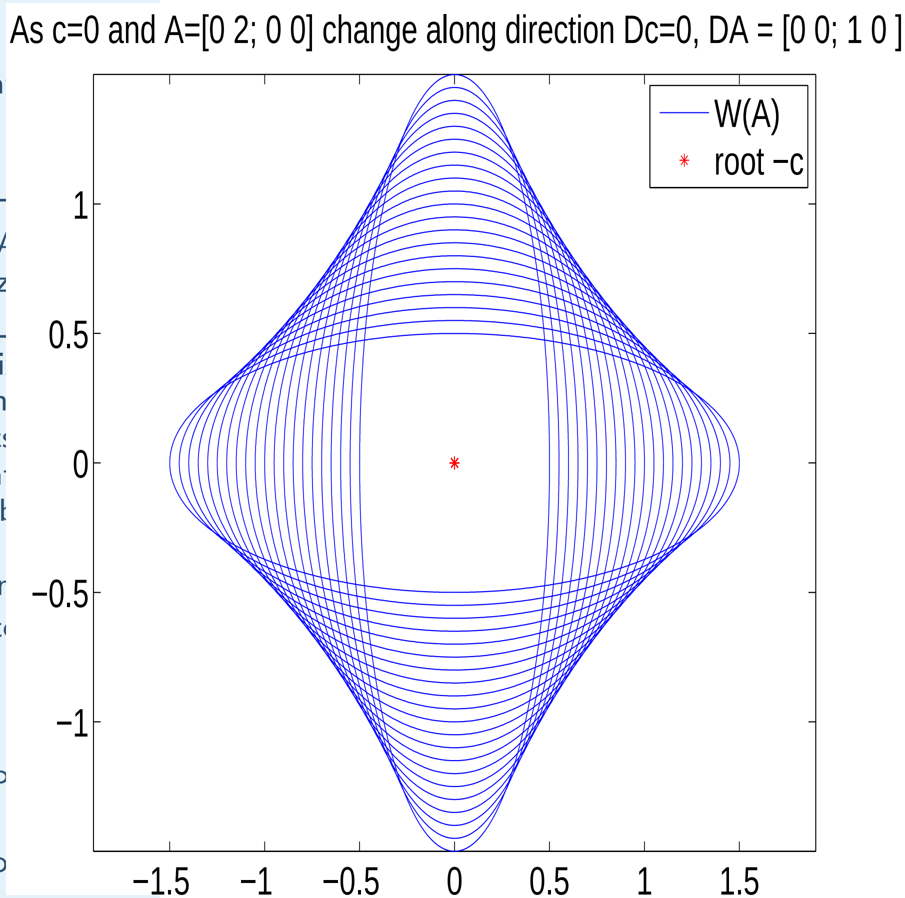
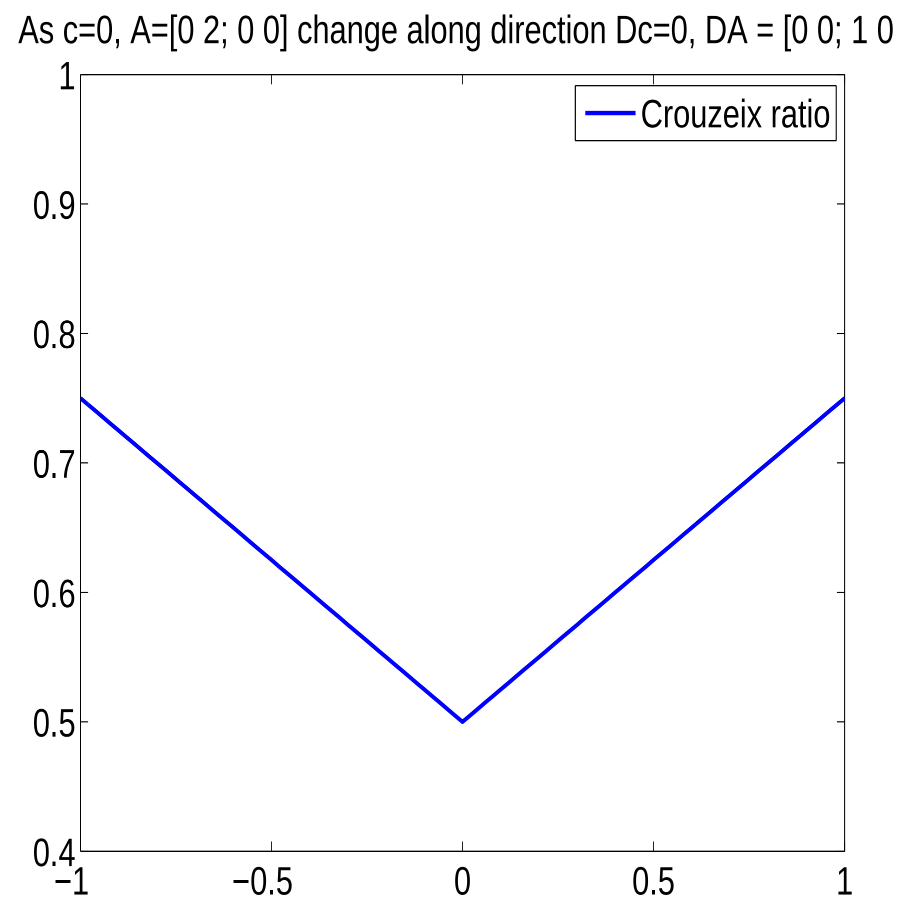




Left: superimposed $W(\hat{A} + t\Delta A)$ and $-c = -(\hat{c} + t\Delta c)$, where $\Delta c = 0$ and $\Delta A = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$, for several $t \in [-1, 1]$.

Varying (c, A) along V_1 Direction





Left: superimposed $W(\hat{A} + t\Delta A)$ and $-c = -(\hat{c} + t\Delta c)$, where $\Delta c = 0$ and $\Delta A = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$, for several $t \in [-1, 1]$.

Right: plot of Crouzeix ratio $f(\hat{c} + t\Delta c, \hat{A} + t\Delta A)$ for $t \in [-1, 1]$.

Varying (c, A) along V_2 Direction

Terry Rocka

Crouzeix's Conjecture

Variational A
of the Crouz
Ratio

The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possit
Sources of
Nonsmoothn
Simplest Int
Case
$(\hat{c}, \hat{A})$ is a
Nonsmooth
Stationary P
f
Partly Smoo
Functions
Partial Smoothness
of the Crouzeix
Ratio
Varying (c, A)
along V_1 Direction
Varying (c, A)
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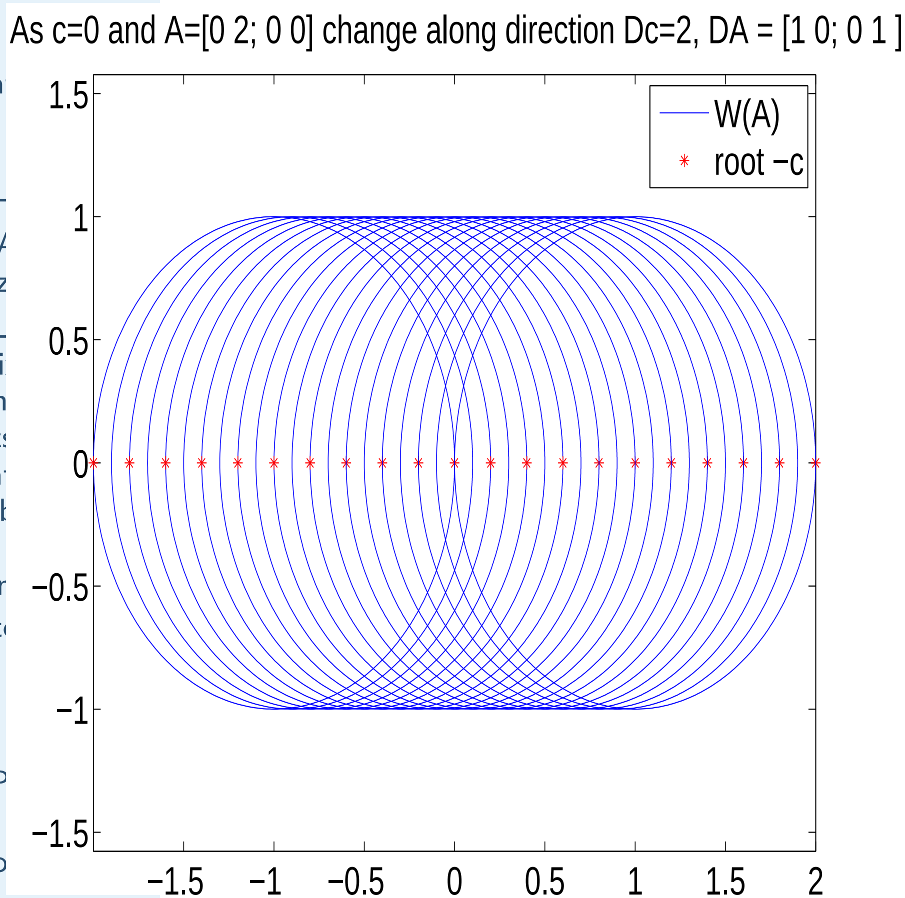

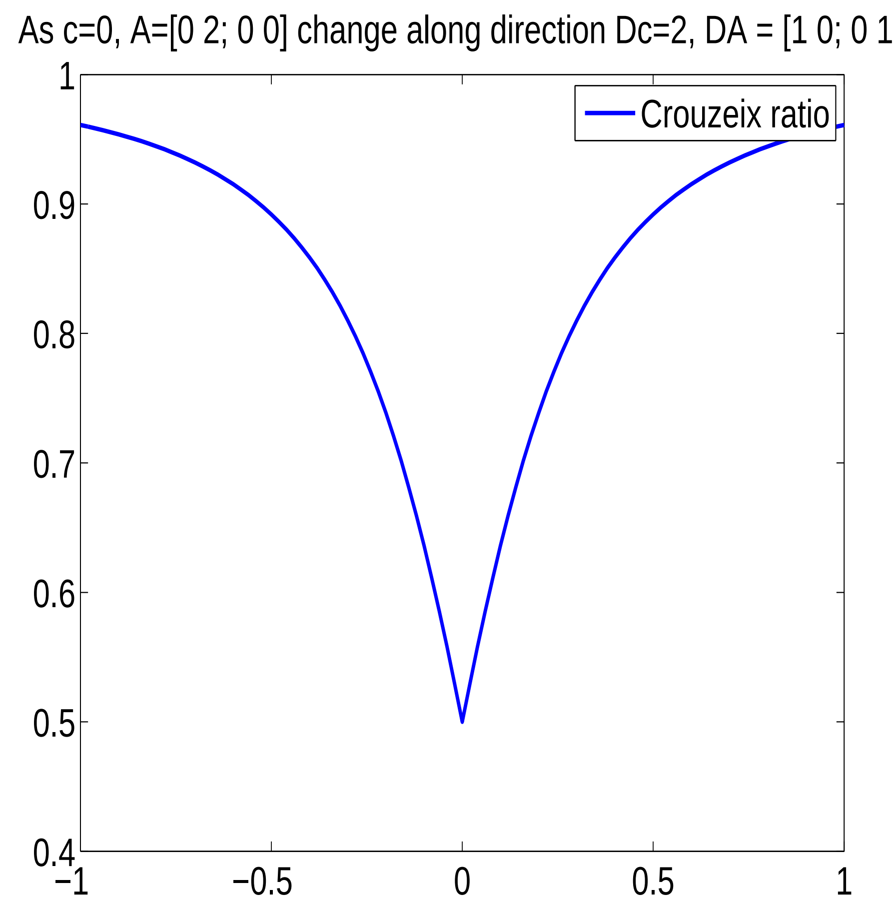

Left: superimposed $W(\hat{A} + t\Delta A)$ and $-c = -(\hat{c} + t\Delta c)$, where $\Delta c = 2$ and $\Delta A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, for several $t \in [-1, 1]$.

Varying (c, A) along V_2 Direction

Terry Rocka
Crouzeix's Conjecture
Variational A of the Crouz Ratio
The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possib Sources of Nonsmoothn
Simplest Inte Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary P f
Partly Smoo Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
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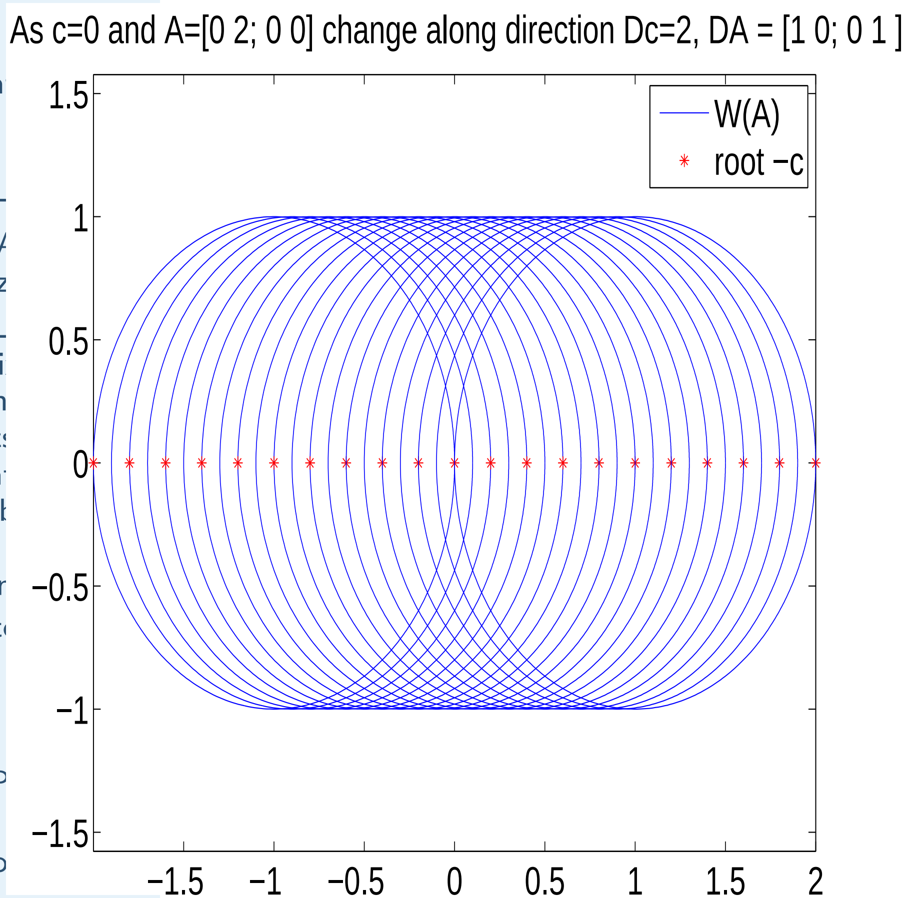

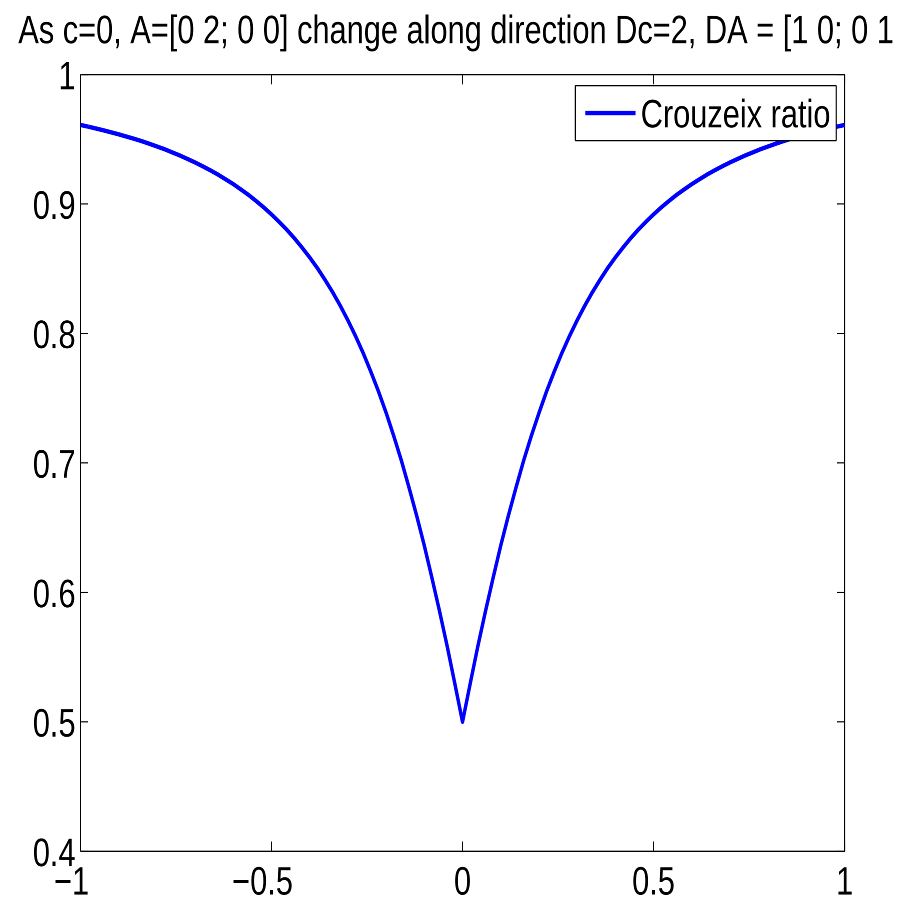

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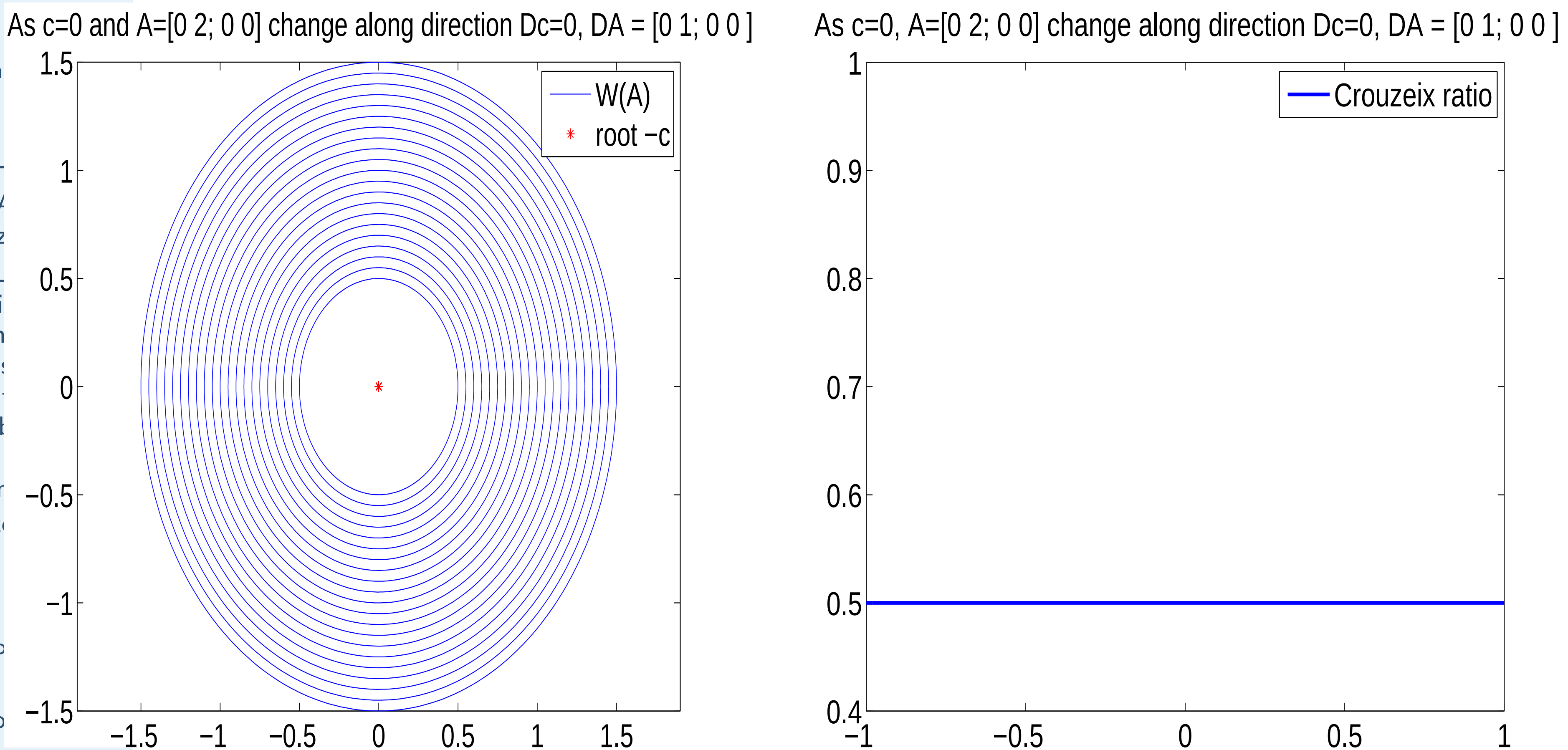

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Terry Rocka
Crouzeix's Conjecture
Variational A of the Crouz Ratio
The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possib Sources of Nonsmoothn
Simplest Int Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary P f
Partly Smoo Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
Varying (c, A) along V_2 Direction
Varying (c, A) along U_1 Direction
Varying (c, A) along U_2 Direction
Varying (c, A)

Varying (c, A) along U_1 Direction

Terry Rocka
Crouzeix's Conjecture
Variational A
of the Crouz
Ratio
The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possib
Sources of
Nonsmoothn
Simplest Int
Case
$(\hat{c}, \hat{A})$ is a
Nonsmooth
Stationary P
f
Partly Smoo
Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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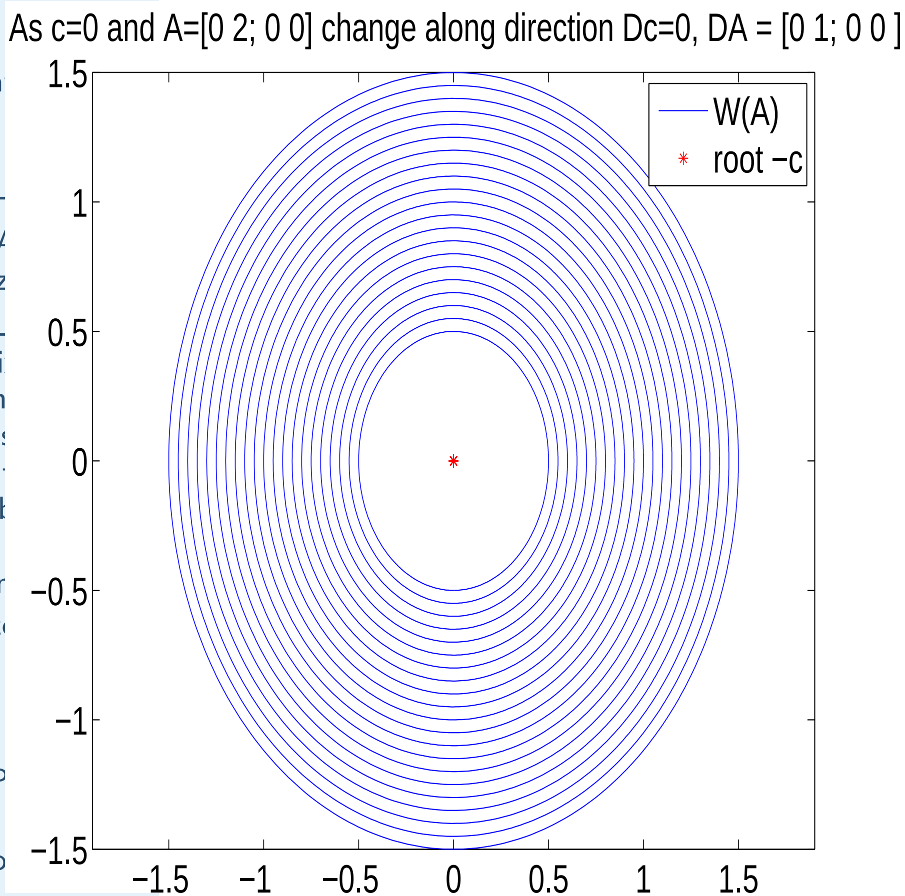

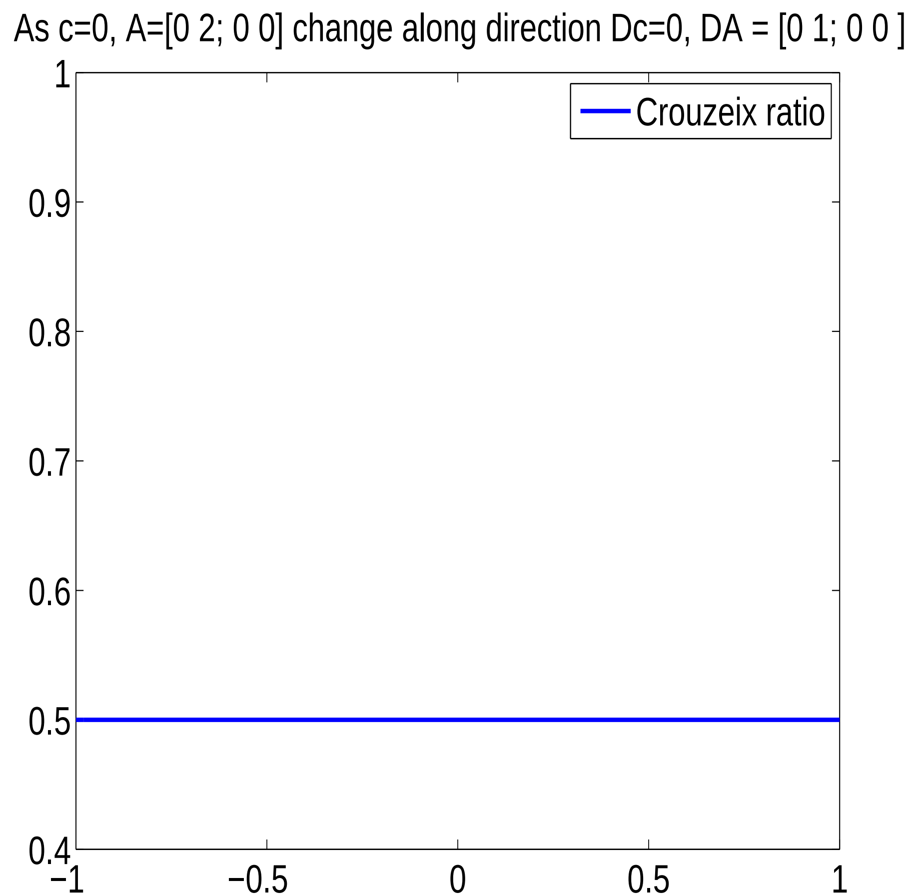

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Terry Rocka
Crouzeix's Conjecture
Variational A of the Crouz Ratio
The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possib Sources of Nonsmoothn
Simplest Int Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary P f
Partly Smoo Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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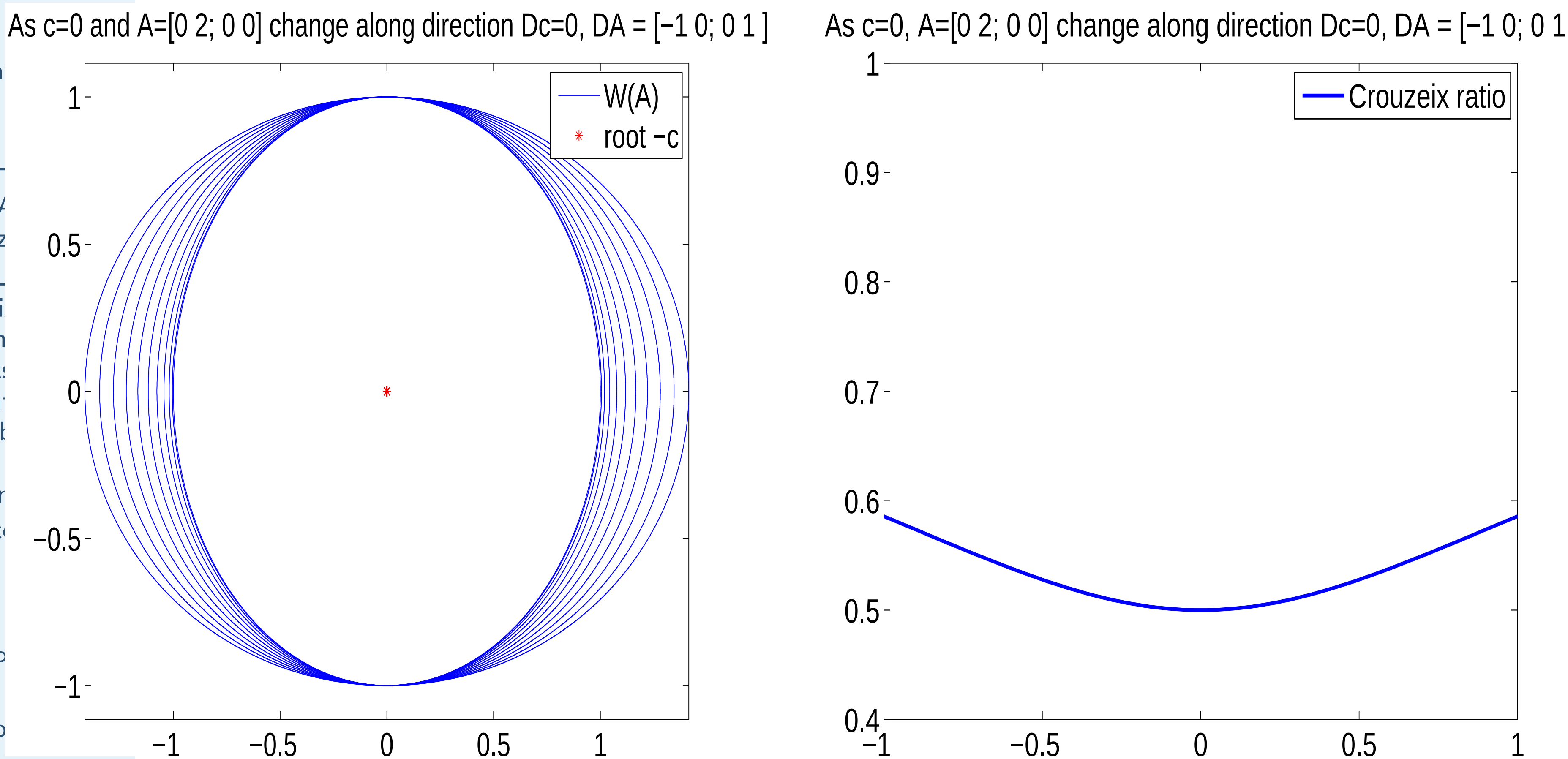

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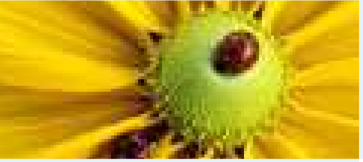

Varying (c, A) along U_2 Direction

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Crouzeix's Conjecture

Variational A
of the Crouz
Ratio

The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possib
Sources of
Nonsmoothn
Simplest Int
Case
$(\hat{c}, \hat{A})$ is a
Nonsmooth
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Functions
Partial Smoothness
of the Crouzeix
Ratio
Varying (c, A)
along V_1 Direction
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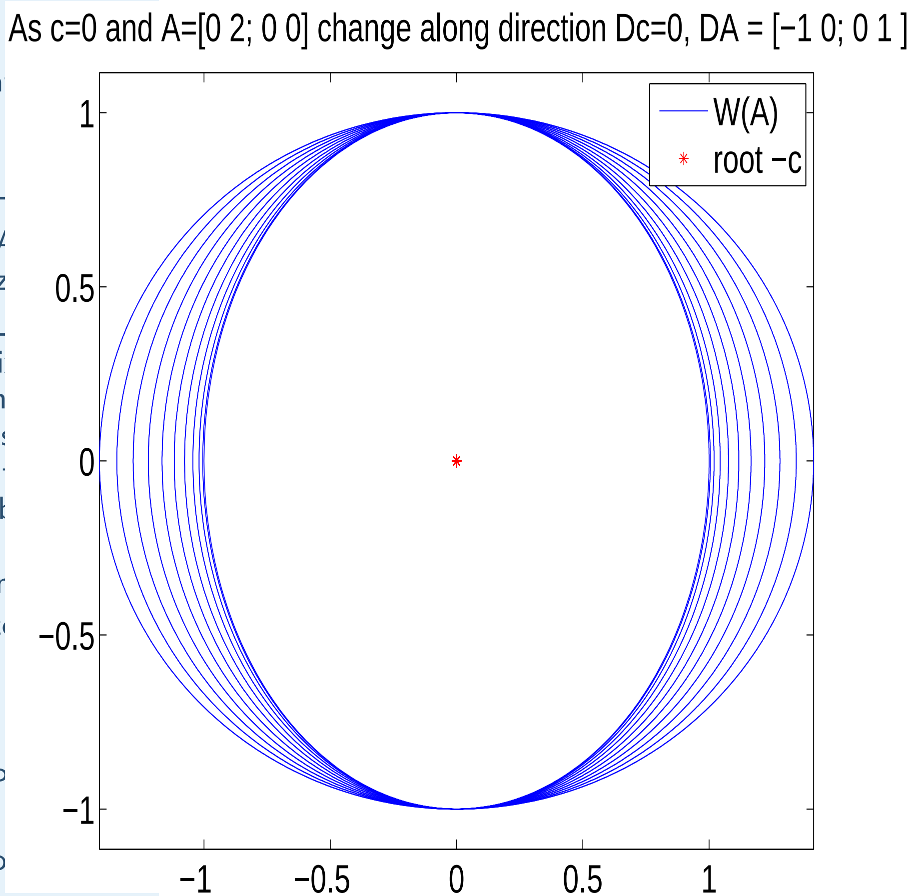

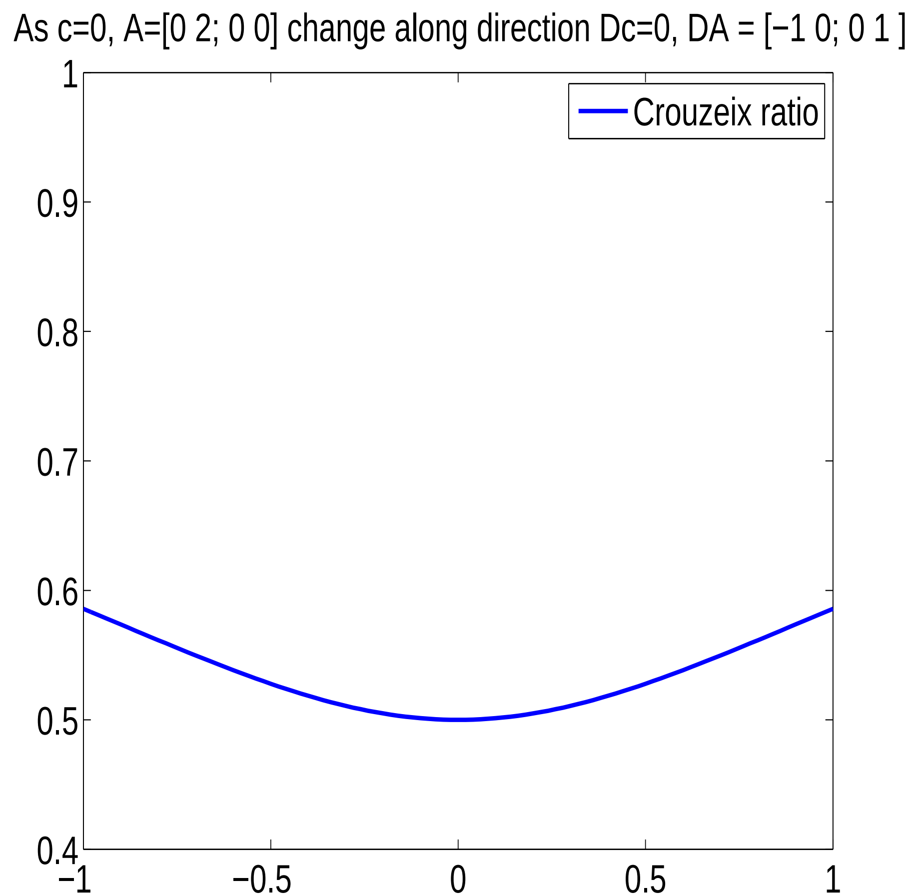

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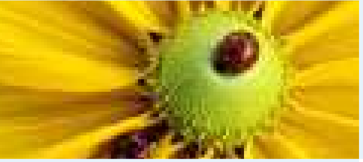
Right: plot of Crouzeix ratio $f(\hat{c} + t\Delta c, \hat{A} + t\Delta A)$ for $t \in [-1, 1]$.



Varying (c, A) along U_3 Direction

Terry Rocka
Crouzeix's Conjecture
Variational A of the Crouz Ratio
The Crouzei
The Gradien
Subgradients
Crouzeix Ra
Three Possib Sources of Nonsmoothn
Simplest Inte Case
$(\hat{c}, \hat{A})$ is a Nonsmooth Stationary P f
Partly Smoo Functions
Partial Smoothness of the Crouzeix Ratio
Varying (c, A) along V_1 Direction
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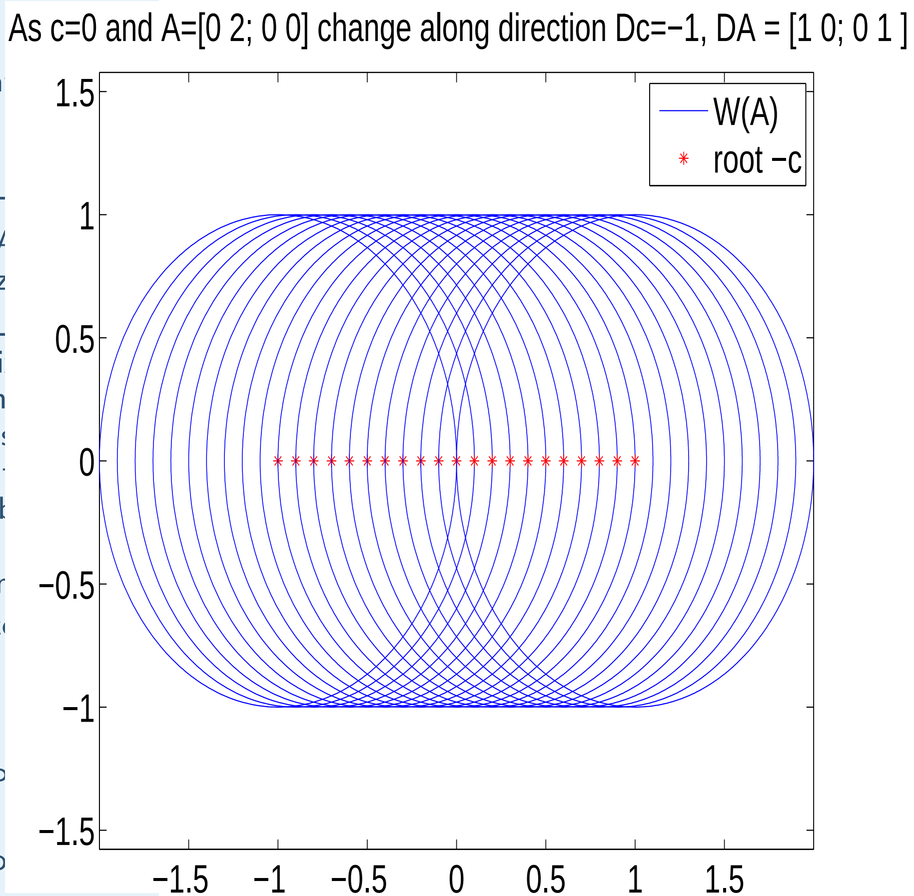
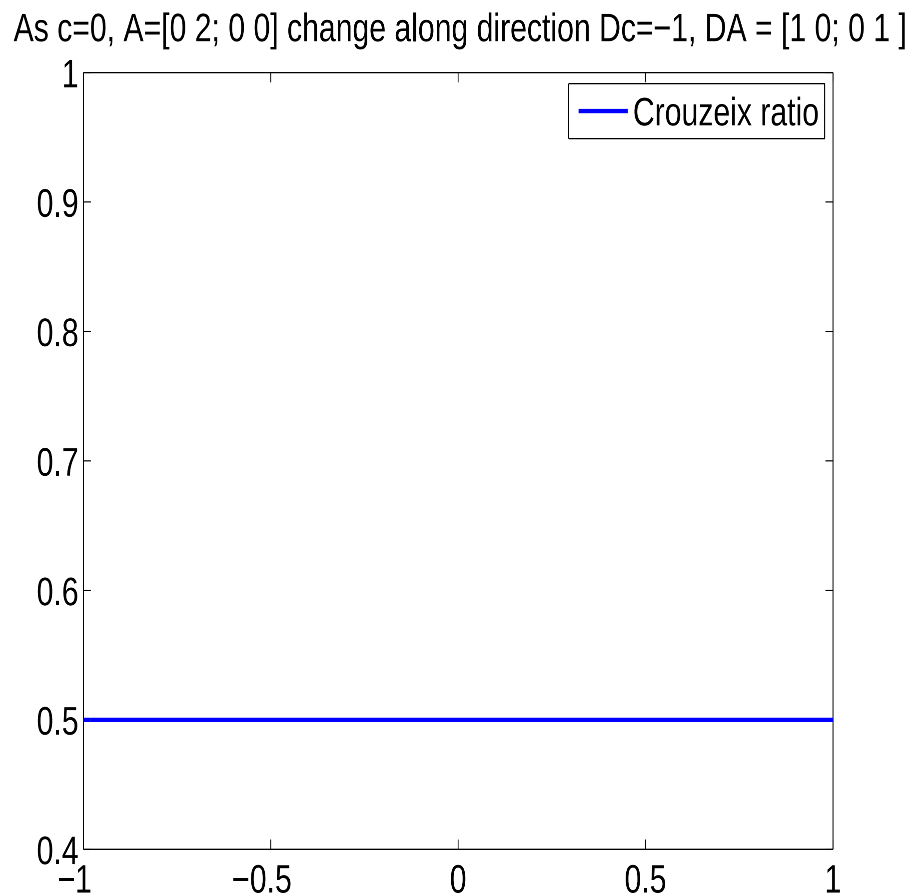
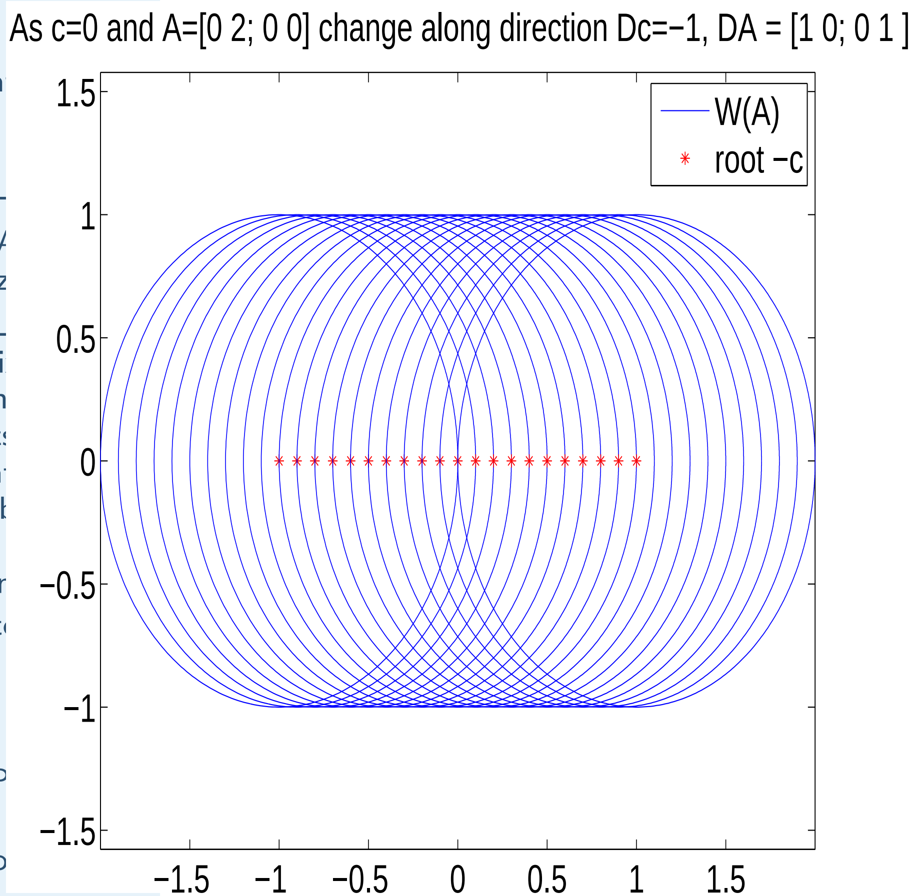
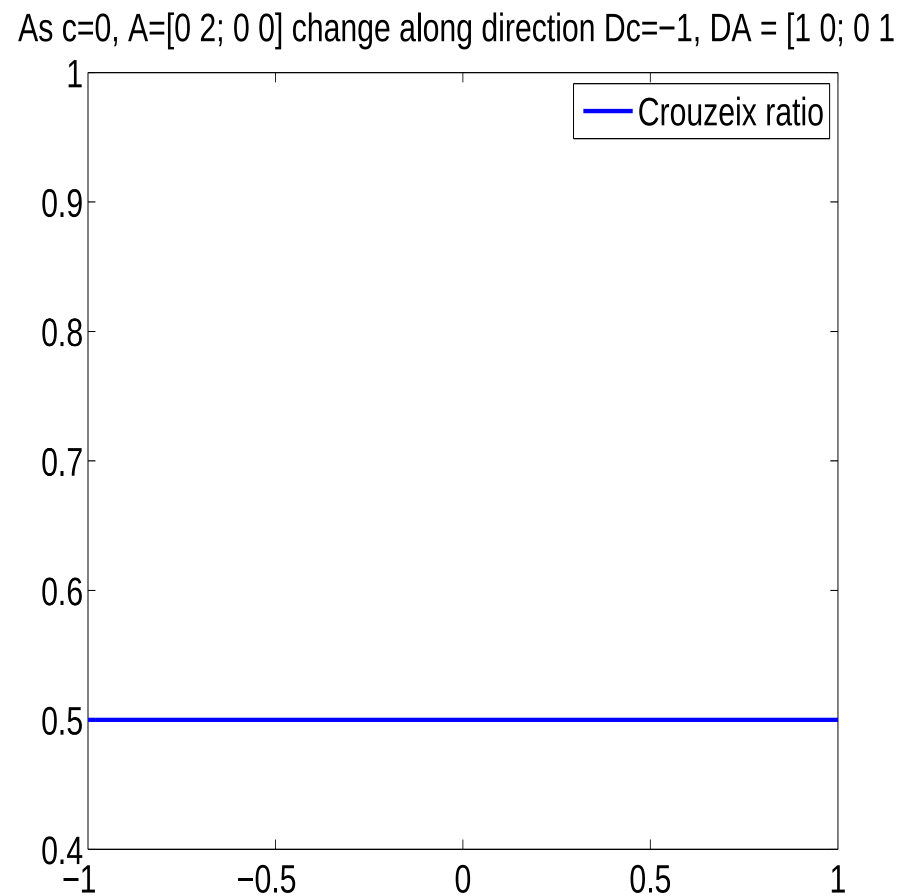




Left: superimposed $W(\hat{A} + t\Delta A)$ and $-c = -(\hat{c} + t\Delta c)$, where $\Delta c = -1$ and $\Delta A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, for several $t \in [-1, 1]$.

Varying (c, A) along U_3 Direction





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Right: plot of Crouzeix ratio $f(\hat{c} + t\Delta c, \hat{A} + t\Delta A)$ for $t \in [-1, 1]$.

Nonsmooth Optimization of the Crouzeix Ratio

Computational Tools

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Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Computational Tools

Experiments

Optimizing over both p (deg. $m \leq 4$) and A $(n = 5)$

Best Solution Found: $f(p, A) = 0.5000000002$

For what (c, A) is the Crouzeix ratio $f(c, A) = 0.5$?

Concluding Remarks

Chebfun (Trefethen et al, 2004-present), for efficiently interpolating the boundary of $W(A)$ to machine precision accuracy using adaptive Chebyshev interpolation

Computational Tools

Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Computational Tools

Experiments

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BFGS (Broyden, Fletcher, Goldfarb, Shanno 1970), a standard method for smooth optimization, which is also an extremely reliable and efficient method to find local minimizers of nonsmooth functions (Lewis-Overton, Math. Programming, 2013)

Experiments

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Computational Tools
Experiments
Optimizing over both p (deg. $m \leq 4$) and A ($n = 5$)
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We have run many experiments searching for local minimizers of the Crouzeix ratio using BFGS.

Experiments

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Several scenarios:

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Computational Tools
Experiments
Optimizing over both p (deg. $m \leq 4$) and A ($n = 5$)
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Experiments

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Several scenarios:

- Fix p with degree m, optimize over A with fixed order n

Terry Rockafellar

Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Computational Tools

Experiments

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Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Computational Tools
Experiments
Optimizing over both p (deg. $m \le 4$) and A ($n = 5$)
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Several scenarios:

- Fix p with degree m, optimize over A with fixed order n
- Fix A with order n, optimize over p with degree $\leq m$
- Optimize over both p with degree $\leq m$ and A with order n

We'll report only the last.

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Computational Tools
Experiments
Optimizing over both p (deg. $m \leq 4$) and A ($n = 5$)
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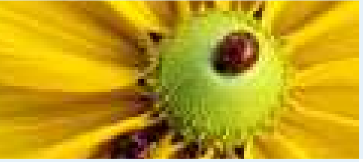

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Several scenarios:

- Fix p with degree m, optimize over A with fixed order n
- Fix A with order n, optimize over p with degree $\leq m$
- Optimize over both p with degree $\leq m$ and A with order n

We'll report only the last.

We restrict p to have real coefficients and A to be real, in Hessenberg form (all but one superdiagonal is zero).

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Computational Tools
Experiments
Optimizing over both p (deg. $m \leq 4$) and A ($n = 5$)
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The next slide shows the *sorted* final values of the Crouzeix ratio after running BFGS for a maximum of 250 iterations from each of 100 randomly generated starting points.

Optimizing over both p (deg. $m \leq 4$) and A $(n = 5)$

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Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Computational Tools

Experiments

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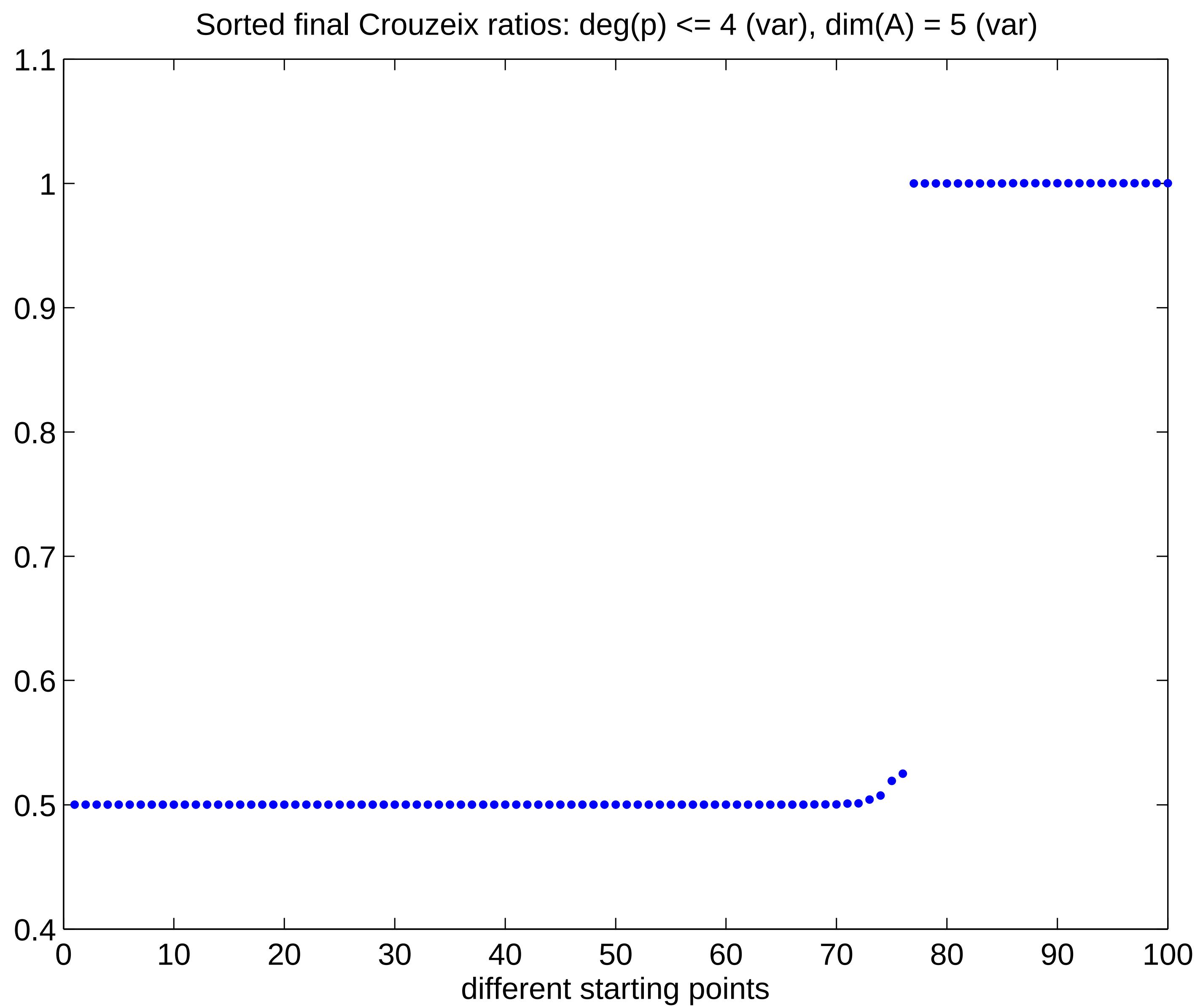

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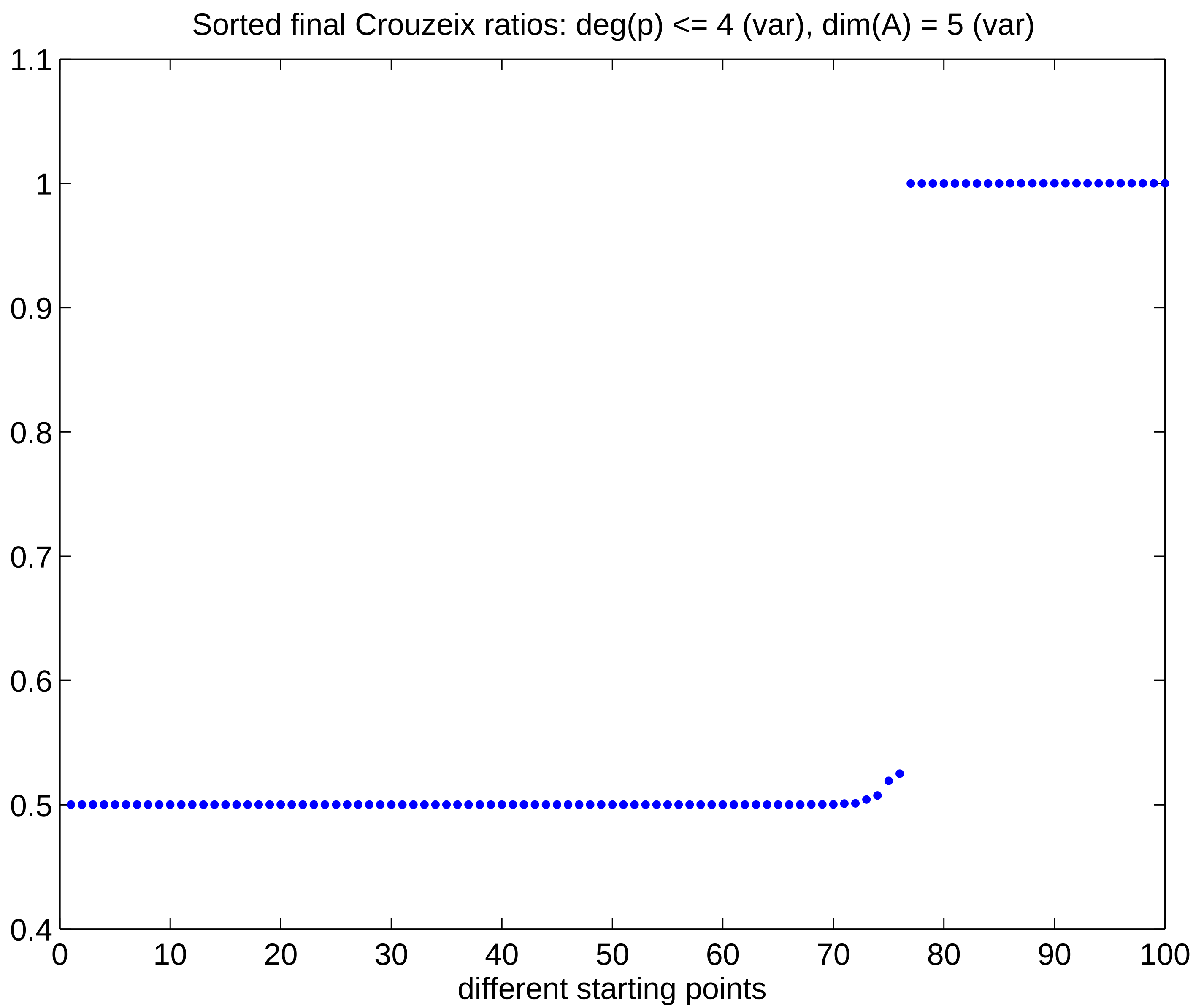

Only locally optimal values found are 0.5 and 1

Best Solution Found: $f(p, A) = 0.5000000002$

Best ratio found was 0.5000000002, with

$$p(z) = -(8.3\times10^{-11})z^4 - (6.6\times10^{-7})z^3 + (1.7\times10^{-5})z^2 + 2.6z - 1.3$$

which is *nearly linear*, with only one moderate sized root: $\mu = 0.49426$, and with A having eigenvalues 0.492 and 0.497, with mean $\lambda = 0.49424$.

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$$p(z) = -(8.3\times10^{-11})z^4 - (6.6\times10^{-7})z^3 + (1.7\times10^{-5})z^2 + 2.6z - 1.3$$

which is *nearly linear*, with only one moderate sized root: $\mu = 0.49426$, and with A having eigenvalues 0.492 and 0.497, with mean $\lambda = 0.49424$.

Using the Generalized Null Space Decomposition[1] we find that

$$A - \lambda I = UDU^T + E$$

where U is unitary, $\|E\| \approx 10^{-3}$, $D = \mathrm{diag}(B_1, B_2)$, B_1 is a scalar multiple of a 2×2 Jordan block and $W(B_2) \subset W(B_1)$, so it fits the example discussed earlier, but with an extra "inactive" block B_2.

[1] Kublanovskaja 1965; Golub-Wilkinson 1976, Guglielmi-Overton-Stewart 2014

For what (c, A) is the Crouzeix ratio $f(c, A) = 0.5$?

Terry Rockafellar
Crouzeix's Conjecture
Variational Analysis of the Crouzeix Ratio
Nonsmooth Optimization of the Crouzeix Ratio
Computational Tools
Experiments
Optimizing over both p (deg. $m \leq 4$) and A $(n = 5)$
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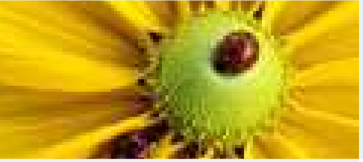

For what (c, A) is the Crouzeix ratio $f(c, A) = 0.5$?

Independently, Crouzeix and Choi showed that the ratio 0.5 is attained if $p(z) = (z - \lambda)^m$ and A is the $m + 1$ by $m + 1$ matrix

$$\begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \text{ if } m = 1, \text{ or } \begin{bmatrix} \lambda & \sqrt{2} & & & & & \\ & \cdot & 1 & & & & \\ & & \cdot & \cdot & & & \\ & & & \cdot & \cdot & & \\ & & & & \cdot & 1 & \\ & & & & & \cdot & \sqrt{2} \\ & & & & & & \lambda \end{bmatrix} \text{ if } m > 1$$

for which $W(A)$ is the unit disk.

For what (c, A) is the Crouzeix ratio $f(c, A) = 0.5$?

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Crouzeix's Conjecture

Variational Analysis of the Crouzeix Ratio

Nonsmooth Optimization of the Crouzeix Ratio

Computational Tools

Experiments

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Concluding Remarks

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for which $W(A)$ is the unit disk.

Based on our experiments, we conjecture that this is essentially the *only* case where 0.5 can be attained (we can change A by applying a unitary similarity transformation, multiplying by a scalar, and appending another diagonal block whose field of values is contained in that of the first block).

Terry Rockafellar
Crouzeix's Conjecture
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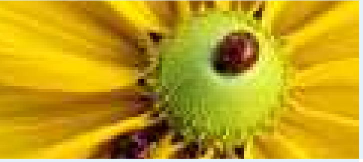
Nonsmooth Optimization of the Crouzeix Ratio
Concluding Remarks
Summary
Happy Birthday Terry

Concluding Remarks



Terry Rockafellar

Crouzeix's Conjecture

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Using variational analysis we have investigated the local behavior of the Crouzeix ratio in the simplest interesting case and we hope to be able to generalize this to higher degree and higher order.

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The results strongly support Crouzeix's conjecture: the globally minimal value of the Crouzeix ratio $f(p, A)$ is 0.5.

Happy Birthday Terry

Using Chebfun: