

**HEATHER WILBER**  
**CAVID SEMINAR, 7 JUNE 2022**

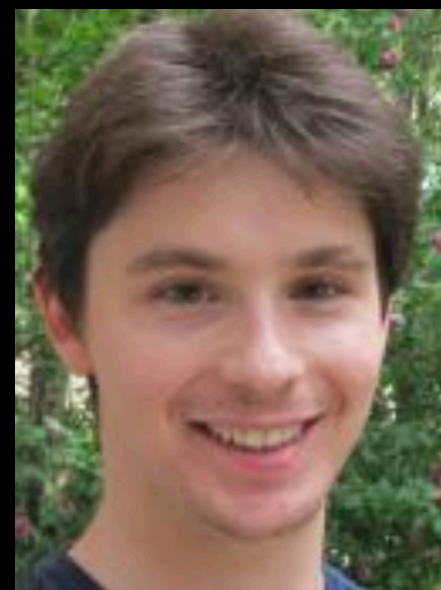
# **LOW RANK NUMERICAL METHODS VIA RATIONAL FUNCTION APPROXIMATION**



**ODEN INSTITUTE**  
FOR COMPUTATIONAL ENGINEERING & SCIENCES



Alex Townsend



Daniel Rubin

**JOINT WITH**



Bernhard Beckermann



Daniel Kressner



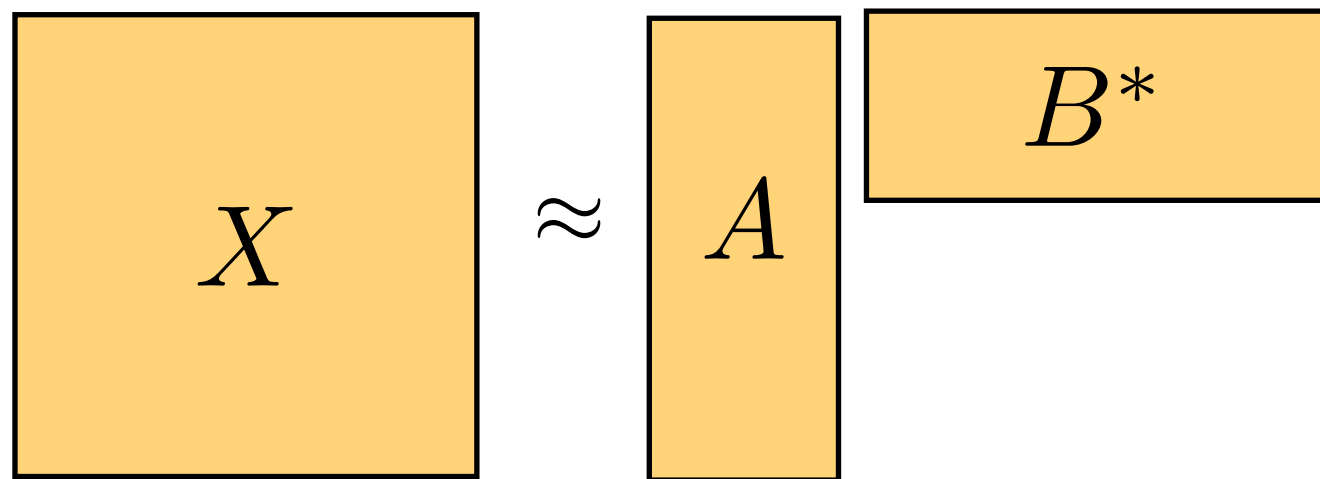
Gunnar Martinsson



Ke Chen

# LOW RANK METHODS IN SCIENTIFIC COMPUTING

"Work ~~smart~~, not hard." –A.P. Morgenstern  
data-sparse



- Discover/observe structures
- Understand them
- Exploit them

Low rank structure is one kind of data-sparsity

# ZOLOTAREV RATIONALS, COMPLEX ANALYSIS, AND LOW RANK METHODS



**Y. I. Zolotarev**

Zolotarev's approximation problems are central in many applications in computational math and numerical linear algebra...

Progress on these problems requires us to venture into the complex plane.



**T. Ganelius**



**E.B. Christoffel**



**K.H. Schwarz**



# ZLOTAREV RATIONAL FUNCTIONS IN SCIENTIFIC COMPUTING

- Analysis of iterative solvers for matrix equations.  
[Druskin, Knizhnerman and Simoninci (2011), Beckermann (2011)]
- Efficient solvers for Sylvester and Ricatti matrix equations.  
[Benner, Bujanović, Kürshcher, and Saak (2018), Wong and Balakrishnan (2005).]
- Singular value decay in matrices with displacement structure.  
[Beckermann and Townsend (2019), Sabino (2006), Rubin, Townsend and W. (2021) ]
- Compression properties in tensors/tensor train compression.  
[Townsend and Shi, 2021]
- Fast solvers for certain linear systems  $Xy = b$ .  
[Martinsson, Rokhlin, and Tygert (2005), Chandrasekaran, Gu, Xia, and Zhu (2007), Xia, Xi, and Gu (2012), Beckermann, Kressner and W. (2021).]
- Optimal complexity solvers for some elliptic PDEs.  
[Olver and Townsend (2013) , Fortunato and Townsend (2018), Townsend, W., Wright (2016,2017), Boule and Townsend (2019)]
- Solvers for PDEs involving the fractional Laplacian.  
[Chen, Martinsson, W. ]
- Matrix evaluation of sign, square root, absolute value, inversion functions.  
[(Gawlik and Nakatsukasa, 2019), (Hale, Higham, and Trefethen 2007)]
- Divide-and-conquer eigensolvers, polar decomposition algorithms.  
[ Nakatsukasa and Freund (2016)]
- Digital filters in signal processing.  
[ Daniels, R. (1974)]



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# ZOLOTAREV'S RATIONAL FUNCTIONS

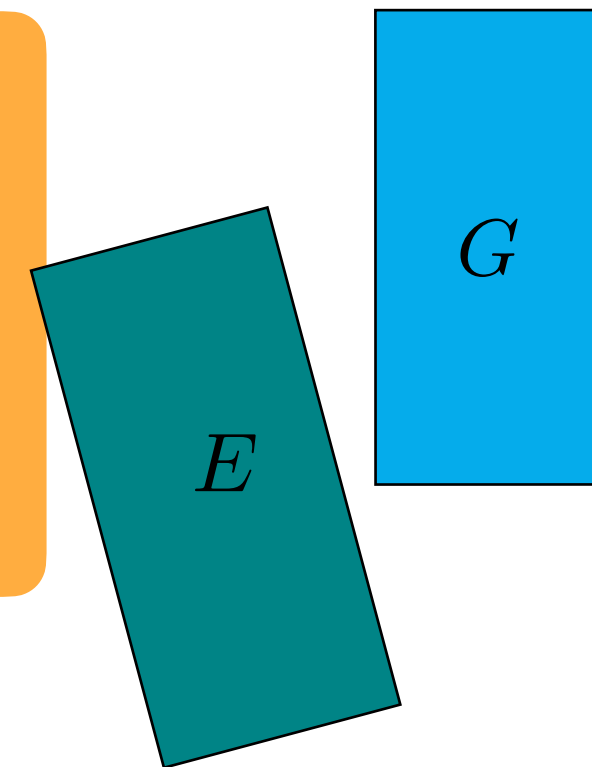
## THE 3RD PROBLEM



Y. I. Zolotarev

Given disjoint sets  $E$  and  $G$  in  $\mathbb{C}$ ,  
find a rational function  $r \in \mathcal{R}_k$  that minimizes the ratio

$$\frac{\sup_{z \in E} |r(z)|}{\inf_{z \in G} |r(z)|}.$$



The  $k$ th Zolotarev number associated with  $E$  and  $G$ :

$$Z_k(E, G) := \inf \frac{\sup_{z \in E} |r(z)|}{\inf_{z \in G} |r(z)|}.$$

# ZOLOTAREV'S RATIONAL FUNCTIONS

## THE 3RD PROBLEM



Y. I. Zolotarev

### Key connection:

$$h = \exp(1/\text{cap}(E, G))$$

When  $E, G$  are disjoint disks in  $\mathbb{C}$ :

- $Z_k(E, G) = h^{-k}$ , poles and zeros of  $r_k$  known.

When  $E, G$  are disjoint intervals on the real line:

- $Z_k(E, G)$  given by an infinite product, poles and zeros of  $r_k$  known.
- $Z_k(E, G) \leq 4h^{-k}$

$E, G$  where  $\mathbb{C} \setminus E \cup G$  is doubly connected:

- $h^{-k} \leq Z_k(E, G)$
- $\lim_{k \rightarrow \infty} (Z_k(E, G))^{1/k} = h^{-1}$



# ZOLOTAREV'S RATIONAL FUNCTIONS

## THE 4TH PROBLEM



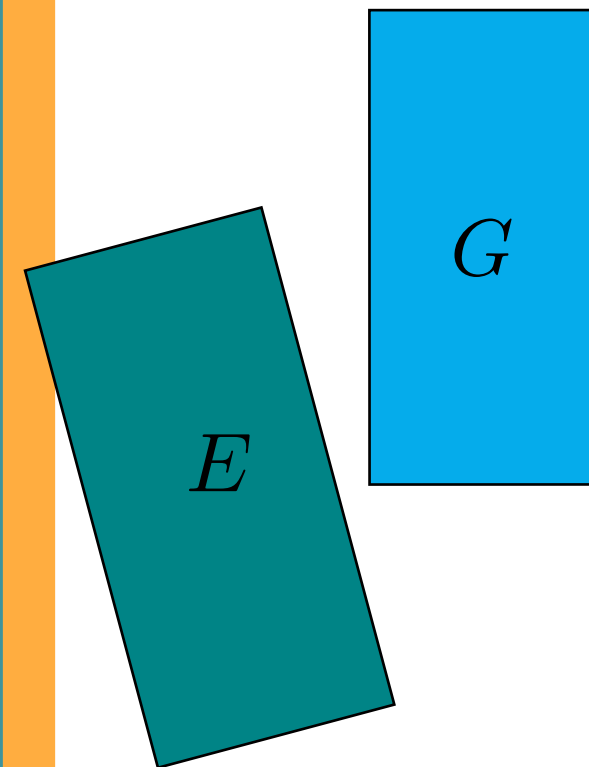
Y. I. Zolotarev

Given sets  $E$  and  $G$  in  $\mathbb{C}$ ,  
find a rational function  $\hat{r} \in \mathcal{R}_k$  that minimizes the error

$$\max_{z \in E \cup G} |\operatorname{sgn}(z) - \hat{r}(z)|,$$

where

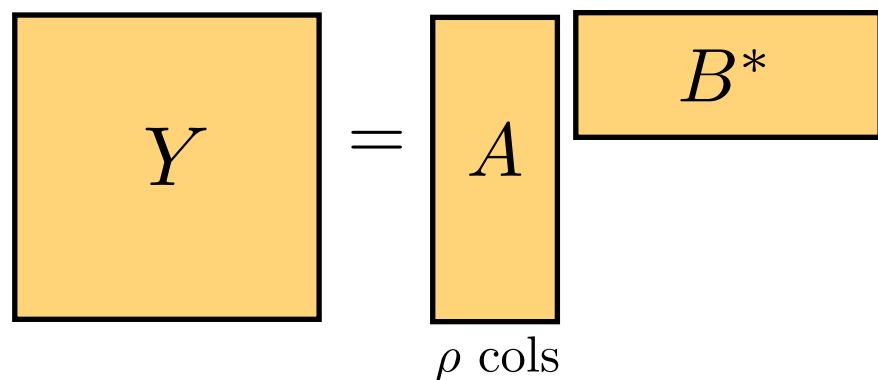
$$\operatorname{sgn}(z) = \begin{cases} 1, & z \in E, \\ -1, & z \in G. \end{cases}$$



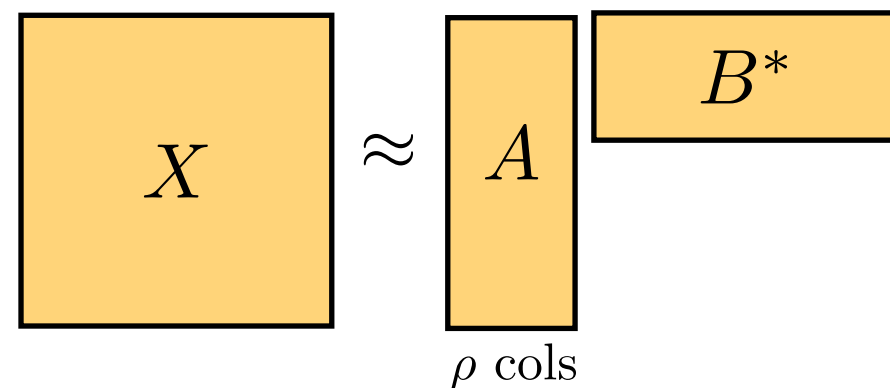
$$\tau_k(E, G) := \min_{\hat{r} \in \mathcal{R}_k} \max_{z \in E \cup G} |\operatorname{sgn}(z) - \hat{r}| = \frac{2\sqrt{Z_k(E, G)}}{1 + Z_k(E, G)}.$$

# LOW RANK APPROXIMATION

$$\text{rank}(Y) \leq \rho$$

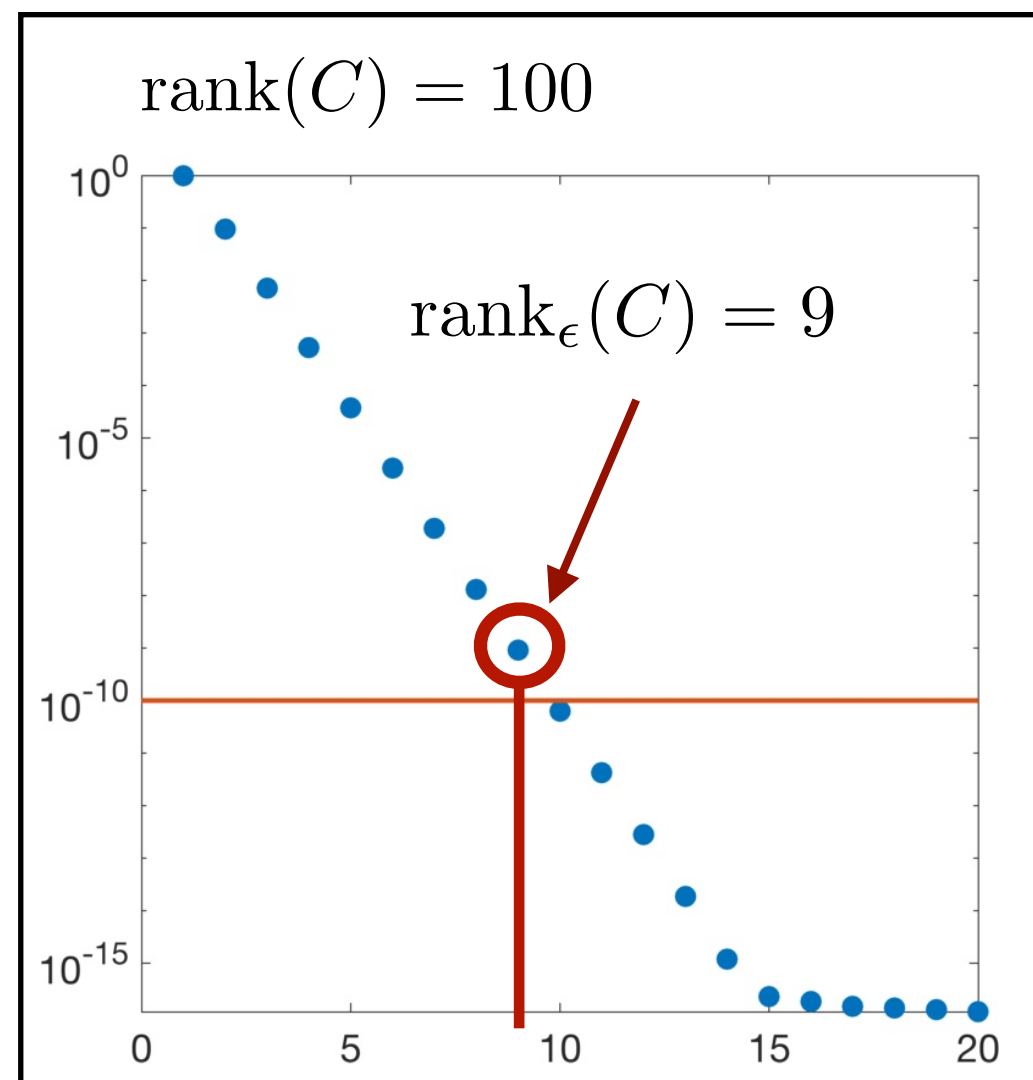


$$\text{rank}_\epsilon(X) \leq \rho$$



$$\sigma_{\rho+1}(X) = \min\{\|X - Y\|_2, \text{rank}(Y) = \rho\}$$

$$\text{rank}_\epsilon(X) = \text{smallest } \rho \text{ where } \sigma_{\rho+1}(X) \leq \epsilon \|X\|_2$$



# MATRICES WITH DISPLACEMENT STRUCTURE

A matrix  $X \in \mathbb{C}^{m \times n}$  is said to have  $(A, B)$  displacement structure if

$$AX - XB = F,$$

where  $A \in \mathbb{C}^{m \times m}$ ,  $B \in \mathbb{C}^{n \times n}$ , and  $F \in \mathbb{C}^{m \times n}$ .

Related formulations:

Block linear equations

$$AX = F \rightarrow Ax_1 = f_1, Ax_2 = f_2, \dots, Ax_n = f_n$$

Sums of Kronecker products

$$AX - XB = F \rightarrow \mathcal{A}\mathbf{x} = \mathbf{f}, \quad \mathcal{A} = I_n \otimes A - B^* \otimes I_m$$



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Sylvester matrix equations appear in:

stability analysis for dynamical systems • discretizations of PDEs • signal processing and time series analysis • eigenvalue assignment problems • iterative solvers for continuous algebraic Ricatti matrix equation • analyses/computations involving special structured matrices (e.g., Toeplitz, Cauchy, Vandermonde)

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In practical settings:

- $A$  and  $B$  are sparse, banded, or structured, so that fast shifted inverses/matrix-vector products are available.
- $F$  is often a low rank matrix (rank 1 or 2).
- $X$  is dense.

# THE LOW RANK PROPERTY

$$AX - XB = F$$

When the spectra of  $A$  and  $B$  are well-separated and  $F$  is low rank,  $X$  is well-approximated by low rank matrices.

1. Why is this true?
2. When is this true?
  - Only in the above circumstances or in greater generality?
  - Can we be precise about how the low rank properties of  $X$  depend on  $A$ ,  $B$ , and  $F$ ?
3. How can we take advantage of it?

[ (Beckermann & Townsend, 2017), (Sabino, 2008 ), (Penzl, 1999), (Benner, Truhar & Li, 2009), (Li & White, 2002), (Druskin, Knizhnerman & Simoninci, 2011), (Peaceman & Rachford, 1955), (Lu & Wachspress, 1991), (Townsend & W., 2018) ]



# A RECIPE FOR LOW RANK APPROXIMATIONS

$$AX - XB = F \qquad A(\textcolor{red}{ZDY}^*) - (\textcolor{red}{ZDY}^*)B = USV^* \quad (\text{S of size } \rho \times \rho)$$

(factored) ADI

$$\begin{aligned} Z^{(k)} &= \begin{bmatrix} \hat{Z}^{(1)} & \hat{Z}^{(2)} & \dots & \hat{Z}^{(k)} \end{bmatrix}, & \begin{cases} \hat{Z}^{(1)} = (A - \beta_1 I)^{-1} US, \\ \hat{Z}^{(i+1)} = (A - \alpha_i I)(A - \beta_{i+1} I)^{-1} Z^{(i)} \end{cases} \\ Y^{(k)} &= \begin{bmatrix} \hat{Y}^{(1)} & \hat{Y}^{(2)} & \dots & \hat{Y}^{(k)} \end{bmatrix}, & \begin{cases} \hat{Y}^{(1)} = (B^* - \alpha_1 I)^{-1} V, \\ \hat{Y}^{(i+1)} = (B^* - \beta_i I)(B^* - \alpha_{i+1} I)^{-1} Y^{(i)} \end{cases} \\ D^{(k)} &= \text{diag}((\beta_1 - \alpha_1)I_\rho, \dots, (\beta_k - \alpha_k)I_\rho) \\ X^{(k)} &= Z^{(k)} D^{(k)} Y^{(k)*} \end{aligned}$$

After k iterations:

- $X^{(k)} = ZW^*, \quad \text{rank}(X^{(k)}) \leq k\rho, \quad \rho = \text{rank}(F)$
- $X - X^{(k)} = r_k(A)Xr_k(B)^{-1}, \quad r(z) = \prod_{j=1}^k \frac{z - \alpha_j}{z - \beta_j}$

$$X^{(k)} = \begin{array}{|c|} \hline Z \\ \hline \end{array} \begin{array}{|c|} \hline W^* \\ \hline \end{array}$$

# A RECIPE FOR BOUNDING SINGULAR VALUES

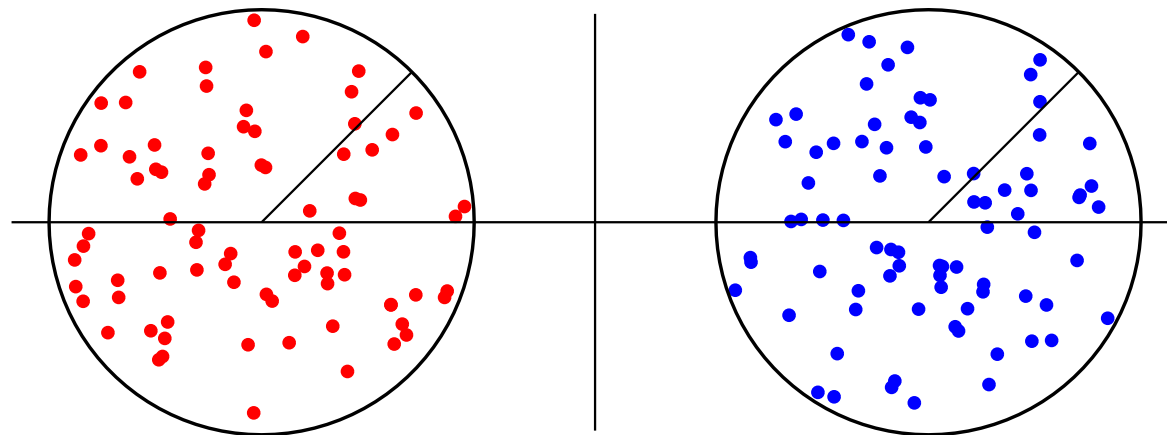
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$$X^{(k)} = \begin{array}{|c|} \hline Z \\ \hline \end{array} \begin{array}{|c|} \hline W^* \\ \hline \end{array}$$

$$\sigma_{k\rho+1}(X) \leq \|X - X^{(k)}\|_2 \leq \|r_k(A)r_k(B)^{-1}\|_2 \|X\|_2 \leq Z_k(E, G) \|X\|_2$$



$$\lambda(A) \subset E$$

$$\lambda(B) \subset G$$

# A RECIPE FOR BOUNDING SINGULAR VALUES

- Explicit bounds on the singular values of  $X$
- A cheap method for constructing low rank approximations  $X^{(k)} = ZW^* \approx X$

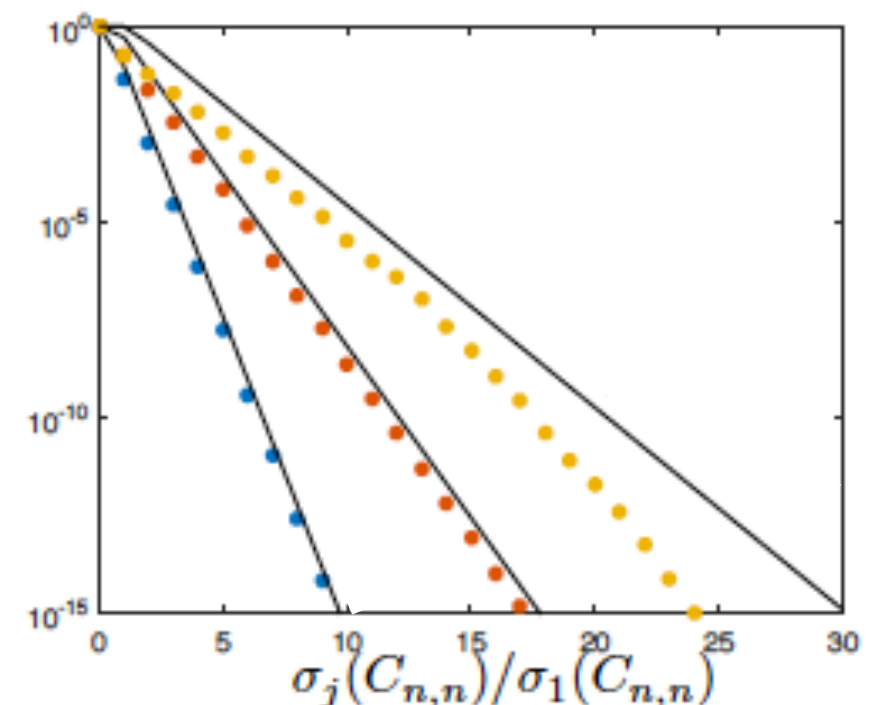
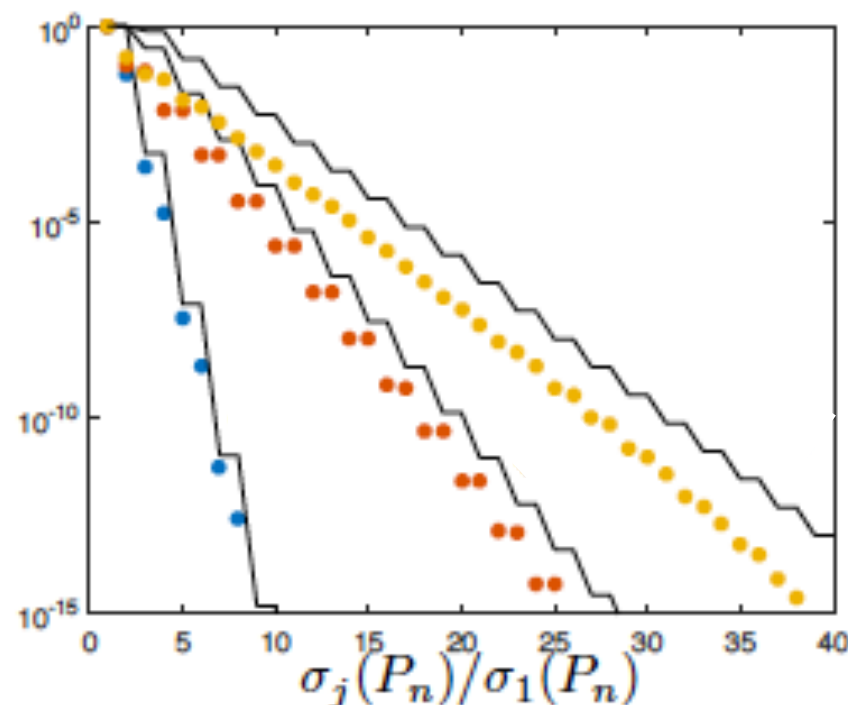
Explains low rank properties in real-valued Vandermonde, Pick, Cauchy, Loewner matrices and more...



**A. Townsend**



**B. Beckermann**





# EXPANDING ADI-BASED METHODS

To bound singular values of  $X$  via fADI, we need...

1.  $\text{rank}(F)$  is small.
2. The spectra of  $A$  and  $B$  are well-separated.
3. A solution to Zolotarev's problem is known for sets  $E, G$ , where  $\lambda(A) \subset E$  and  $\lambda(B) \subset G$ .

**Problem: Many practical applications do not satisfy these constraints!**

# EXPANDING ADI-BASED METHODS

1. ~~rank( $F$ ) is small.~~

$F$  has decaying singular values.

Townsend, W., (2018):

ADI with high-rank right-hand sides.

- low rank solver for  $AX - XB = F$ ,  $F$  is full rank.
- bounds on numerical ranks of matrices, e.g., multidimensional Vandermonde

2. ~~The spectra of  $A$  and  $B$  are well separated.~~

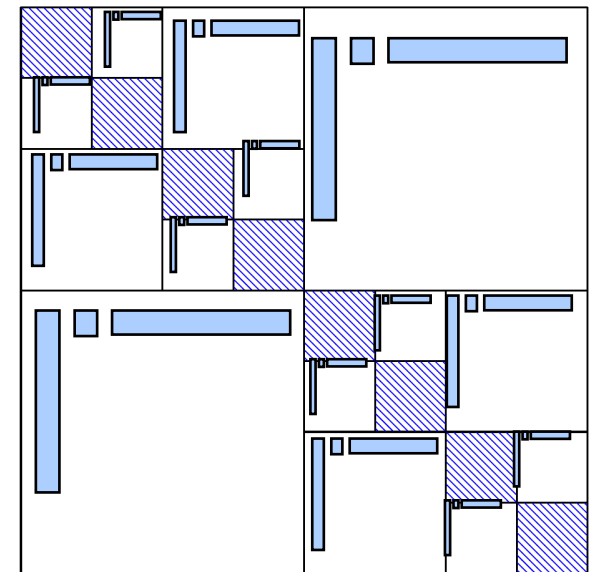
Subsets of the spectra of  $A$  and  $B$  are well-separated.

Beckermann, Kressner, W., (2021)

superfast solvers for Toeplitz system  $Tx = b$ .

ADI-based hierarchical compression.

- extends to other related linear systems (e.g., NUDFT, Toeplitz+Hankel)
- explicit approx. error bounds + competitive with state-of-the-art.



# EXPANDING ADI-BASED METHODS

3. ~~A solution~~ to Zolotarev's problem is known for sets  $E, G$ , where  $\lambda(A) \subset E$  and  $\lambda(B) \subset G$ .

## An approximate solution

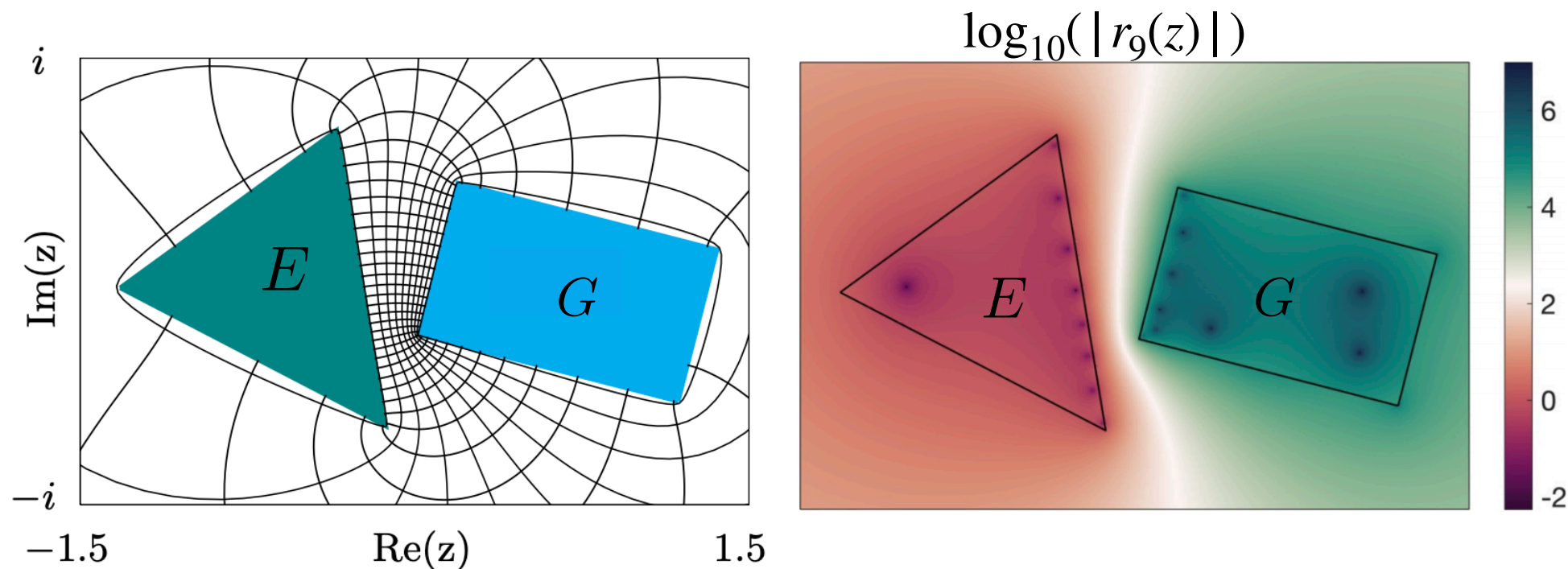
Zolotarev's third problem:

$$Z_k(E, G) := \inf_{r \in \mathcal{R}^k} \frac{\sup_{z \in E} |r(z)|}{\inf_{z \in G} |r(z)|}$$

Solution is known for:

- Intervals of the real line
- Disks in the complex plane

For more general sets in  $\mathbb{C}$ ...



[(Zolotarev, 1877), (Sabino, 2008), (Beckermann & Townsend, 2017, 2019), (Starke, 1992) (Ganelius, 1976, 1979)]

# ZOLOTAREV'S 3RD PROBLEM IN THE COMPLEX PLANE



$$h = \exp(1/\text{cap}(E, G))$$

$$\Phi : \Omega \rightarrow \mathcal{A} = \{z \in \mathbb{C}, 1 \leq |z| \leq h\}$$

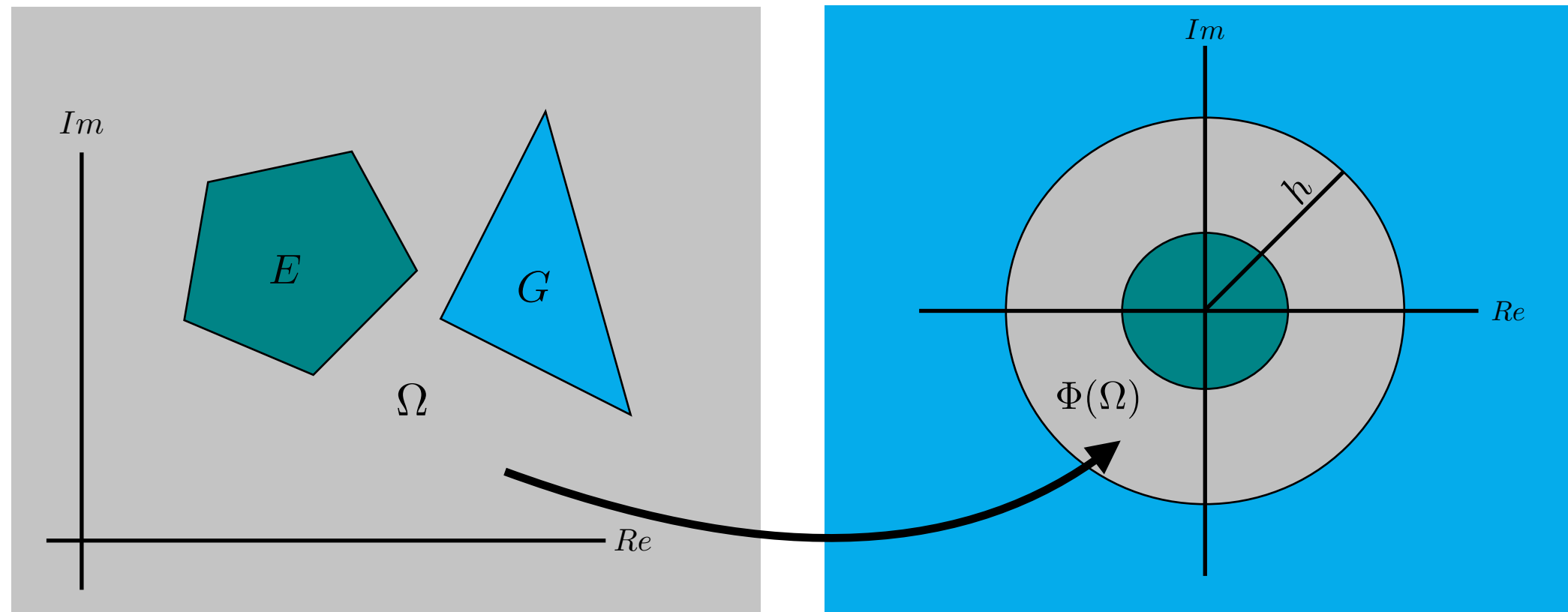
Suppose that  $\Phi$  is a type  $(1, 1)$  rational function...

$\Phi^k$  is a type  $(k, k)$  rational function.

$$h^{-k} \leq Z_k(E, G) \leq \frac{\sup_{z \in E} \Phi^k(z)}{\inf_{z \in G} \Phi^k(z)} \leq \frac{1}{h^k} = h^{-k}.$$

$$\implies Z_k(E, G) = h^{-k}$$

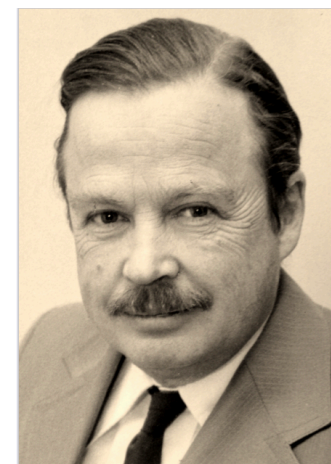
# THE FABER RATIONAL FUNCTIONS



$$\Phi : \Omega \rightarrow \mathcal{A} = \{z \in \mathbb{C}, 1 \leq |z| \leq h\}$$

When  $\Phi$  isn't a rational function, the story gets more complicated...

- Apply a special “filtering” process to  $\Phi^k(z)$ ,
- Results in a type  $(k, k)$  rational  $\tilde{r}(z)$  (Faber rational),
- Bound  $\frac{\sup_{z \in E} |\tilde{r}_k(z)|}{\inf_{z \in G} |\tilde{r}_k(z)|}$  from above.



(T. Ganelius)



(G. Faber)

# ZLOTAREV'S 3RD PROBLEM IN THE COMPLEX PLANE

Theorem (Rubin, Townsend, W., 2021) If  $E, G$  are disjoint, bounded open convex sets in  $\mathbb{C}$ , then there is  $k_0$  where for  $k > k_0$ ,

$$Z_k(E, G) \leq 16h^{-k} + \mathcal{O}(h^{-2k}).$$

\*We have an inelegant explicit upper bound and expression for  $k_0$ .





# ZOLOTAREV'S 3RD PROBLEM IN THE COMPLEX PLANE

Disjoint sets $E$ and $G$	Bound	Reference
finite intervals of $\mathbb{R}$	$Z_k(E, G) \leq 4h^{-k}$	Beckermann, Townsend (2017)
disks in $\mathbb{C}$	$Z_k(E, G) \leq h^{-k}$	Starke (1992)
arcs on a circle $\mathbb{C}$	$Z_k(E, G) \leq 4h^{-k}$	Beckermann, Kressner, W. (2021)
more general sets in $\mathbb{C}$	$Z_k(E, G) \leq 16h^{-k} + \mathcal{O}(h^{-2k})$	

- Bounds on singular values for families of matrices.
- Bounds for rational approximation to  $\text{sign}(z)$  on  $E, G$ .
- New ideas for computing ADI shift parameters.

**CONFORMAL MAPS  
+ NUMERICS =  
HEURISTICS**

Many modern tools available to compute  $\Phi$  (and  $h$ )

Lightning Laplace solver (Trefethen, Gopal, Baddoo)

Integral formulations (Gaier, Schiffer, Nasser)

Schwarz-Christoffel methods (Delillo, Elcrat, Driscoll, Crowdy, many more...)

To compute/evaluate  $\Phi^{-1}$

Construct a complex-valued barycentric rational interpolant to samples  $(\Phi(z), z)$ .

# ZOLOTAREV'S 4TH PROBLEM AND THE MATRIX/OPERATOR-VALUED SQUARE ROOT FUNCTION

Consider a matrix  $A \in \mathbb{R}^{n \times n}$  and let  $\lambda(A) \subset [\alpha, 1]$ .

Compute  $\sqrt{A}$ .

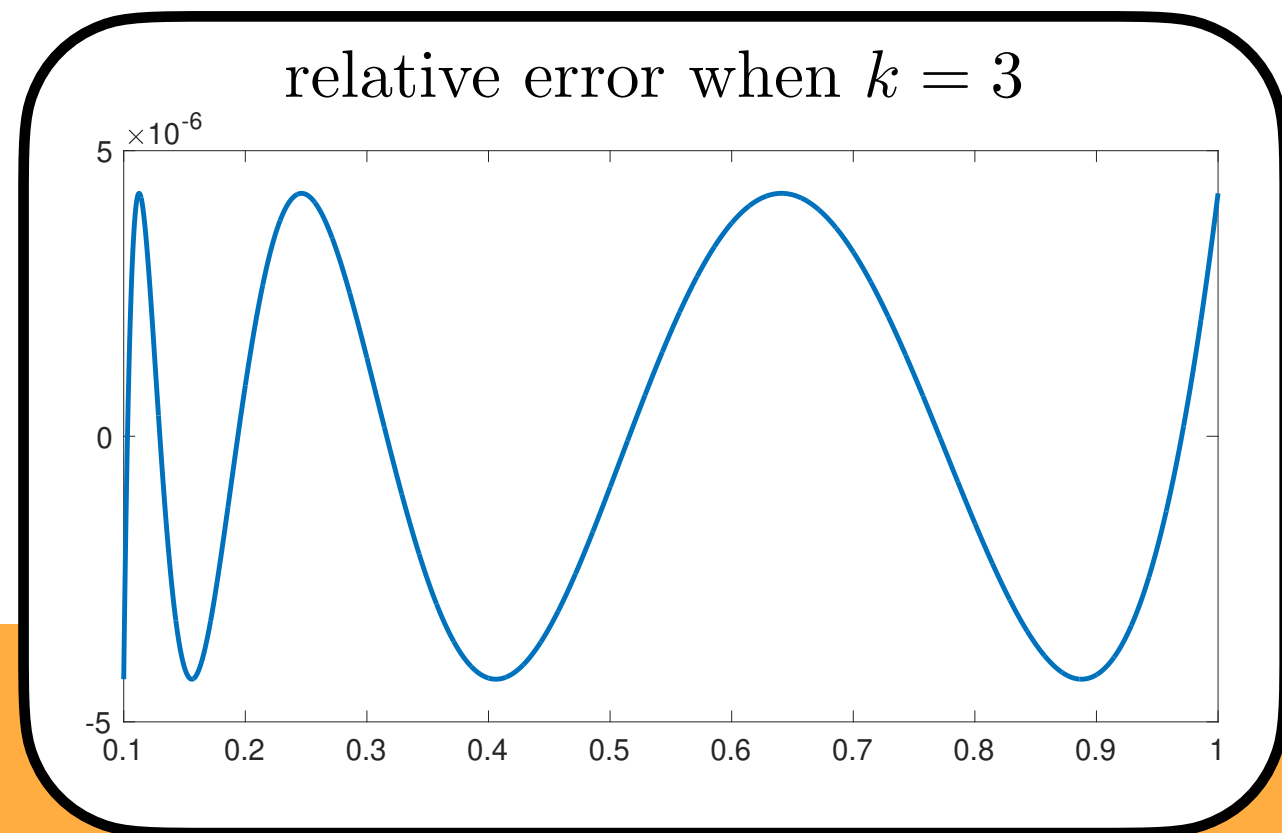
Let  $\hat{r}_k$  be the best type  $(2k+1, 2k)$  approx. to  $\operatorname{sgn}(z)$ ,  $z \in [-1, -\alpha^2] \cup [\alpha^2, 1]$ .

$$E_{2k+1, 2k} := |\operatorname{sgn}(z) - \hat{r}_k(z)| = \left| \frac{z}{|z|} - z \frac{p_k(z^2)}{q_k(z^2)} \right|$$

Letting  $x = z^2$ ,

$$E_{2k+1, 2k} = \left| \sqrt{x} - x \frac{p_k(x)}{q_k(x)} \right| / |\sqrt{x}|, \quad x \in [\alpha, 1]$$

Gives the best type  $(k+1, k)$  relative rational approximation to  $\sqrt{x}$  on  $[\alpha, 1]$ .



# ZOLOTAREV'S 4TH PROBLEM AND THE MATRIX/OPERATOR-VALUED SQUARE ROOT FUNCTION

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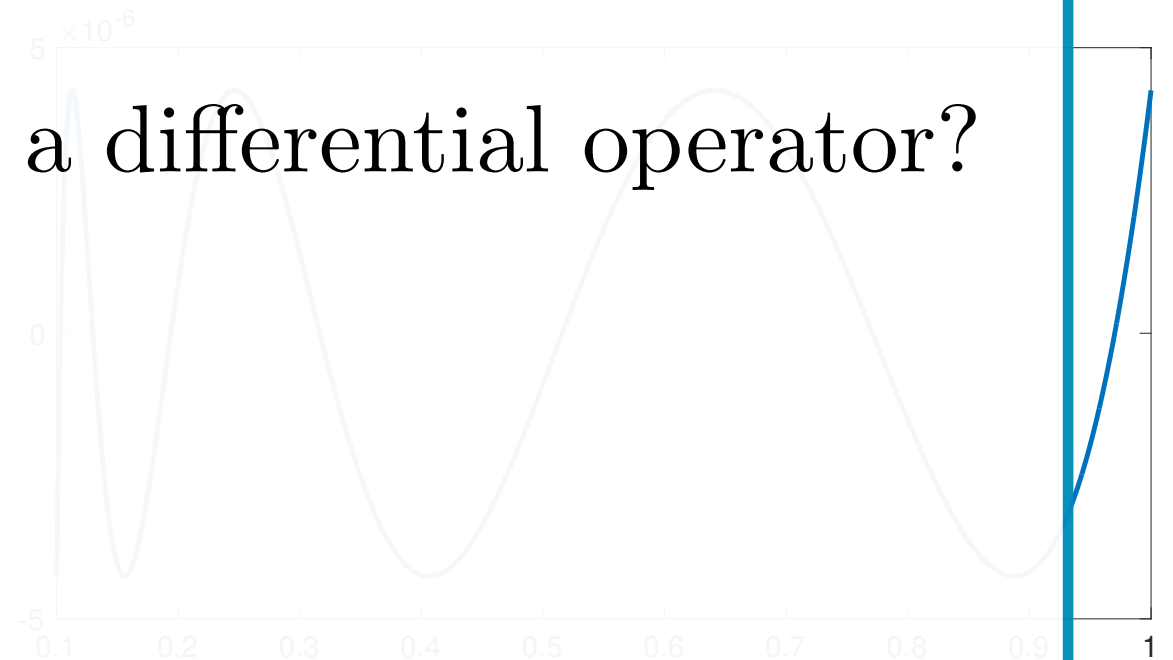
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What about  $\sqrt{\mathcal{L}}$ , where  $\mathcal{L}$  is a differential operator?

Letting  $x = z^2$ ,

$$E_{2k+1, 2k} = \left| \sqrt{x} - \frac{p_k(x)}{q_k(x)} \right| / |\sqrt{x}|, \quad x \in [\alpha, 1].$$

relative error when  $k = 3$



Gives the best type  $(k, k)$  relative rational approximation to  $\sqrt{x}$  on  $[\alpha, 1]$ .

# THE SPECTRAL FRACTIONAL LAPLACE OPERATOR

Let  $\Omega$  be a bounded, simply connected, open subset of  $\mathbb{R}^d$ .

$$\Delta u = - \left( \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2} \right)$$

For  $0 < \alpha \leq 2$ , we define  $\mathcal{L}_\alpha : H_0^2(\Omega) \rightarrow L^2(\Omega)$  as follows:

$$\mathcal{L}_\alpha u = \sum_{j=1}^{\infty} \lambda_j^{\alpha/2} \langle e_j, u \rangle e_j,$$

where  $\Delta e_j = \lambda_j e_j$ , and  $e_j|_{\partial\Omega} = 0$ .

When  $\alpha \neq 2$ ,  $\mathcal{L}_\alpha$  is a nonlocal operator arising from physical problems involving anomalous diffusion:

**“Diffusion of particles with spattering”**

**-C. Pozrikidis (The Fractional Laplacian)**

# THE SPECTRAL FRACTIONAL LAPLACE OPERATOR

## SPECTRAL FRACTIONAL POISSON EQUATION

$$\begin{aligned}\mathcal{L}_\alpha u &= f, & x \in \Omega, \\ u(x) &= 0, & x \in \partial\Omega\end{aligned}$$



Gunnar Martinsson



Ke Chen

$$\mathcal{L}_\alpha u = \sum_{j=1}^{\infty} \lambda_j^{\alpha/2} \langle e_j, u \rangle e_j, \quad \rightarrow \quad \mathcal{L}_\alpha^{-1} f = \sum_{j=1}^{\infty} \lambda_j^{-\alpha/2} \langle e_j, f \rangle e_j$$

Naive method: Discretize  $\Delta$ , represent with a matrix  $L$ . Find the eigendecomposition of  $L$ .

Ex.  $\Omega = [0, 1]$

$$e_k(x) = \sqrt{2} \sin(k\pi x) \quad \lambda_k = (\pi k)^2 \quad \langle 1, e_k \rangle = \frac{2\sqrt{2}}{\pi k}$$

➡ For  $\alpha = 1$ ,  $k \sim (4/\epsilon)^2$  to achieve error tolerance  $\epsilon$ .

# RATIONAL FUNCTIONS AND FAST DIRECT SOLVERS TO THE RESCUE

## SPECTRAL FRACTIONAL POISSON EQUATION

$$\begin{aligned}\mathcal{L}_\alpha u &= f, & x \in \Omega, \\ u(x) &= 0, & x \in \partial\Omega\end{aligned}$$



Gunnar Martinsson



Ke Chen

Let  $r_k(x) = \sum_{\ell=1}^k \frac{\gamma_\ell}{x-p_\ell}$ ,  $r_k(x) \approx x^{-\alpha/2}$  for  $x \in [1, \infty)$ .

Now  $\mathcal{L}_\alpha^{-1} f \approx r_k(\Delta) f = \sum_{j=1}^k \gamma_\ell (\Delta - p_\ell I)^{-1} f$ .

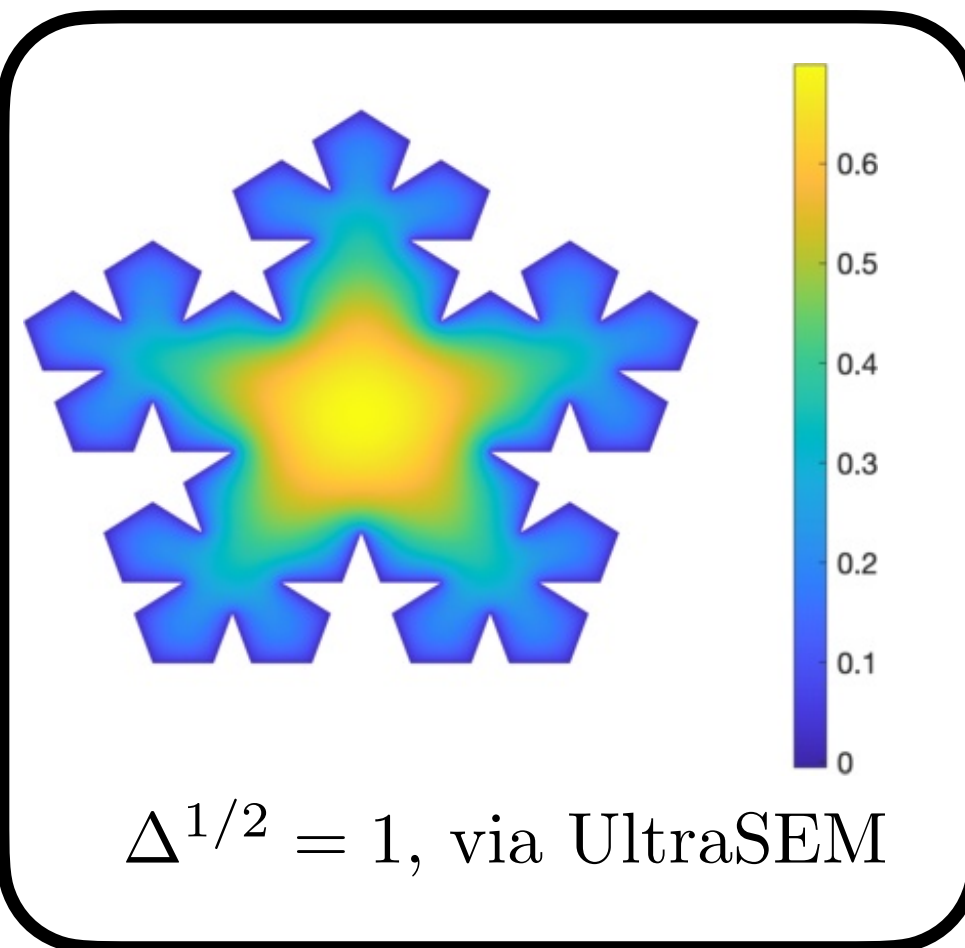
For each  $\ell$ , solve

---

$$\begin{aligned}\Delta u_\ell - p_\ell u_\ell &= \gamma_\ell f, & x \in \Omega \\ u_\ell(x) &= 0, & x \in \partial\Omega.\end{aligned}$$

---

Then 
$$u \approx \sum_{\ell=1}^k u_\ell.$$





# CONSTRUCTING RATIONAL FUNCTIONS

Transform to a finite interval:

$$\tilde{r}_k(y) \approx y^{\alpha/2}, \quad y \in [0, 1].$$

Let  $r_k(x) = \tilde{r}_k(1/y)$ .

$$\text{H. Stahl: For } \alpha = 2/n, n \in \mathbb{Z}^+, e^{-c_1(n)\sqrt{k}} \leq \max_{x \in [0,1]} |r_k(x) - x^{\alpha/2}| \leq e^{-c_2(n)\sqrt{k}}$$

## How to build such a rational function?

- sampling methods/least-squares fitting:

Error blows up in locations off sampling grid as  $x \rightarrow 0$ .

- Analytical construction (e.g., contour integration) on interval  $[m, 1]$ , where  $m$  is small and  $r_k$  “behaves well” on  $[0, m]$ .

# RATIONALS VIA CONTOUR INTEGRATION

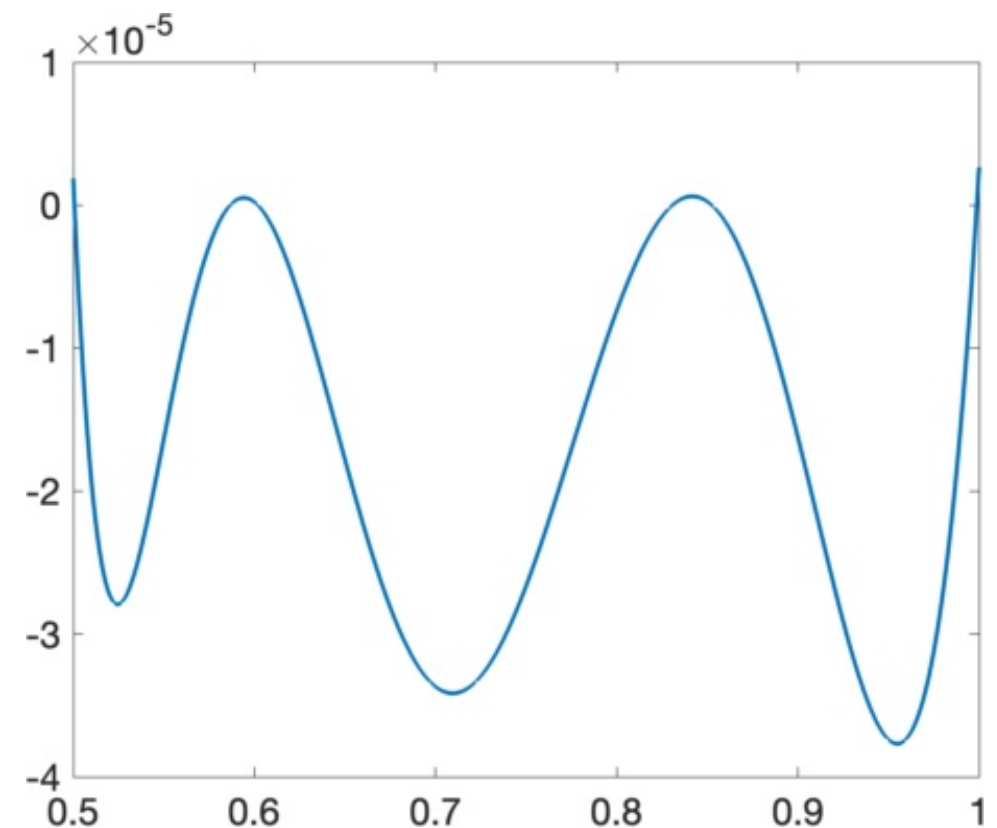
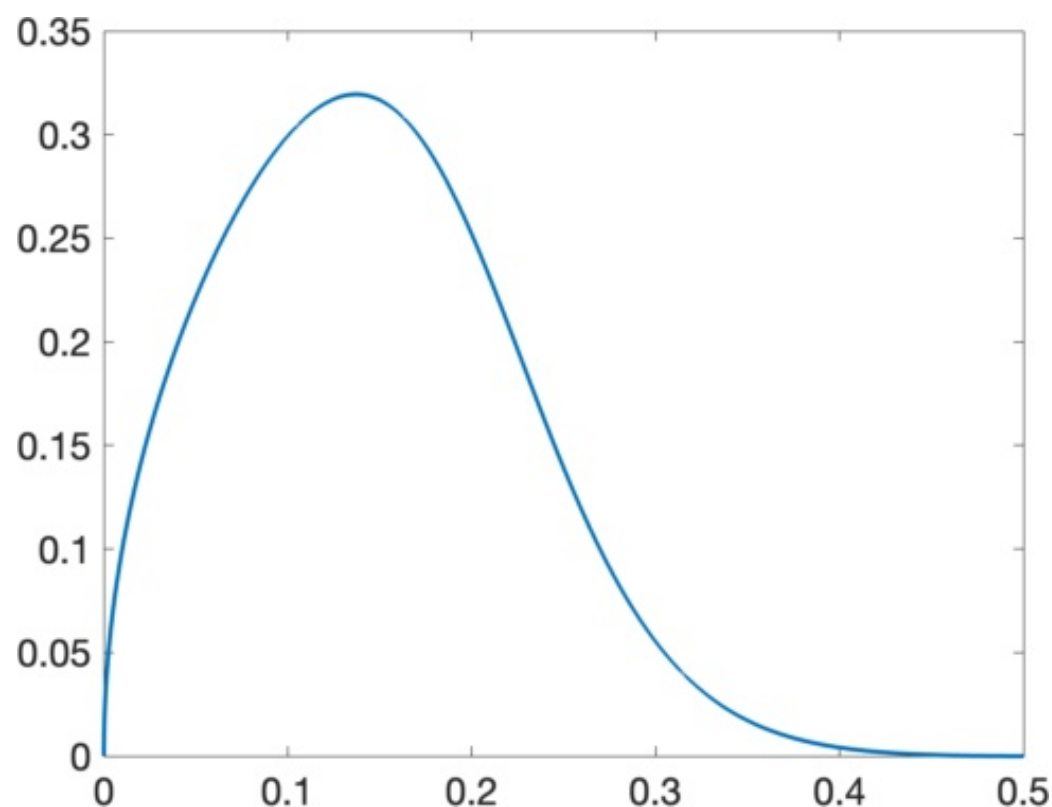
## RESOLVENT METHODS

$$f(x) = \frac{x}{2\pi i} \int_{\gamma} z^{-1} f(z) (z - x)^{-1} dz, \quad x \in [m, 1].$$

Apply a quadrature rule consisting of  $k$  weight-node pairs,  $\{(w_j, z_j)\}_{j=1}^k$ :

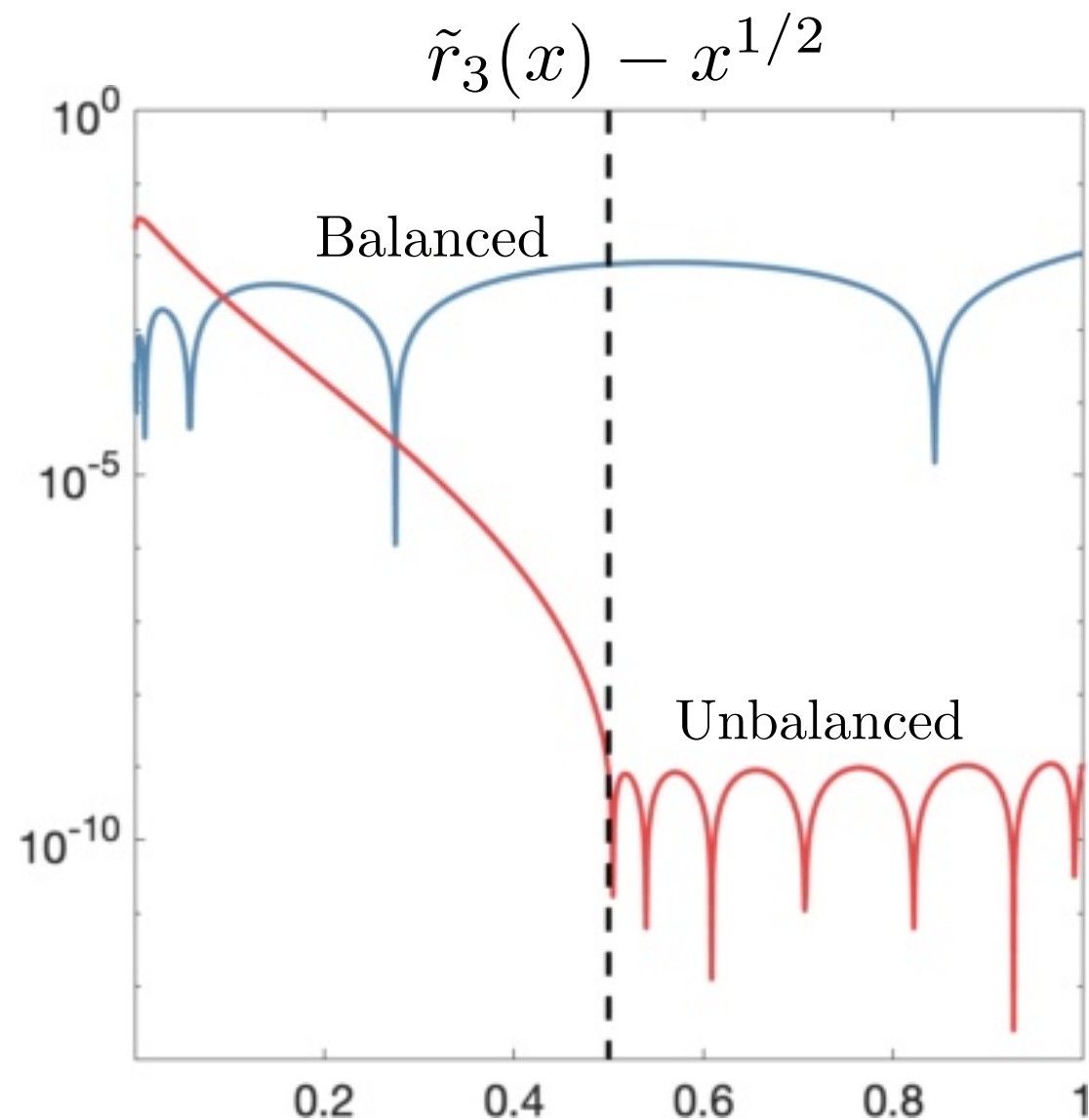
$$f(x) \approx \frac{x}{2\pi i} \sum_{j=1}^k \frac{-\gamma_j}{x - p_j}, \quad \text{where, } \gamma_j = w_j z_j^{-1} f(z_j) dz_j.$$

Choose the contour and quadrature points cleverly via conformal mapping.



# THE SQUARE ROOT CASE

For  $\Delta^{-1/2}f$ , we can construct  $r_k$  via the solution via Zolotarev's 4th problem.



Each  $r_k$  is bounded and small on  $[0, m]$ .

For fixed  $k$ , we optimize the choice of  $m$ :

Approximants converge to  $\sqrt{x}$  like  $e^{-c\sqrt{k}}$ .

# EXTENSIONS VIA SPECIALIZED CONTOUR INTEGRALS

Let  $f(x) = x^{1/2}$ .

$$f(x) = \frac{x}{2\pi i} \int_{\gamma} z^{-1} f(z) (z - x)^{-1} dz, \quad x \in [m, 1].$$

Let  $v^2 = z$ :

$$f(x) = \frac{x}{\pi i} \int_{\gamma_v} (v^2 - x)^{-1} dv$$

Map conformally to a rectangle  $R$ :

$$v = m^{1/2} \operatorname{sn}(t|q), \quad q = m^{1/2}.$$

Apply trapezoidal quadrature rule.



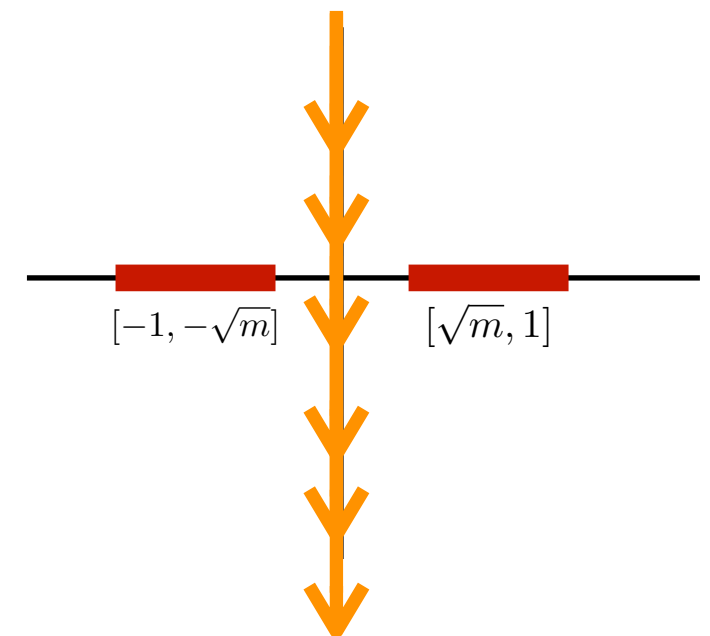
N. Higham



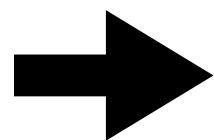
N. Trefethen



N. Hale



The resulting rational approximation is the best relative approximation to  $\sqrt{x}$  on  $[m, 1]$ !



A blueprint for approximations to  $x^{1/n}$  on  $[0, 1]$ .

# EXTENSIONS VIA SPECIALIZED CONTOUR INTEGRALS

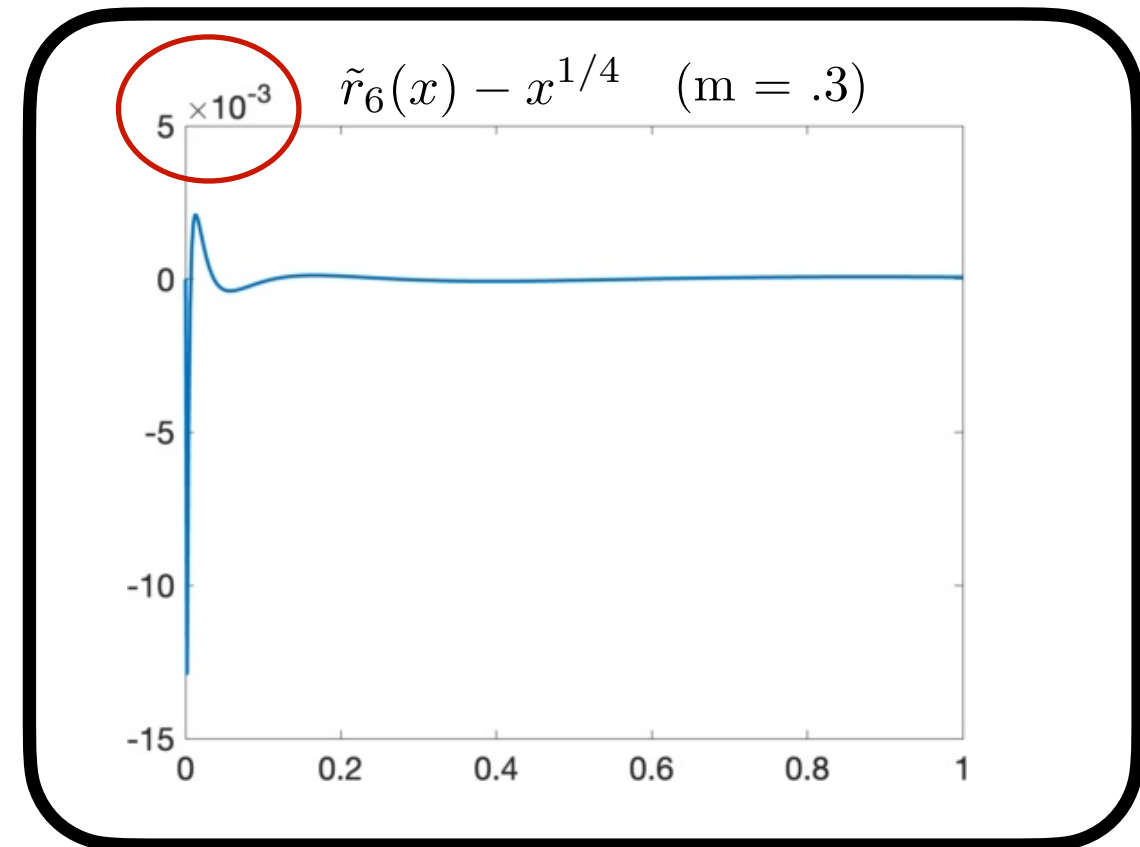
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Let  $v^n = z$ :

$$f(x) = \frac{nx}{2\pi i} \int_{\gamma_v} (v^n - x)^{-1} dv$$

Map conformally to a rectangle  $R$ :  
Apply trapezoidal quadrature rule.



- poles along  $(-\infty, 0]$  in  $z$  plane
- formulation via elliptic functions

# SUMMARY

We can **explain** and **exploit** low rank properties in several computational applications by...

Expanding our understanding of the Zolotarev rational functions

Revisiting and expanding upon our understanding of classical tools like contour integration and conformal mapping

Developing new computational methods for constructing rational approximations to functions

Code, papers, slides, and more:  
[heatherw3521.github.io](https://heatherw3521.github.io)

