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Zolotarev numbers and the

nonuniform discrete Fourier transform

Heather Wilber 4 November 2024 PACM Seminar, Princeton University

In collaboration with...



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Today's focus: the nonuniform discrete Fourier transform

Solve Vx = b, where V is a Vandermonde matrix, with $\{\gamma_1, \ldots, \gamma_m\}$ on the unit circle.

Related highly structured matrix families

Toeplitz, Hankel, Toeplitz+Hankel

Numerical PDEs

Covariance matrices in signal processing

Time series and dynamical systems

Function approximation

Cauchy-like, Loewner, Pick

Semi-separable function representation

Matrix equations

Dynamical systems

Rational approximation methods

$$T = \begin{pmatrix} t_0 & t_{-1} & \cdots & \cdots & t_{-(n-1)} \\ t_1 & t_0 & \ddots & \ddots & t_{-(n-2)} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ t_{n-1} & \cdots & \cdots & t_1 & t_0 \end{pmatrix}$$

$$C = \begin{pmatrix} \frac{1}{x_1 - y_1} & \frac{1}{x_1 - y_2} & \cdots & \frac{1}{x_1 - y_n} \\ \frac{1}{x_2 - y_1} & \frac{1}{x_2 - y_2} & \cdots & \frac{1}{x_2 - y_n} \\ \vdots & & & \vdots \\ \frac{1}{x_n - y_1} & \frac{1}{x_n - y_2} & \cdots & \frac{1}{x_n - y_n} \end{pmatrix}$$

What do all these matrices have in common?

1. They share a very special kind of *displacement structure*, enabling a *sparse representation*.

2. They are all just a *fast transform* away from *hierarchical low rank structure*.

Example: Solve $n \times n$ linear system in as few operations as possible.

FastLevinson Algorithm [Levinson (1947) Durbin (1962)] $\mathcal{O}(n^2)$ Schur Algorithm [Lev-Ari (1983), Kailath and Sayed (1991)]Displacement-based GE [Heinig (1995), Gohberg, Kailath and Olshevsky(1995)]

Example: Solve $n \times n$ linear system in as few operations as possible.

Superfast

 $\mathcal{O}(n\log^p(n)\log^q(1/\epsilon))$

The square Toeplitz case

Heinig (1998) Chandrasekaran, Gu, Xia, Zhu (2007) Martinsson, Rokhlin, Tygert (2005) Xia, Xi, Gu (2007)

Overdetermined Toeplitz system

Xi, Xia, Cauley, Balakrishnan (2014)

Can we adapt these ideas to Vandermonde systems, and beyond?

Example: Solve $n \times n$ linear system in as few operations as possible. Template for superfast solver for Ax = b: 1) Apply fast transform: $A \to \hat{A}, b \to \hat{b}$ 2) Compress rank-structured matrix: $\hat{A} \approx H$ 3) Solve: $H\hat{x} = \hat{b}$ 4) Transform solution: $\hat{x} \to x$ **Displacement structure** +

Zolotarev rationals for low rank approximation

Zolotarev rationals and low rank approximation

The inverse nonuniform discrete Fourier transform

Zolotarev's rational approximation problems



Zolotarev's third problem:

Rational analogue to Chebyshev polynomial approximation problem

Zolotarev's fourth problem: Rational analogue to polynomial filtering

Y. Zolotarev (1847-1878) Rational approximation to sign function on disjoint intervals, square root function on $[\beta, 1]$.

[Acheiser (1901), Todd (1984), Gončar (1969), Istace & Thiran (1995)]

Zolotarev's rational approximation problems



Y. Zolotarev (1847-1878) Iterative solvers for matrix equations

- Low rank approximation and bounds on the decay of singular values of certain matrices
- Eigensolvers, polar decompositions, the SVD
- Tensor compression
- Nonlinear approximation schemes (e.g., via rationals or exponential sums)
- Spectral methods and PDE solvers
- Digital and analog filter design

[See Simoncini (2016), Beckermann & Townsend (2019), Nakatsukasa & Freund (2016) for overviews]

Zolotarev's third problem



Zolotarev's third problem



Zolotarev's third problem



Known results: Disks and Intervals

- When E, G are intervals on $\mathbb{R}, r(z)$ is known exactly and can be expressed in terms of its poles and zeros, which are computed via elliptic integrals (Zolotarev, 1877).
- When E, G are disks in $\mathbb{C}, r(z)$ is known exactly and can be expressed in terms of a repeated pole and zero (Starke, 1992).
- $Z_k(E,G)$ is invariant under Möbius transformations.

$$h = \exp\left(\frac{1}{\operatorname{cap}(E,G)}\right)$$

Disjoint sets E and G	Bound	Reference
finite intervals of \mathbb{R}	$Z_k(E,G) \le 4h^{-k}$	Townsend & Beckermann (2016)
disks in \mathbb{C}	$Z_k(E,G) \le h^{-k}$	Starke (1992)
arcs on a circle $\mathbb C$	$Z_k(E,G) \le 4h^{-k}$	Useful for NUDFT
I	```'	(W., Epperly, Barnett, 2024)

Known results: More general sets

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

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

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



[(Gončar, 1969), (Ganelius, 1977, 1979), (Rubin, Townsend, & W., 2022)]

Computing Zolotarev rationals



Key ideas:

- Use equivalency with best sign function approximation
- New developments in AAA rational approximation algorithm for accurate approximations to sgn(z) (Trefethen, W., 2024).

[(Trefethen & W., 2024), (Nakatsukasa, Sète & Trefethen, 2018)]

The low rank connection:

Displacement, Zolotarev, and singular value decay

Matrices with displacement structure

$$A \in \mathbb{C}^{m \times m}, \ B \in \mathbb{C}^{n \times n}, \ X, F \in \mathbb{C}^{m \times n},$$
$$AX - XB = F$$

"X has (A, B) displacement structure"

Appears with X as an unknown: discretization of PDEs, reduced order modeling, signal processing (see Simoncini SIAM REV, 2016 + ref. therein).

Special (A, B, F) triplets characterize properties of X for structured matrices: e.g., X = Toeplitz, Hankel, Cauchy, Vandermonde, and more.

[(Beckermann & Townsend, 2019), (Kailath & Sayed, 1995) (Heinig, 1995)]

Example: Vandermonde matrix

The low rank connection

$$A \in \mathbb{C}^{m \times m}, \ B \in \mathbb{C}^{n \times n}, \ X, F \in \mathbb{C}^{m \times n}, AX - XB = F$$

 \boldsymbol{X} is well-approximated by a low rank matrix when

(1) $\lambda(A)$ and $\lambda(B)$ are "well-separated" (2) F is low rank



[(Beckermann & Townsend, 2019), (Sabino, 2008), (Penzl, 1999), (Benner, Truhar & Li, 2009), (Li & White, 2002), (Druskin, Knizhnerman & Simoncini, 2011), (Peaceman & Rachford, 1955), (Lu & Wachspress, 1991), (Townsend & W., 2018), (Rubin, Townsend, & W., 2022)]

The factored ADI method

$$AX - XB = F$$

<u>Factored ADI:</u> $A(ZDY^*) - (ZDY^*)B = USV^*$ U, V have ρ columns.

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

 $k\rho$ columns

<u>After k iterations</u>: $X^{(k)} = Z^{(k)}(W^{(k)})^*$,

[(Li & White, 2002), (Benner, Li & Truhar, 2009)]

Bounding the ADI error

$$X - X^{(k)} = r_k(A) X r_k(B)^{-1}, \quad r_k(z) = \prod_{j=1}^k \frac{z - \alpha_j}{z - \beta_j}$$
$$X - X^{(k)} \|_2 \le \|r_k(A) r_k(B)^{-1}\|_2 \|X\|_2 \le \|r_k(\lambda(A))\|_2 \|r_k(\lambda(B))^{-1}\|_2 \|X\|_2$$



[(Beckermann & Townsend, 2017), (Sabino, 2008), (Penzl, 1999), (Benner, Truhar & Li, 2009), (Li & White, 2002), (Druskin, Knizhnerman & Simoncini, 2011), (Peaceman & Rachford, 1955), (Lu & Wachspress, 1991), (Townsend & W., 2018), (Rubin, Townsend, & W., 2022)]

Bounding the Zolotarev numbers

$$AX - XB = F$$

Theorem (informal):

If rank $(F) \leq \rho$, and $\lambda(A)$, $\lambda(B)$ are each arcs on the unit circle disjoint from one-another, then there are Z, W, each with ρk columns such that

$$||ZW^* - X||_2 / ||X||_2 \le 4 \exp\left(\frac{\pi^2}{2\log 16\gamma}\right)^{-\lfloor k/\rho \rfloor},$$

where γ is the cross-product of the arcs.

Key Idea: Use fADI to construct $ZW^* \approx X$

[(W., 2021), (W., Epperly, & Barnett, 2024)]



[Forward problem: (Barnett, see FINUFFT package), (Potts, Kunis, see NFFT package) (Greengard and Inati, 2006), (Townsend and Ruiz, 2017), Other direct inversion solvers: (Kircheis and Potts, 2019), (Dutt and Rokhlin, 1993)]



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Solve a (overdetermined) linear system Vc = b

<u>Goal</u>: Solve a linear system Vc = b

When $\gamma_1, \ldots, \gamma_m$ are equally spaced on the unit circle and m = n...



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When $\gamma_1, \ldots, \gamma_m$ are equally spaced on the unit circle and m = n...

$$V^{-1} = V^*, \ c = V^*b$$

Compute in $\mathcal{O}(n \log n)$ flops via FFT



<u>Goal</u>: Solve a linear system Vc = b

When $\gamma_1, \ldots, \gamma_m$ are equally spaced on the unit circle and m = n...

$$V^{-1} = V^*, \ c = V^*b$$

Compute in $\mathcal{O}(n \log n)$ flops via FFT

Small perturbation, structure breaks!

Solution: Find a new structure



 V^*V is Toeplitz

Iterative approach:

(1) Form $V^*Vc = V^*b$.

(2) Apply iterative method with fast matrix-vector multiply

Problem:

Depends on
$$\kappa(V^*V) = \|V^*V\|_2 \|(V^*V)^{-1}\|_2 !$$

Solution: Fast direct solvers

Solve cost does not depend on $\kappa(V)$ Also good for multiple right-hand sides!



When the problem compels it, use a direct solver!

<u>Our wishlist</u>

- (1) (Super)fast!
- (2) Do not square condition number
- (3) Can handle overdetermined case
- (4) "Black box"

x = inufft(samplelocs, n, rhs, acc)

[Related ideas: (Greengard and Inati, 2006), (Kircheis and Potts, 2019), (Dutt and Rokhlin, 1993), (Heinig, 1995)]

The fast Cauchy-like transformation family

AX - XB = F, with F low rank +

A, B are diagonal or "very easily diagonalizable".

The Cauchy-like transformation

$$V \to C = VF^*$$
$$DV - VQ = uw^*$$
$$D(VF^*) - (VF^*)FQF^* = uw^*F^*$$
$$FQF^* = \Lambda = \operatorname{diag}(\omega^2, \omega^4, \cdots, \omega^{2n}), \quad \omega = e^{i\pi/n}.$$

 $DC - C\Lambda = u\tilde{w}^*$ $\frac{\text{Cauchy-like}}{\text{``diagonal'' displacement structure with low rank RHS.}}$

$$C_{jk} = \frac{(u\tilde{w}^*)_{jk}}{D_{jj} - \Lambda_{kk}}$$

If $V \in \mathbb{C}^{m \times n}$, only 1 length-n FFT to (implicitly represent C.

C has hierarchical low rank structure (C is an HSS matrix)



The Cauchy-like transformation

C has heirarchical low rank structure (C is an HSS matrix)



Low rank submatrices



Low rank submatrices



ADI-based hierarchical compression

$$D_J C' - C' \Lambda_L = [u(Fv)^*]_{JL}$$

$$||C' - ZW^*||_2 \le \epsilon ||C'||_2,$$

Z, W have $k = \mathcal{O}(\log n \log 1/\epsilon)$ columns.

We construct Z, W via one-sided ADI-based interpolative decomposition.

$$Z^{(k)} = \begin{bmatrix} \hat{Z}^{(1)} & \hat{Z}^{(2)} & \cdots & \hat{Z}^{(k)} \end{bmatrix}, \quad \begin{cases} \hat{Z}^{(1)} = (A - \beta_1 I)^{-1} US, \\ \hat{Z}^{(i+1)} = (A - \alpha_i I)(A - \beta_{i+1} I)^{-1} Z^{(i)} \end{cases}$$
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$$D^{(k)} = \operatorname{diag}\left((\beta_1 - \alpha_1) I_{\rho}, \cdots, (\beta_k - \alpha_k) I_{\rho}\right)$$
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ADI-based hierarchical compression

$$D_J C' - C' \Lambda_L = [u(Fv)^*]_{JL}$$

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Z, W have $k = \mathcal{O}(\log n \log 1/\epsilon)$ columns.

We construct Z, W via one-sided ADI-based interpolative decomposition.

Total cost for low rank compression: $\mathcal{O}((n+m)\log^2 n\log^2(1/\epsilon))$

ADI-based hierarchical solver

Algorithm 1 A superfast least squares solver for Vc = b. (Type-II NUDFT inversion) (Transforms to Cy = b, solves, transforms back)

- 1: Compute w = Fv.
- 2: Use ADI on $DC C\Lambda = uw^*$ to generate H, an approximate hierarchical factorization of C.
- 3: Solve Hy = b in the least squares sense
- 4: Compute $c = F^* y$.
 - $\mathcal{O}((m+n)\log^2(n)\log^2(1/\epsilon))$ flops, where ϵ is an accuracy parameter.
 - Construction of H is automatic.
 - Toeplitz version for normal equations.
 - Especially effective for multiple RHSs

[A least-squares Toeplitz solver: (Xi, Xia, Cauley, Balakrishnan, 2014)]

When do iterative solvers work well?

1. Jittered grid (almost equispaced)



3. Random iid from uniform distribution



2. Clenshaw-Curtis quadrature nodes





When iterative methods work well





When a direct solver is needed



When a direct solver is needed



Systems with many right-hand sides



[(Kircheis and Potts, 2019)]

Solution properties



1D signal reconstructed using samples from Grid 3

Ongoing work

The 2D NUDFT

$$V_{2D} = V_{\epsilon} * V_{\eta}, * =$$
 the "face-splitting" product.

Requires working with block-structured matrices

Blocks of Cauchy-like matrices, linked compression properties across blocks. \rightarrow one large HSS matrix.

Several related block-structured matrices in other applications (e.g., block–Toeplitz with Toeplitz blocks)

Noise and related issues

Basic Tikhonov regularization is straightforward.

Various constrained optimization problems with rank-structured matrices?

Designing preconditioners, fast matvecs, etc.

Zolotarev rationals on general sets via interpolation (with L.N. Trefethen)

Inverse-free iterative solvers for Sylvester matrix equations via Akheizer polynomials (with T. Trogdon and C. Ballew)

Resources and software

Paper on NUDFT inversion: https://arxiv.org/abs/2404.13223

Code for solver: https://github.com/heatherw3521/NUDFT

Paper on computing Zolotarev rationals: <u>https://arxiv.org/abs/2408.14092</u>

heatherw3521.github.io

Begin Extra Slides

Constructing low rank approximations



[Factored ADI: (Benner, Li, Truhar, 2009), Interpolative decomposition: (Cheng, Gimbutas, Martinsson, Rokhlin, 2005)]

The ADI method

One ADI iteration:

1. Solve
$$(A - \beta_{j+1}I)X^{(j+1/2)} = X^{(j)}(B - \beta_{j+1}I) + F$$
 for $X^{(j+1/2)}$.

- 2. Solve $X^{(j+1)}(B \alpha_{j+1}I) = (A \alpha_{j+1}I)X^{(j+1/2)} F$ for $X^{(j+1)}$.
- Developed as a method for solving the heat equation by applying a splitting scheme to Crank-Nicholson.
 - Running ADI on the heat equation at steady state leads to an ADI-based Poisson solver.
 - Systems and control theory groups + numerical linear algebra groups generalized and applied the Poisson solver to develop low rank solvers for Lyapunov and Sylvester matrix equations.
 - Studied by optimization community as a special instance of the alternating direction method of multipliers (ADMM).

Low rank structures





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

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