Approximation of singular functions using frames

Marcus Webb

Joint with Daan Huybrechs, Vincent Coppé and Roel Matthysen

NUMA Seminar, KU Leuven
25 Oct 2018

    

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Motivation: why singular functions?

- Some differential equations naturally have solutions with singularities:
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  - Corner singularities
  - Endpoint singularities
  - Discontinuous media: fractures/interfaces
  - Singular integral equations/fractional differential equations

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  - Rational collocation (Weidemann 1998)
  - Enriched finite elements (Belytschko et al 1999)

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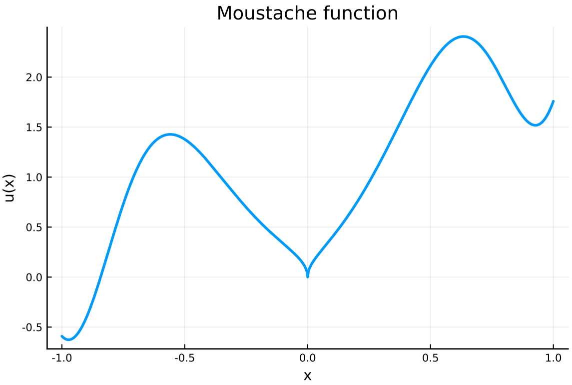
  - Enriched finite elements (Belytschko et al 1999)
- Traditional spectral methods struggle in these situations.

Model problem

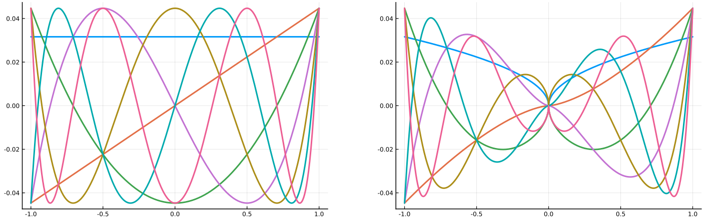
- Consider a function u of the form $u(x) = f(x) + |x|^{1/2} g(x)$
- f and g are smooth functions
- We can only sample u



- More generally, $u(x) = w_1(x) f_1(x) + \cdots + w_p(x) f_p(x)$

Approximating $u(x) = f(x) + |x|^{1/2}g(x)$

1. $u(x) \approx \sum_{k=0}^{N-1} a_k T_k(x)$
2. $u(x) \approx \sum_{k=0}^{N-1} b_k |x|^{1/2} T_k(x)$
3. $u(x) \approx \sum_{k=0}^{N/2-1} c_{2k} T_k(x) + c_{2k+1}|x|^{1/2} T_k(x)$



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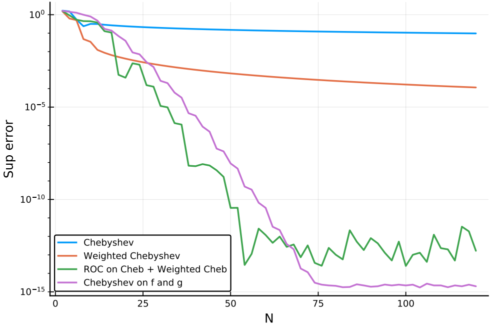

What are we computing?

- We seek the N coefficients $\mathbf{c} \in \mathbb{R}^N$ which form the least squares interpolant at $M = \gamma N$ Gauss-Chebyshev nodes $\{x_{1,M}, \ldots, x_{M,M}\}$:

$$\operatorname*{arg\,min}_{\mathbf{c} \in \mathbb{R}^N} \sum_{k=1}^{M} \left| \sum_{j=0}^{N/2-1} c_{2j} T_j(x_{k,M}) + c_{2j+1} |x_{k,M}|^{1/2} T_j(x_{k,M}) - f(x_{k,M}) \right|^2$$

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- AKA **oversampled collocation**
- Equivalent to the least squares solution of the tall, skinny linear system, $A\mathbf{c} = \mathbf{b}$, where $A \in \mathbb{R}^{M \times N}$,

$$A_{k,2j} = T_j(x_{k,M}), \qquad A_{k,2j+1} = |x_{k,M}|^{1/2} T_j(x_{k,M}),$$

$$b_k = f(x_{k,M}), \qquad k = 1, 2, \ldots, M, j = 0, 1, \ldots, N/2 - 1.$$

FrameFun vs ApproxFun (Chebfun)

- The collocation matrix A is a **transform** between **coefficients** $\mathbf{c}$ and **values** of the function with those coefficients.

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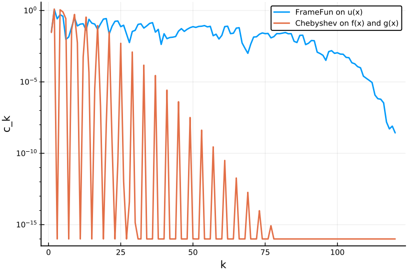

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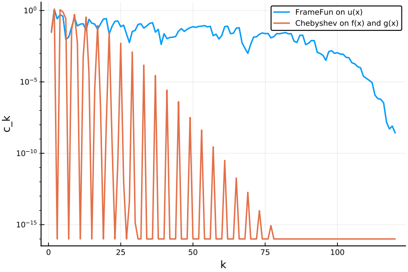

Adaptivity and frames: Coppé-Huybrechs (in prep.)

Solving ill-conditioned systems

- Ill-conditioned least squares problem: $A \in \mathbb{R}^{M \times N}$, $\mathbf{b} \in \mathbb{R}^M$ $(M = \gamma N)$,

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- Many solutions with small residual. The ε-**regularised** SVD solution is,

$$A = U \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & & \\ & & & \ddots & \\ & & & & \sigma_N \end{bmatrix} V^*, \quad \mathbf{x} = V \begin{bmatrix} \sigma_1^{-1} & & & & \\ & \ddots & & & \\ & & \sigma_r^{-1} & & \\ & & & \ddots & \\ & & & & 0 \end{bmatrix} U^* b$$

where $\sigma_k < \varepsilon \iff k > r$.

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- Backslash computes the ε-regularised pivoted-QR solution
- $O(N^3)$ flops – **very slow!**

Adcock-Huybrechs Theorems

Oversampled Collocation Theorem (Adcock–Huybrechs 2018)

Let $\Phi = \{\varphi_k\}_{k=1}^{\infty}$ be a **frame** for $L^2(\Omega)$ and let $\{w_{k,M} f(x_{k,M})\}_{k=1}^{M}$ be "good" samples for any $f \in L^2(\Omega)$.
If the entries of $A \in \mathbb{R}^{M \times N}$ are $a_{k,j} = w_{k,M}\varphi_j(x_{k,M})$, and $b_k = w_{k,M} u(x_{k,M})$, then the ε-regularised solution $u^{\varepsilon,M,N}(x)$ satisfies

$$\|u^{\varepsilon,M,N} - u\|_{L^2(\Omega)} \leq C^{\varepsilon}_{M,N} \left(\left\| \sum_{k=1}^{N} v_k \varphi_k - u \right\|_{L^2(\Omega)} + \varepsilon \|\mathbf{v}\|_2 \right),$$

for any $\mathbf{v} \in \ell^2$, where $\sup_N \limsup_{M \to \infty} C^{\varepsilon}_{M,N} \leq C < \infty$.

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for any $\mathbf{v} \in \ell^2$, where $\sup_N \limsup_{M\to\infty} C^{\varepsilon}_{M,N} \leq C < \infty$.

Furthermore, the RHS converges to $\mathcal{O}(\varepsilon)$ as $N \to \infty$, with **sufficient oversampling** M.

What is a frame?

- A **frame** is a set of functions $\Phi = \{\varphi_k\}_{k=1}^{\infty} \subset \mathcal{H}$ (inner product space) such that

$$f \mapsto \|\left(\langle \varphi_k, f \rangle\right)_{k=1}^{\infty}\|_{\ell^2} \quad \text{and} \quad f \mapsto \|f\|_{\mathcal{H}}$$

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- The set $\varphi_{2k} = T_k$, $\varphi_{2k+1} = w \cdot T_k$, satisfies

$$\|f\|^2 \inf_{x \in [-1,1]} |1+|w(x)|^2| \leq \sum_{k=0}^{\infty} |\langle \varphi_k, f \rangle|^2 \leq \|f\|^2 \sup_{x \in [-1,1]} |1+|w(x)|^2|$$

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- We have a frame if $1 + |w(x)|^2$ is **bounded above** and **below**

Dual frames

- Typical focus: dual frame or "inversion of the frame operator"
- A dual frame $\tilde{\Phi} = \{\tilde{\varphi}_k\}_{k=1}^{\infty}$ satisfies

$$f = \sum_{k=1}^{\infty} \langle \tilde{\varphi}_k, f \rangle \varphi_k$$

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$$f = \sum_{k=1}^{\infty} \langle \tilde{\varphi}_k, f \rangle \varphi_k$$

$$\Phi = \{T_k(x)\}_{k=1}^{\infty} \cup \{w(x)T_k(x)\}_{k=1}^{\infty}$$

$$\tilde{\Phi} = \left\{ \frac{T_k(x)}{1 + |w(x)|^2} \right\}_{k=1}^{\infty} \cup \left\{ \frac{w(x)T_k(x)}{1 + |w(x)|^2} \right\}_{k=1}^{\infty}$$

- These coefficients, $c_k = \langle \tilde{\varphi}_k, f \rangle$, converge too slowly! ROC gives better approximations.

Aside: Solving a low-rank system fast

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Randomised least squares solver for $A\mathbf{x} = \mathbf{b}$

1. $W = \mathrm{randn}(N, r + 20)$
2. Least squares solve for $\mathbf{y} \in \mathbb{R}^{r+20}$: $(AW)\mathbf{y} = \mathbf{b}$
3. $\mathbf{x} = W\mathbf{y} \in \mathbb{R}^N$

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Theorem (Using techniques in Halko, Martinsson, Tropp 2011)

The computed solution $\mathbf{x}$ satisfies,

$$\|A\mathbf{x} - b\|_2 \leq \|A\mathbf{v} - b\|_2 + \kappa_{r,N} \cdot \left(\sum_{k>r} \sigma_k^2\right)^{1/2} \cdot \|\mathbf{v}\|_2, \qquad \forall \mathbf{v} \in \mathbb{R}^N,$$

where $\kappa_{r,N}$ is a random variable such that
$\mathbb{P}\left[\kappa_{r,N} > 16 + 5\sqrt{r}\right] < 2.89 \times 10^{-9}$.

The plunge region

- Let $A \in \mathbb{R}^{M \times N}$ be the collocation matrix in M Gauss-Chebyshev points for the N-truncated frame, $\{T_k\}_{k=0}^{N/2-1} \cup \{|x|^{1/2} T_k(x)\}_{k=0}^{N/2-1}$.

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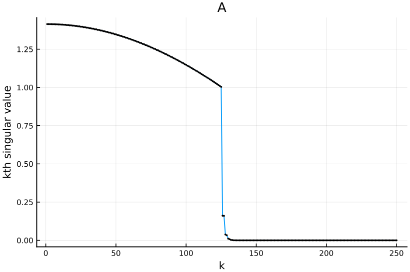

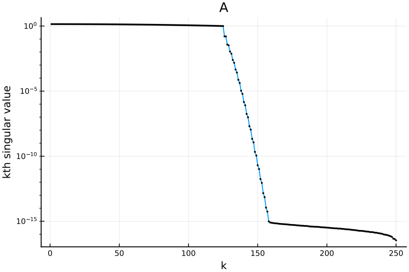

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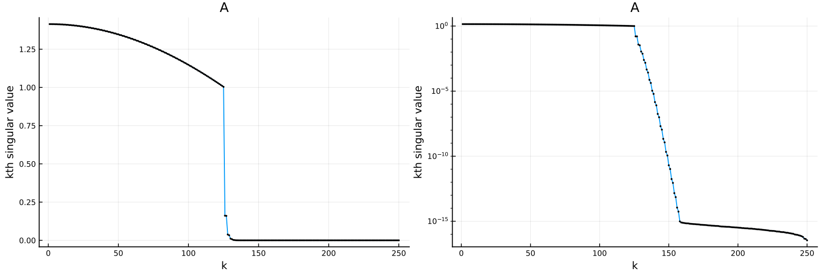

- For weighted sums of trigonometric bases, the number of singular values in $(\varepsilon, 1-\varepsilon)$ is $\mathcal{O}(\log(N))$ (see Adcock-Huybrechs FNA paper and Webb (in prep.)).
- The big-$\mathcal{O}$ depends on ε and the BV norms of the weights. Precise dependence is an **open problem**.

Dual frame isolates plunge region

Let $A \in \mathbb{R}^{M\times N}$ be the collocation matrix in M Gauss-Chebyshev points for the N-truncated frame, $\{T_k\}_{k=0}^{N/2-1} \cup \{|x|^{1/2}T_k(x)\}_{k=0}^{N/2-1}$.
Let $Z \in \mathbb{R}^{M\times N}$ be the collocation matrix in M Gauss-Chebyshev points for the N-truncated **dual frame**,
$\{T_k(x)/(1+|x|)\}_{k=0}^{N/2-1} \cup \{|x|^{1/2}T_k(x)/(1+|x|)\}_{k=0}^{N/2-1}$.

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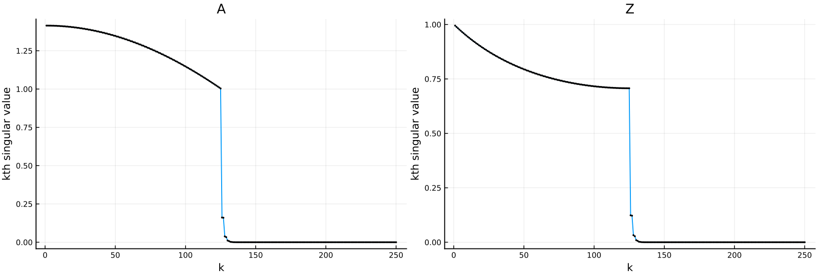

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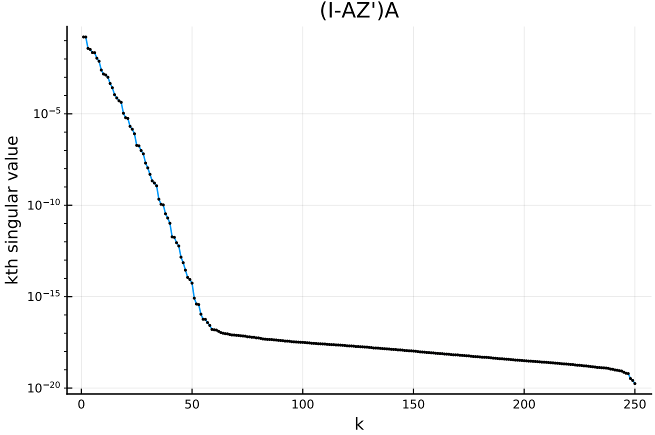

The AZ algorithm - $A, Z \in \mathbb{R}^{M \times N}$, $b \in \mathbb{R}^M$

AZ Algorithm for a least squares solution to $A\mathbf{x} = b$:

1. Solve $(I - AZ^*)A\mathbf{x}_1 = (I - AZ^*)b$
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- Residual:
$$\begin{aligned} b - A\mathbf{x} &= b - A\mathbf{x}_1 - A\mathbf{x}_2 \\ &= b - A\mathbf{x}_1 - AZ^*(b - A\mathbf{x}_1) \\ &= (I - AZ^*)(b - A\mathbf{x}_1). \end{aligned}$$

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- If $\mathrm{rank}_\varepsilon((I - AZ^*)A) = \mathrm{rk}_N$, and $A\mathbf{v}$, $Z^*\mathbf{w}$ require mul_N operations, then, in total,

$$\mathcal{O}(\mathrm{mul}_N \cdot \mathrm{rk}_N + N \cdot \mathrm{rk}_N^2) \text{ operations.}$$

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AZ Algorithm for a least squares solution to $A\mathbf{x} = b$:

1. Solve $(I - AZ^*)A\mathbf{x}_1 = (I - AZ^*)b$
2. $\mathbf{x}_2 = Z^*(b - A\mathbf{x}_1)$
3. $\mathbf{x} = \mathbf{x}_1 + \mathbf{x}_2$

- Residual:
$$\begin{aligned} b - A\mathbf{x} &= b - A\mathbf{x}_1 - A\mathbf{x}_2 \\ &= b - A\mathbf{x}_1 - AZ^*(b - A\mathbf{x}_1) \\ &= (I - AZ^*)(b - A\mathbf{x}_1). \end{aligned}$$
- If $\mathrm{rank}_\varepsilon((I - AZ^*)A) = \mathrm{rk}_N$, and $A\mathbf{v}$, $Z^*\mathbf{w}$ require mul_N operations, then, in total,
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- See Coppé-Huybrechs-Matthysen-Webb (in prep.)

Discussion

Effective algorithms:

- Adcock-Huybrechs: for frames use regularised oversampled collocation
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Several papers in prep.!