KU LEUVEN

Efficient Approximation in Enriched Bases

Astrid Herremans

jointly with Daan Huybrechs and Lloyd N. Trefethen

September 21, 2023

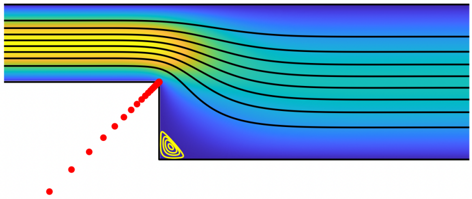
Enriched basis

$$\Phi_{N+K} = \underbrace{\{\varphi_n\}_{n=1}^{N}}_{\text{conventional basis}} \cup \underbrace{\{\psi_k\}_{k=1}^{K}}_{\text{extra functions}}$$

Extra functions capture known features of function to be approximated
$\rightarrow$ **expert-driven approximation**

- Singular behaviour
- Oscillatory behaviour
- ...

Example: lightning approximation



Expert knowledge: solution exhibits corner singularities

$$f(z) \quad \approx \quad r(z) \quad = \quad \sum_{n=0}^{N} b_n z^n \quad + \quad \sum_{k=1}^{K} \frac{a_k}{z - p_k}$$

$f(z)$ $\downarrow$ contains branch point singularities

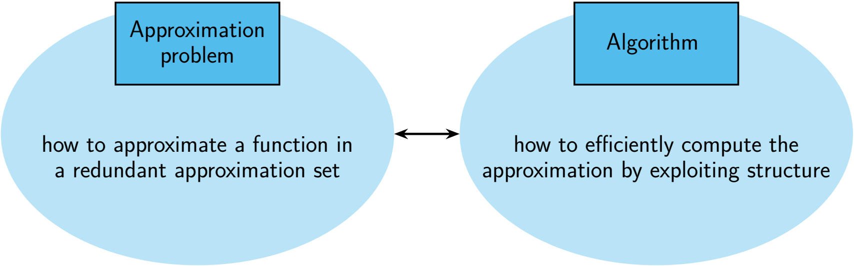
$\sum_{n=0}^{N} b_n z^n$ $\downarrow$ smooth term

$\sum_{k=1}^{K} \frac{a_k}{z - p_k}$ $\downarrow$ clustered poles

[Gopal and Trefethen, 2019], [Brubeck and Trefethen, 2022], [Herremans, Huybrechs, and Trefethen, 2023]

Enriched approximation scheme

$$\Phi_{N+K} = \underbrace{\{\varphi_n\}_{n=1}^{N}}_{\text{conventional basis}} \cup \underbrace{\{\psi_k\}_{k=1}^{K}}_{\text{extra functions}}$$



Enriched approximation scheme

$$\Phi_{N+K} = \underbrace{\{\varphi_n\}_{n=1}^{N}}_{\text{conventional basis}} \cup \underbrace{\{\psi_k\}_{k=1}^{K}}_{\text{extra functions}}$$

Approximation problem

how to approximate a function in a redundant approximation set

$\longleftrightarrow$

Algorithm

how to efficiently compute the approximation by exploiting structure

1 Approximation problem

Find

$$\underset{\hat{f}\in H_{N+K}}{\arg\min} \left\| f - \hat{f} \right\|_{\mathcal{H}}$$

with $H_{N+K} = \mathsf{span}(\Phi_{N+K}) \subset \mathcal{H}$

1 Approximation problem

Find

$$\arg\min_{\hat{f}\in H_{N+K}} \left\| f - \hat{f} \right\|_{\mathcal{H}}$$

with $H_{N+K} = \mathsf{span}(\Phi_{N+K}) \subset \mathcal{H}$

In practice we only have access to limited information $\mathcal{M}_M : f \mapsto \{\xi_m(f)\}_{m=1}^{M}$ and the discrete error $\mathcal{M}_M(f - \hat{f})$

1 Approximation problem

Find

$$\underset{\hat{f} \in H_{N+K}}{\arg\min} \left\| f - \hat{f} \right\|_{\mathcal{H}}$$

with $H_{N+K} = \mathrm{span}(\Phi_{N+K}) \subset \mathcal{H}$

In practice we only have access to limited information $\mathcal{M}_M : f \mapsto \{\xi_m(f)\}_{m=1}^{M}$ and the discrete error $\mathcal{M}_M(f - \hat{f})$

In what follows, I use $\|f\|_M^2 = \|\mathcal{M}_M f\|^2 = \sum_{m=1}^{M} |\xi_m(f)|^2$

1 Discrete approximation in enriched bases

Least squares approximation $\mathcal{P}$

$$\mathcal{P}f = \underset{\hat{f} \in H_{N+K}}{\arg\min} \left\| f - \hat{f} \right\|_M$$

$$\|f - \mathcal{P}f\|_M \leq \inf_{\mathbf{x} \in \mathbb{C}^{N+K}} \{ \|f - \Phi_{N+K}\, \mathbf{x}\|_M \}$$

1 Influence of the representation and finite precision

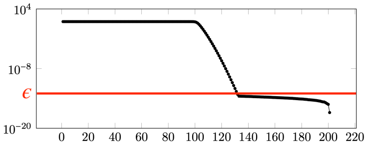
Using the enriched basis, $\mathcal{P}f = \Phi_{N+K}\,\mathbf{c}$ with

$$A\mathbf{c} \approx \mathbf{b}$$

where $(A)_{m,i} = \xi_m(\phi_i), (\mathbf{b})_m = \xi_m(f)$

[Adcock and Huybrechs, 2019]

The coefficients $\mathbf{c}$ are increasingly underdetermined



$\rightarrow$ "regularized approximation space" (truncated SVD at a threshold ϵ)

$$H^{\epsilon}_{\xi,N+K} \subseteq H_{N+K}$$

1 Discrete approximation in enriched bases

Least squares approximation $\mathcal{P}$

$$\mathcal{P}f = \underset{\hat{f} \in H_{N+K}}{\arg\min} \left\| f - \hat{f} \right\|_M$$

$$\|f - \mathcal{P}f\|_M \leq \inf_{\mathbf{x} \in \mathbb{C}^{N+K}} \left\{ \|f - \Phi_{N+K}\mathbf{x}\|_M \right\}$$

Regularized least squares approximation $\mathcal{P}^\epsilon$

$$\mathcal{P}^\epsilon f = \underset{\hat{f} \in H^\epsilon_{\xi, N+K}}{\arg\min} \left\| f - \hat{f} \right\|_M$$

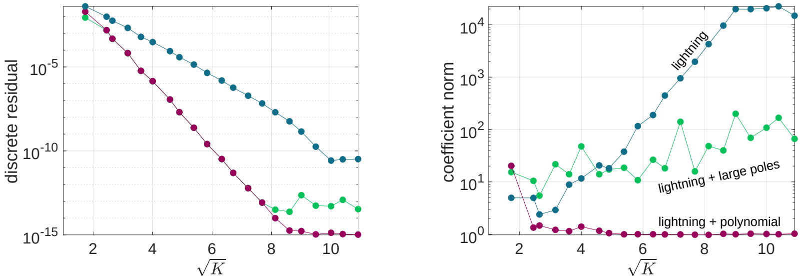
$$\|f - \mathcal{P}^\epsilon f\|_M \leq \inf_{\mathbf{x} \in \mathbb{C}^{N+K}} \left\{ \|f - \Phi_{N+K}\mathbf{x}\|_M + \epsilon \|\mathbf{x}\|_2 \right\}$$

[Coppé, Huybrechs, Matthysen, and Webb, 2020]

1 Example: lightning approximation

$$\|f - \mathcal{P}^{\epsilon} f\|_M \leq \inf_{\mathbf{x} \in \mathbb{C}^{N+K}} \left\{ \|f - \Phi_{N+K}\,\mathbf{x}\|_M + \epsilon\, \|\mathbf{x}\|_2 \right\}$$

Approximation of $\sqrt{x}$ on $[0,1]$:



[Herremans, Huybrechs, and Trefethen, 2023]

1 Approximation error in enriched bases

What does $\|f - \mathcal{P}^\epsilon f\|_M$ tell us about $\|f - \mathcal{P}^\epsilon f\|_{\mathcal{H}}$?

[Adcock and Huybrechs, 2020]

$$
\begin{aligned}
&\|f - \mathcal{P}^\epsilon f\|_{\mathcal{H}} \\
&\leq \inf_{\mathbf{x}\in\mathbb{C}^{N+K}} \left\{ \|f - \Phi_{N+K}\,\mathbf{x}\|_{\mathcal{H}} + \frac{1}{\sqrt{A_{\xi,N+K}}} \left(\|f - \Phi_{N+K}\,\mathbf{x}\|_M + \epsilon\, \|\mathbf{x}\|_2 \right) \right\}
\end{aligned}
$$

1 Approximation error in enriched bases

What does $\|f - \mathcal{P}^\epsilon f\|_M$ tell us about $\|f - \mathcal{P}^\epsilon f\|_\mathcal{H}$?

[Adcock and Huybrechs, 2020]

$$\|f - \mathcal{P}^\epsilon f\|_\mathcal{H}$$
$$\leq \inf_{\mathbf{x}\in\mathbb{C}^{N+K}} \left\{ \|f - \Phi_{N+K}\,\mathbf{x}\|_\mathcal{H} + \frac{1}{\sqrt{A_{\xi,N+K}}} \left(\|f - \Phi_{N+K}\,\mathbf{x}\|_M + \epsilon\,\|\mathbf{x}\|_2 \right) \right\}$$

where

$$A_{\xi,N+K}\,\|f\|_\mathcal{H}^2 \leq \|f\|_M^2 \qquad \forall f \in H_{N+K}$$

$\rightarrow$ choose $\mathcal{M}_M$ such that $A_{\xi,N+K}$ is bounded from below

1 Example: lightning approximation

[Cohen and Migliorati, 2017]

For $\mathcal{H} = L^2$, you can compute a (weighted) sample distribution based on Φ_D which is near-optimal in the sense that

$$A_{\xi,D} \geq 1/2 \text{ using only } M = \mathcal{O}(D \log D) \text{ random samples}$$

with high probability

1 Example: lightning approximation

[Cohen and Migliorati, 2017]

For $\mathcal{H} = L^2$, you can compute a (weighted) sample distribution based on Φ_D which is near-optimal in the sense that

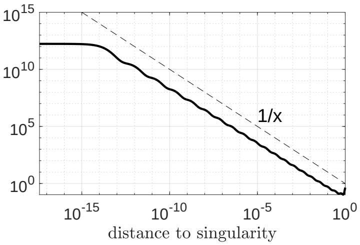
$$A_{\xi,D} \geq 1/2 \text{ using only } M = \mathcal{O}(D \log D) \text{ random samples}$$

with high probability

Experiment

(near-)optimal sampling distribution for 20 lightning poles

$\rightarrow$ many samples needed close to the singularity



Enriched approximation scheme

$$\Phi_{N+K} = \underbrace{\{\varphi_n\}_{n=1}^{N}}_{\text{conventional basis}} \cup \underbrace{\{\psi_k\}_{k=1}^{K}}_{\text{extra functions}}$$

Approximation problem

how to approximate a function in a redundant approximation set

$\longleftrightarrow$

Algorithm

how to efficiently compute the approximation by exploiting structure

2 AZ algorithm [Coppé, Huybrechs, Matthysen, and Webb, 2020]

Goal

efficient computation of $A\mathbf{c} \approx \mathbf{b}$ $\quad A : \mathbb{C}^N \to \mathbb{C}^M$

Idea

assume efficient solver $Z^* : \mathbb{C}^M \to \mathbb{C}^N$ exists for a subset of problems

$$A\mathbf{c} = \mathbf{v} \text{ for } \mathbf{c} = Z^*\mathbf{v}, \qquad \forall\, \mathbf{v} \in V \subset \mathrm{Col}(A)$$

$$\Big\downarrow\ V = \mathrm{Null}(I - AZ^*)$$

only perform least squares fitting in $\mathrm{Col}(A) \setminus V$

$$(I - AZ^*)A\tilde{\mathbf{c}} \approx (I - AZ^*)\mathbf{b} \qquad \mathrm{rank}((I - AZ^*)A) \leq \mathrm{rank}(A) - \dim(V)$$

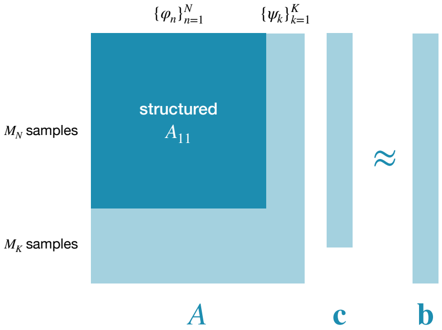
comprehensive algebraic + analytic interpretation [Herremans and Huybrechs, 2023]

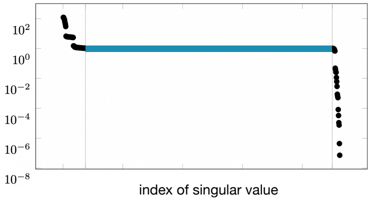
2 AZ algorithm [Coppé, Huybrechs, Matthysen, and Webb, 2020]

1. $(I - AZ^*)A\mathbf{c_1} \approx (I - AZ^*)\mathbf{b}$ — new least squares problem
2. $\mathbf{c_2} = Z^*(\mathbf{b} - A\mathbf{c_1})$ — efficient solver
3. $\mathbf{c} = \mathbf{c_1} + \mathbf{c_2}$

- Efficiency
  low rank can be exploited via randomized NLA
  $\rightarrow$ A and Z^* should have fast matrix-vector products
- Accuracy
  the system $A\mathbf{c} \approx \mathbf{b}$ is only solved approximately
  $\rightarrow$ error can grow with a factor $\|I - AZ^*\|_2$

2 Structure of the least squares problem



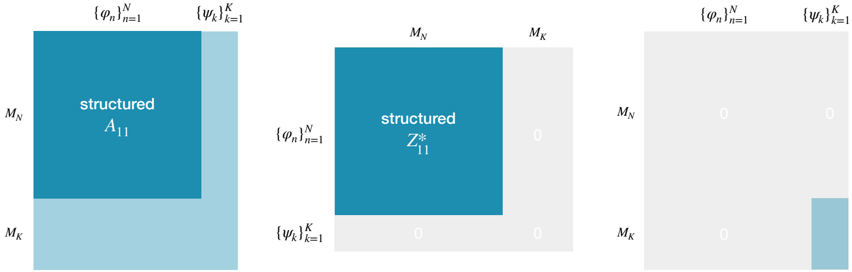


M_N samples $\rightarrow$ linked to conventional basis, structured
M_K samples $\rightarrow$ linked to extra functions, unstructured

2 AZ algorithm for enriched bases [Herremans and Huybrechs, 2023]

Efficient solver $Z_{11}^* : \mathbb{C}^{M_N} \to \mathbb{C}^N$ generally exists for approximation in conventional basis

Example: $Z_{11}^* = A_{11}^{-1}$

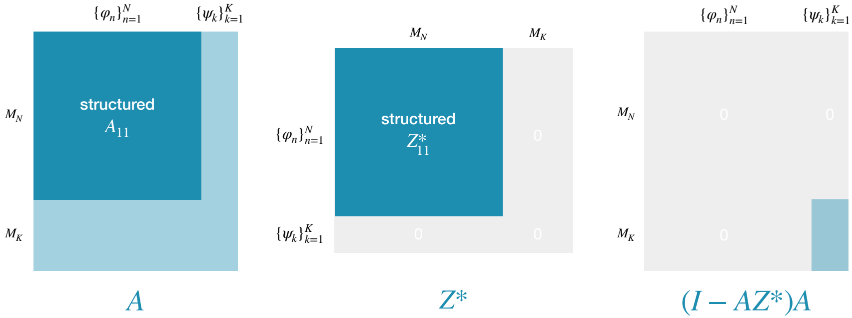


A Z^* $(I - AZ^*)A$

2 AZ algorithm for enriched bases [Herremans and Huybrechs, 2023]

- constructing the system matrix: $\mathcal{O}(\text{cost}(Z_{11}^*)K)$ flops
- solving the new least squares problem: $\mathcal{O}(M_K K^2)$ flops

$\leftrightarrow$ solving the original system: $\mathcal{O}(M(N+K)^2)$



2 Example: approximation of Green's function

Green's function of the 2D gravity Helmholtz equation

$$G(\mathbf{x},\mathbf{y}) = A(\mathbf{x},\mathbf{y})\frac{1}{\log|\mathbf{x}-\mathbf{y}|} + B(\mathbf{x},\mathbf{y})$$

Approximate with polynomials + weighted polynomials

$$\Phi_{N+K} = \{\varphi_n(\mathbf{x},\mathbf{y})\}_{n=1}^{N} \cup \left\{\frac{1}{\log|\mathbf{x}-\mathbf{y}|}\varphi_k(\mathbf{x},\mathbf{y})\right\}_{k=1}^{K}$$

<u>Experiment</u>

- parametrise both $\mathbf{x} = \boldsymbol{\gamma}(s_x)$ and $\mathbf{y} = \boldsymbol{\gamma}(s_y)$ on a semicircle
- use tensor-product Chebyshev polynomials

$$\{\varphi_n\}_{n=1}^{\sqrt{N}\times\sqrt{N}} = \{T_i(s_x)T_j(s_y)\}_{i,j=(0,0)}^{(\sqrt{N}-1,\sqrt{N}-1)}$$

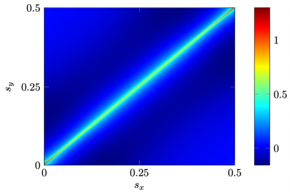
2 Example: approximation of Green's function

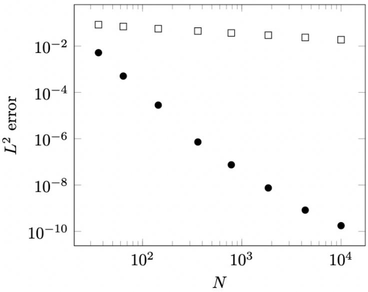
$M_N = 4N, M_K = 0$

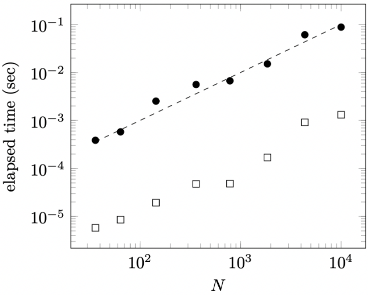
squares: Chebyshev approximation $(K = 0)$

dots: Chebyshev + weighted

Chebyshev approximation $(K = 5^2)$







Main conclusions

Approximation problem

how to approximate a function in a redundant approximation set

↔

Algorithm

how to efficiently compute the approximation by exploiting structure

- regularization makes the approximation space smaller
- non-standard approximation spaces require non-standard samples

- AZ algorithm combines least squares fitting with a fast solver
- AZ algorithm for enriched bases is efficient when $N \gg K$

Ben Adcock and Daan Huybrechs. Frames and numerical approximation. *SIAM Rev.*, 61 (3):443–473, 2019.

Ben Adcock and Daan Huybrechs. Frames and numerical approximation II: Generalized sampling. *J. Fourier Anal. Appl.*, 26(6):87–114, 2020.

Pablo D. Brubeck and Lloyd N. Trefethen. Lightning Stokes solver. *SIAM J. Sci. Comput.*, 44(3):A1205–A1226, 2022.

Albert Cohen and Giovanni Migliorati. Optimal weighted least-squares methods. *SMAI J. Comput. Math.*, 3:181–203, 2017.

Vincent Coppé, Daan Huybrechs, Roel Matthysen, and Marcus Webb. The AZ Algorithm for Least Squares Systems with a Known Incomplete Generalized Inverse. *SIAM J. Matrix Anal. Appl.*, 41(3):1237–1259, 2020.

Abinand Gopal and Lloyd N. Trefethen. Solving Laplace problems with corner singularities via rational functions. *SIAM J. Numer. Anal.*, 57(5):2074–2094, 2019.

Astrid Herremans and Daan Huybrechs. Efficient function approximation in enriched approximation spaces. *arXiv:2308.05652*, 2023.

Astrid Herremans, Daan Huybrechs, and Lloyd N. Trefethen. Resolution of singularities by rational functions. *SIAM J. Numer. Anal.*, 2023. (to appear).