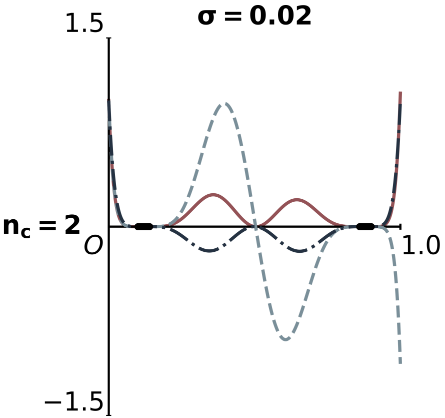
Sharpened CG Iteration Bound for High-contrast Heterogeneous Scalar Elliptic PDEs

Going Beyond Condition Number

P. Soliman[1]

EEMCS-DIAM Numerical Analysis MSc. Thesis Presentation, August, 2025

[1] Delft University of Technology



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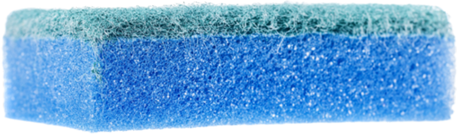
Opening

Darcy Problem



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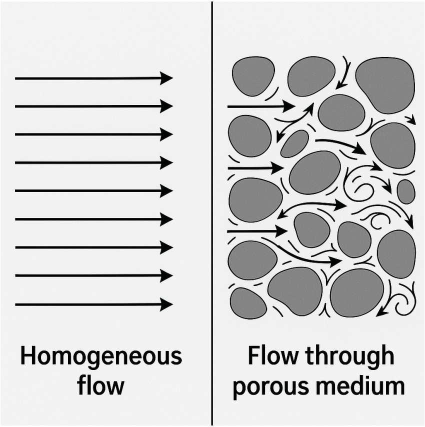

Opening
Darcy Problem

- Simpler case; high-contrast diffusion problem for $u, u_D \in H^1(\Omega)$, $f \in L^2(\Omega)$ and $\mathcal{C} \in L^\infty(\Omega)$

$$
\begin{aligned}
-\nabla \cdot (\mathcal{C}\nabla u) &= f \quad \text{in } \Omega \\
u &= u_D \quad \text{on } \partial\Omega
\end{aligned}
$$

Opening

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$$u = u_D \quad \text{on } \partial\Omega$$

- Find $u \in V = \{u \in H^1(\Omega) | u_{\delta\Omega} = u_D\}$

$$a(u, w) = \int_\Omega \mathcal{C}\nabla u \cdot \nabla w \, dx = \int_\Omega fw \, dx = (f, w) \quad \text{for all } w \in H_0^1(\Omega).$$

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- Introduce some computational mesh $\mathcal{T}_h$ with DOFs $\mathcal{N}$
- Discretize $V_h \subset V$ and $V_{h,0} = V_h \cap H_0^1(\Omega) = \text{span}\{\phi_k\}_{\in\mathcal{N}}$

$$A\mathbf{u} = \mathbf{b} \quad A_{ij} = a(\phi_j, \phi_i)_{L^2} \quad b_i = (f, \phi_i) \quad \forall i, j \in \mathcal{N}$$

Structure

- Research Questions
- Background & Literature
- Preliminary Results
- Outlook

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Research Questions

Main Research Question

How can we refine the CG iteration bound for Schwarz-preconditioned high-contrast heterogeneous elliptic problems beyond the classical condition number-based bound?

Research Questions

Subsidiary Research Questions

Q1 What other spectral characteristics like the condition number can we consider?

Q2 How to estimate the characteristics from **Q1**?

Q3 Given a toy eigenspectrum, how can we sharpen the CG iteration bound?

Q4 How does the sharpened bound from **Q3** compare to the classical CG bound?

Q5 How does the performance described in **Q4** depend on the characteristics found in **Q1**?

Q6 Can the sharpened bound from **Q3** distinguish between preconditioners?

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Algorithm Conjugate Gradient Method [1]

$\mathbf{r}_0 = \mathbf{b} - A\mathbf{u}_0$, $\mathbf{p}_0 = \mathbf{r}_0$, $\beta_0 = 0$

for $j = 0, 1, 2, \ldots, m$ **do**

  $\alpha_j = (\mathbf{r}_j, \mathbf{r}_j)/(A\mathbf{p}_j, \mathbf{p}_j)$

  $\mathbf{u}_{j+1} = \mathbf{u}_j + \alpha_j \mathbf{p}_j$

  $\mathbf{r}_{j+1} = \mathbf{r}_j - \alpha_j A\mathbf{p}_j$

  $\beta_j = (\mathbf{r}_{j+1}, \mathbf{r}_{j+1})/(\mathbf{r}_j, \mathbf{r}_j)$

  $\mathbf{p}_{j+1} = \mathbf{r}_{j+1} + \beta_j \mathbf{p}_j$

end for

[1] Y. Saad. *Iterative Methods for Sparse Linear Systems*. Second. Society for Industrial and Applied Mathematics, 2003. DOI: 10.1137/1.9780898718003. eprint: https://epubs.siam.org/doi/book/10.1137/1.9780898718003

Background & Literature

Conjugate gradient method: residual polynomial

- Iterative, projection method onto a Krylov subspace $\mathcal{K}_m(A_0, \mathbf{r}_0)$ given by

$$\text{span}\{\mathbf{r}_0, A\mathbf{r}_0, A^2\mathbf{r}_0, \ldots, A^{m-1}\mathbf{r}_0\}$$

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- Approximate solution can be expressed as

$$\mathbf{u}_m = \mathbf{u}_0 + \sum_{i=0}^{m-1} c_i A^i \mathbf{r}_0 = \mathbf{u}_0 + q_{m-1}(A)\mathbf{r}_0$$

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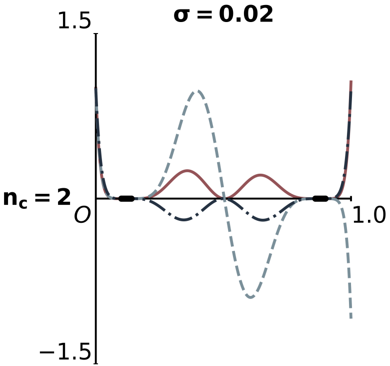

Figure: Residual polynomial $r_m(\lambda) = 1 - \lambda q_{m-1}(\lambda)$

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- Minimize residual polynomial on eigenvalues of A

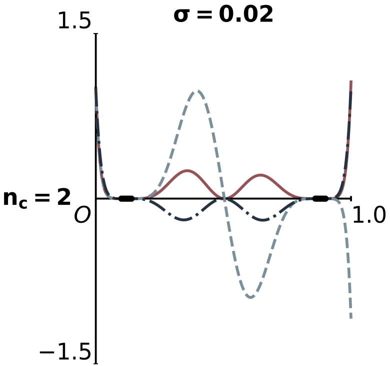

Figure: Residual polynomial $r_m(\lambda) = 1 - \lambda q_{m-1}(\lambda)$

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Conjugate gradient method: convergence

- Classical (condition number) convergence bound:

Theorem

The error of the m^{th} iterate of the CG algorithm is bounded by

$$||\mathbf{e}_m||_A \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^m ||\mathbf{e}_0||_A,$$

where $\kappa = \lambda_{max}/\lambda_{min}$ is the condition number of (symmetric matrix) A.

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- Only sharp for uniform eigenvalue distributions!

$$||\mathbf{e}_m||_A \leq \min_{r\in\mathcal{P}_{m-1}, r(0)=1} \max_{\lambda\in[\lambda_{\min},\lambda_{\max}]} |r(\lambda)|||\mathbf{e}_0||_A \overset{\text{uniform } \sigma(A)}{=} \frac{||\mathbf{e}_0||}{C_m\left(\frac{\kappa+1}{\kappa-1}\right)}$$

Background & Literature

Conjugate gradient method: spectral distribution

Setting $\lambda_{\text{min}} = 0.1$ and $\lambda_{\text{max}} = 0.9$ gives $m_{\text{classical}} = 26$. Worst case distribution:

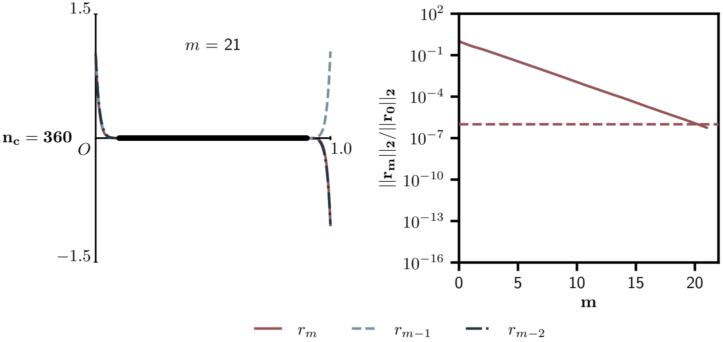

Figure: CG convergence for uniform spectrum.

Background & Literature

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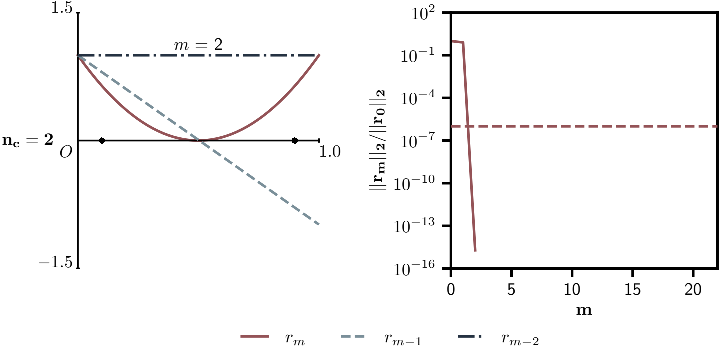

Figure: CG convergence for spectrum with two distinct eigenvalues.

Background & Literature

Conjugate gradient method: non-uniform spectra

- Clusterpoint distribution ($0 < \rho \leq 1$)[2]

$$\lambda_i = \lambda_1 + \frac{i-1}{N-1}(\lambda_N - \lambda_1)\rho_i^{N-i},$$

For $i = 1, \ldots, N$

[2] Z. Strakoš. "On the real convergence rate of the conjugate gradient method". In: *Linear Algebra and its Applications* 154-156 (1991), pp. 535–549. ISSN: 0024-3795. DOI: https://doi.org/10.1016/0024-3795(91)90393-B

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$$\lambda_i = \lambda_1 + \frac{i-1}{N-1}(\lambda_N - \lambda_1)\rho_i^{N-i},$$

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- $\rho = 1$ gives uniform distribution

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For $i = 1, \dots, N$

- $\rho = 1$ gives uniform distribution
- $\rho = 0$ gives two distinct eigenvalues
- $0 < \rho < 1$ gives a spectrum with a clusterpoint at λ_1.

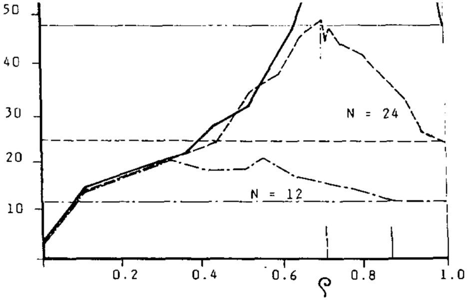

Figure: CG iterations versus ρ

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Background & Literature

Conjugate gradient method: non-uniform spectra

- Let $0 < a < b < c < d < 1$ and consider[3]

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Background & Literature

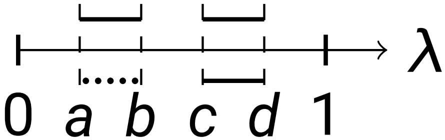
Conjugate gradient method: non-uniform spectra

- Let $0 < a < b < c < d < 1$ and consider[3]
  - Two disjoint clusters

$$\sigma_1(A) = [a, b] \bigcup [c, d]$$

  - Cluster with tail

$$\sigma_2(A) = [c, d] \bigcup_{\substack{i=1 \\ \lambda_i \in [a,b]}}^{N_{\text{tail}}} \lambda_i$$



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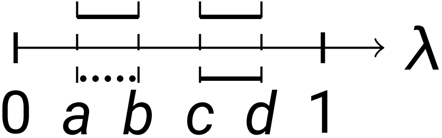
Background & Literature

Conjugate gradient method: non-uniform spectra

- A-norm optimality of CG

$$\|\mathbf{e}_m\|_A = \min_{r \in \mathcal{P}_m, r(0)=1} \sum_{i=1}^{m} \frac{r(\lambda_i)^2}{\lambda_i} \rho_{0,i}^2$$



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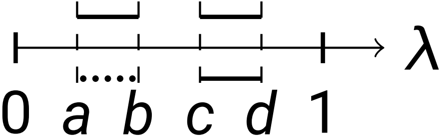

- We look for $r_{\bar{m}} = \hat{r}_p \hat{r}_{\bar{m}-p} \in \mathcal{P}_{\bar{m}}$[3]

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Let $\epsilon = \frac{\|\mathbf{e}_m\|_A}{\|\mathbf{e}_0\|_A}$ relative error

$$1 \leq p = \min\left\{ \left\lceil \frac{1}{2}\sqrt{\frac{b}{a}} \ln \epsilon + 1 \right\rceil, N_{\text{tail}} \right\}$$

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Background & Literature

Schwarz preconditioners

- Derived from the Alternating Schwarz method[4]

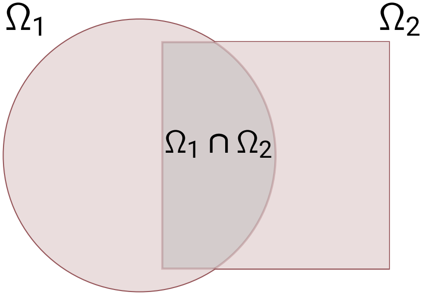

Figure: Domain decomposition with overlapping subdomains.

[4] V. Dolean, P. Jolivet, and F. Nataf. *An Introduction to Domain Decomposition Methods*. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2015. DOI: 10.1137/1.9781611974065. eprint: https://epubs.siam.org/doi/pdf/10.1137/1.9781611974065

Background & Literature

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- Convergence rate depends on the overlap δ and the wave number of eigenmodes k

2D Alternating Schwarz Example

Let $\Omega_1 = (-\infty, \delta) \times \mathbb{R}$, $\Omega_2 = (\delta, \infty) \times \mathbb{R}$

$$-(\eta - \Delta)u = f \text{ in } \mathbb{R}^2,$$
$$u \text{ bounded at infinity.}$$

Then the convergence rate is given by

$$\rho_{2D}(k; \eta, \delta) = e^{-\delta\sqrt{\eta + k^2}}$$

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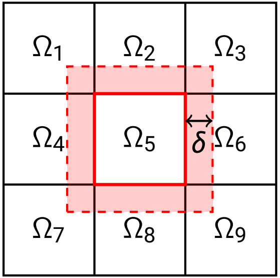

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- As a preconditioner $M_{\text{OAS-1}} = \sum_{i=1}^{N_{\text{sub}}} R_i^T A_i^{-1} R_i$
- Need a coarse space R_0 to counter slowly converging modes

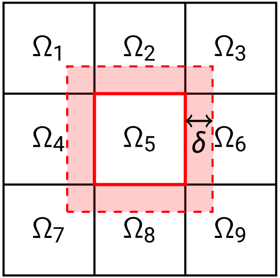

Figure: Domain decomposition with N_{sub} subdomains.

[4] V. Dolean, P. Jolivet, and F. Nataf. *An Introduction to Domain Decomposition Methods*. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2015. DOI: 10.1137/1.9781611974065. eprint: https://epubs.siam.org/doi/pdf/10.1137/1.9781611974065

Background & Literature

Schwarz preconditioners

- Derived from the Alternating Schwarz method[4]
- Convergence rate depends on the overlap δ and the wave number of eigenmodes k
- As a preconditioner $M_{\text{OAS-1}} = \sum_{i=1}^{N_{\text{sub}}} R_i^T A_i^{-1} R_i$
- Need a coarse space R_0 to counter slowly converging modes

2-level Additive Schwarz Preconditioner

$$M_{\text{OAS-2}} = {R_0}^T A_0^{-1} R_0 + M_{\text{OAS-1}}$$

[4] V. Dolean, P. Jolivet, and F. Nataf. *An Introduction to Domain Decomposition Methods*. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2015. DOI: 10.1137/1.9781611974065. eprint: https://epubs.siam.org/doi/pdf/10.1137/1.9781611974065

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

- MsFEM-based: robust for high-contrast, but computationally expensive[5]

[5] Heinlein (2018)

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

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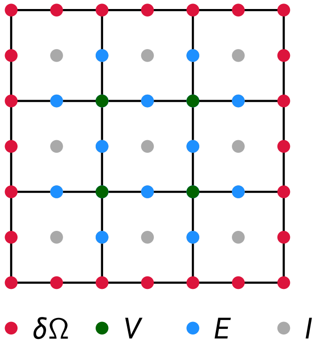
- Generalized framework: GDSW[6], RGDSW[7]



[5] Heinlein (2018)
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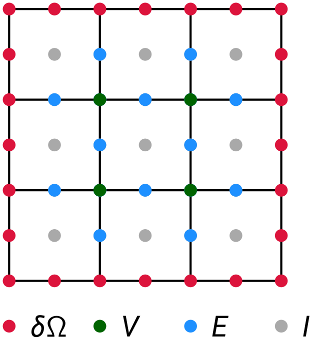
[7] Dohrmann and Widlund (2017)

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

- MsFEM-based: robust for high-contrast, but computationally expensive[5]
- Generalized framework: GDSW[6], RGDSW[7]
- Hybrid: AMS[8]

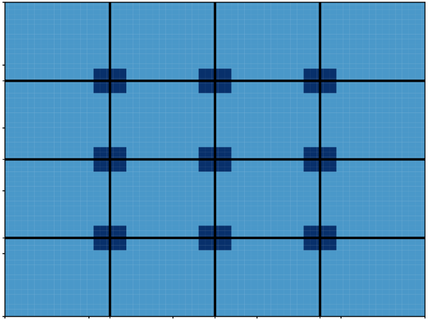


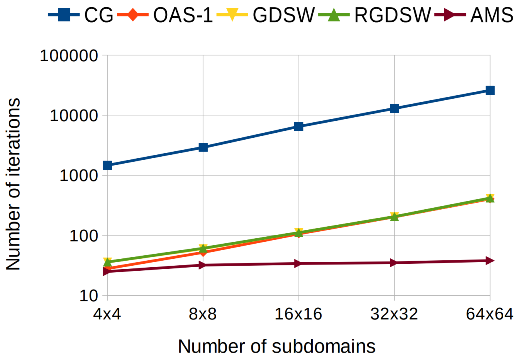
[5] Heinlein (2018)
[6] Dohrmann, Klawonn, and Widlund (2008)
[7] Dohrmann and Widlund (2017)
[8] Alves, Heinlein, and Hajibeygi (2024)

Background & Literature

Tailored Coarse Spaces for High-Contrast Problems

Figures obtained from [5]





[5] F. A. C. S. Alves, A. Heinlein, and H. Hajibeygi. *A computational study of algebraic coarse spaces for two-level overlapping additive Schwarz preconditioners*. 2024. arXiv: 2408.08187 [math.NA]

Background & Literature

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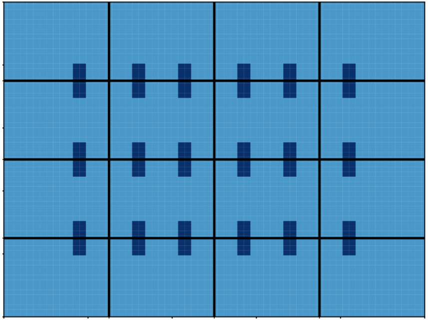

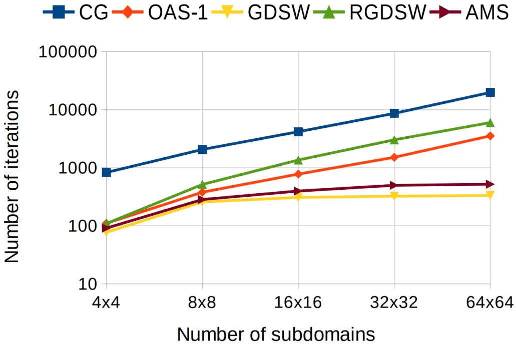

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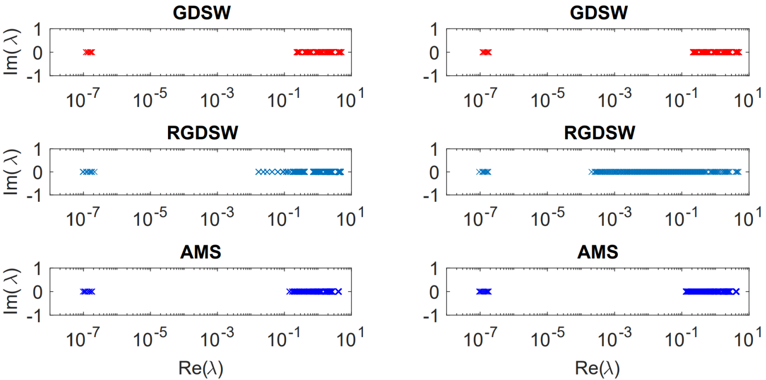

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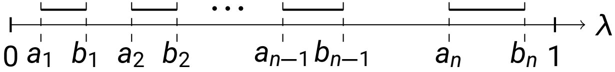
Structure

- Research Questions
- Background & Literature
- Preliminary Results
- Outlook

Preliminary Results

Generalization to multiple clusters



Preliminary Results

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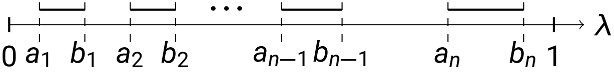


Building on the work of Axelsson we can imagine $r_{\bar{m}} = \hat{r}_{p_1}\hat{r}_{p_2}\dots\hat{r}_{p_n} \in \mathcal{P}_{\bar{m}}$ with

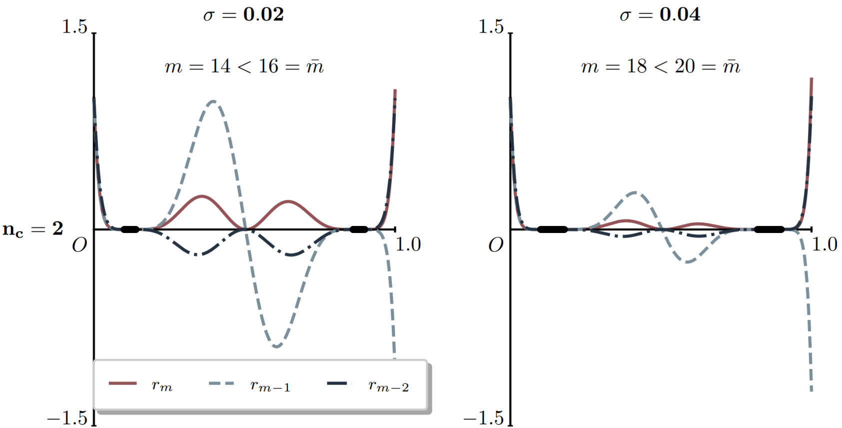
$$p_i \leq \left\lceil \log_{f_i} \frac{\epsilon}{2} + \sum_{j=1}^{i-1} p_j \log_{f_i} \frac{\zeta_2^{(j)}}{\zeta_1^{(i,j)}} \right\rceil \quad \text{and} \quad f_i = \frac{\sqrt{K_i} - 1}{\sqrt{K_i} + 1}.$$

Sharpened bound given by

$$\bar{m} = \sum_{i=1}^{n} p_i.$$

Preliminary Results

Generalization to multiple clusters



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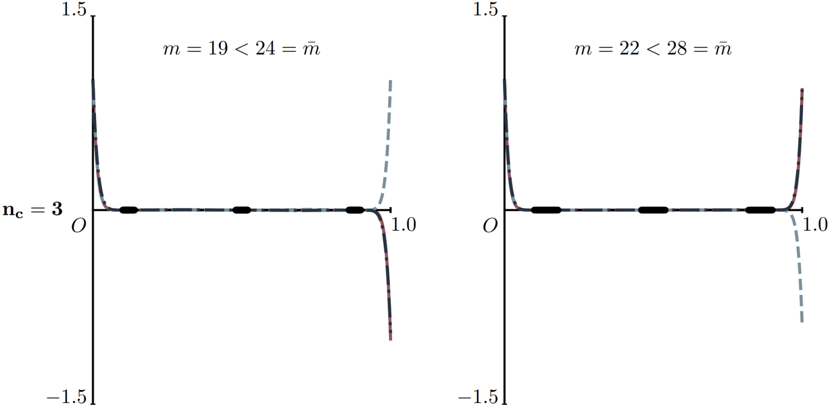

Preliminary Results

Demo

Structure

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Outlook

Progress

Q1 What other spectral characteristics like the condition number can we consider?

Q3 Given a toy eigenspectrum, how can we sharpen the CG iteration bound?

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Q5 How does the performance described in **Q4** depend on the characteristics found in **Q1**?

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Outlook

Progress

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