

A Chebyshev-based two-stage iterative method as an alternative to the direct solution of linear systems

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Outline

- Problems with Preconditioning
- Techniques for improving the solvers
- The two phase algorithm
- Error Analysis
- Influence of the different parameters
- Numerical experiments

Problems with Preconditioning

$$Au = b$$

$$A \in \mathbf{R}^{N \times N} \text{ SPD}$$

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$$\hat{\mathbf{A}} = \mathbf{R}^{-T} \mathbf{A} \mathbf{R}^{-1}, \mathbf{x} = \mathbf{R} \mathbf{u}, \hat{\mathbf{b}} = \mathbf{R}^{-T} \mathbf{b}.$$

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A PDE example

$\Omega \subset \mathbf{R}^2$ simply connected bounded polygonal. Let

$$a(\mathbf{u}, \mathbf{v}) \quad \forall \mathbf{u}, \mathbf{v} \in H_0^1(\Omega)$$

be a continuous and coercive bilinear form, and

$$L(\mathbf{v}) \in H^{-1}(\Omega).$$

The problem

$$\begin{cases} \text{Find } \mathbf{u} \in H_0^1(\Omega) \text{ such that} \\ a(\mathbf{u}, \mathbf{v}) = L(\mathbf{v}), \quad \forall \mathbf{v} \in H_0^1(\Omega), \end{cases}$$

has a unique solution.

A PDE example

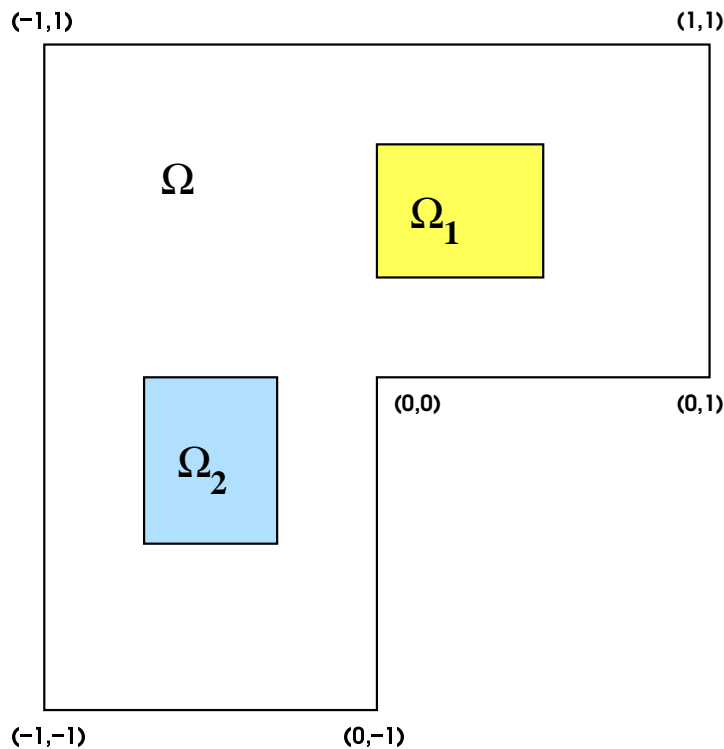
$$a(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \mathcal{K}(\mathbf{x}) \nabla \mathbf{u} \cdot \nabla \mathbf{v} d\mathbf{x}, \quad \forall \mathbf{u}, \mathbf{v} \in H_0^1(\Omega)$$

$$L(\mathbf{v}) = \int_{\Omega} 10\mathbf{v} d\mathbf{x}, \quad \forall \mathbf{v} \in H_0^1(\Omega)$$

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$$\mathcal{K}(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in \Omega \setminus \{\Omega_1 \cup \Omega_2\}, \\ 10^6 & \mathbf{x} \in \Omega_1, \\ 10^4 & \mathbf{x} \in \Omega_2. \end{cases}$$

A PDE example

Using **pdetool**[©], we generated a mesh satisfying the usual regularity conditions of Ciarlet and we computed a finite-element approximation of the problem with the use of continuous piece-wise linear elements. The approximated problem is equivalent to the following system of linear equations:

$$\mathbf{A}\mathbf{u} = \mathbf{b}.$$

In our mesh, the largest triangle has an area of 3.123×10^{-4} , therefore, the resulting linear system has 16256 triangles, 8289 nodes, and 7969 degrees of freedom.

A PDE example

We used three kinds of preconditioners: the classical Jacobi diagonal matrix, $\mathbf{M} = \text{diag}(\mathbf{A})$, the incomplete Cholesky decomposition of \mathbf{A} with zero fill-in, and the incomplete Cholesky decomposition of \mathbf{A} with drop tolerance 10^{-2} . Using the incomplete Cholesky decompositions, we computed the upper triangular matrix \mathbf{R} such that $\mathbf{M} = \mathbf{R}^T \mathbf{R}$.

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\mathbf{M}	$\kappa(\mathbf{M}^{-1} \mathbf{A})$	λ_{\min}	λ_{\max}
\mathbf{I}	$2.6 \cdot 10^9$	$3.7 \cdot 10^{-3}$	$9.6 \cdot 10^6$
Jacobi	$6.8 \cdot 10^8$	$3.1 \cdot 10^{-9}$	2.08
Inc. Cholesky(0)	$9.4 \cdot 10^7$	$1.7 \cdot 10^{-8}$	1.6
Inc. Cholesky(10^{-2})	$6.2 \cdot 10^6$	$1.8 \cdot 10^{-7}$	1.1

A PDE example

	Preconditioner M		
μ	Jacobi	Inc. Cholesky(0)	Inc. Cholesky(10^{-2})
$\lambda_{\max}/10^3$	3		
$\lambda_{\max}/500$	5		
$\lambda_{\max}/200$	18		
$\lambda_{\max}/100$	43	3	
$\lambda_{\max}/50$		11	
$\lambda_{\max}/20$		32	
$\lambda_{\max}/10$	>200	68	3
$\lambda_{\max}/5$			9
$\lambda_{\max}/2$			40

Number of eigenvalues in $[\lambda_{\min}, \mu]$.

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- Implicit matrix

Techniques for improving the solvers

- Deflation: compute the invariant space corresponding to the smallest eigenvalues

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- Filtering + Lanczos

The two-phase iterative approach

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- Start with an initial set of s randomly generated vectors (s is the **block-size**), and “*damp*”, in these starting vectors, the eigenfrequencies associated with all the eigenvalues in $[\mu, \lambda_{\max}(\hat{\mathbf{A}})]$.

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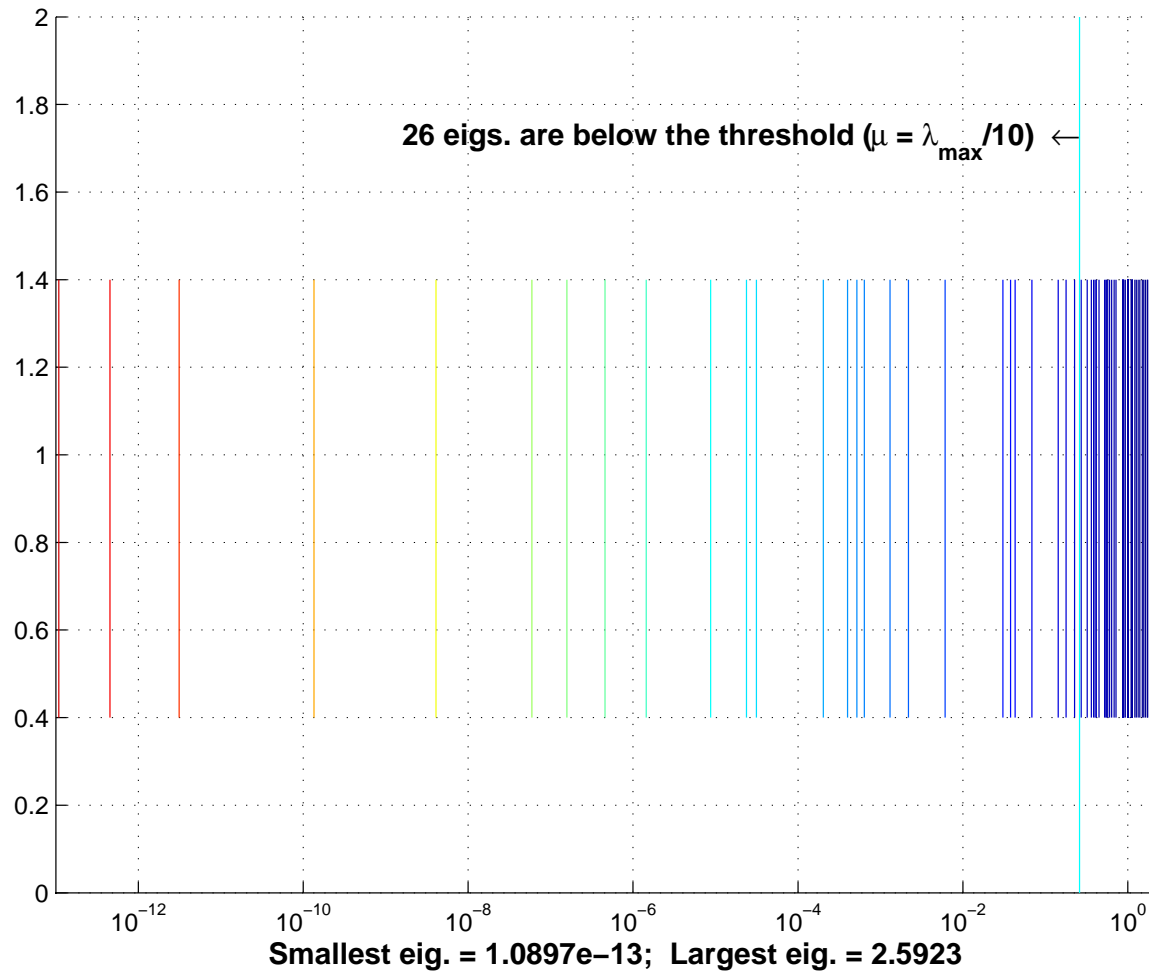
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If the eigenvalues are well clustered the number of remaining eigenvalues in $[\lambda_{\min}(\hat{\mathbf{A}}), \mu]$, with reasonable μ ($\lambda_{\max}/100$, or $\lambda_{\max}/10$), should be small compared to the size of the linear system.

The two-phase iterative approach



The two-phase iterative approach

We can use Chebyshev polynomials to *damp*

$$\begin{cases} T_0(\omega) = 1, & T_1(\omega) = \omega \\ T_{n+1}(\omega) = 2\omega T_n(\omega) - T_{n-1}(\omega) & n \geq 1. \end{cases} \cdot$$

If we consider $d > 1$ and

$$H_n(\omega) = \frac{T_n(\omega)}{T_n(d)},$$

then H_n has minimum l_∞ norm on the interval $[-1, 1]$ over all polynomials Q_n of degree less than or equal to n and satisfying the condition $Q_n(d) = 1$, and we have

$$\max_{\omega \in [-1, 1]} H_n(\omega) = \frac{1}{T_n(d)}.$$

The two-phase iterative approach

$$\lambda \in \mathbb{R} \mapsto \omega_\mu(\lambda) = \frac{\lambda_{\max}(\hat{\mathbf{A}}) + \mu - 2\lambda}{\lambda_{\max}(\hat{\mathbf{A}}) - \mu},$$

with $\lambda_{\min}(\hat{\mathbf{A}}) < \mu < \lambda_{\max}(\hat{\mathbf{A}})$ given above.

This transformation maps $\lambda_{\max}(\hat{\mathbf{A}})$ to -1 , μ to 1 , and 0 to

$$\omega_\mu(0) = d_\mu = \frac{\lambda_{\max}(\hat{\mathbf{A}}) + \mu}{\lambda_{\max}(\hat{\mathbf{A}}) - \mu} > 1.$$

Then,

$$\mathcal{P}_n(\lambda) = \frac{T_n(\omega_\mu(\lambda))}{T_n(d_\mu)},$$

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with $\xi_i = \mathbf{u}_i^T \mathbf{z}$, $i = 1, \dots, n$,

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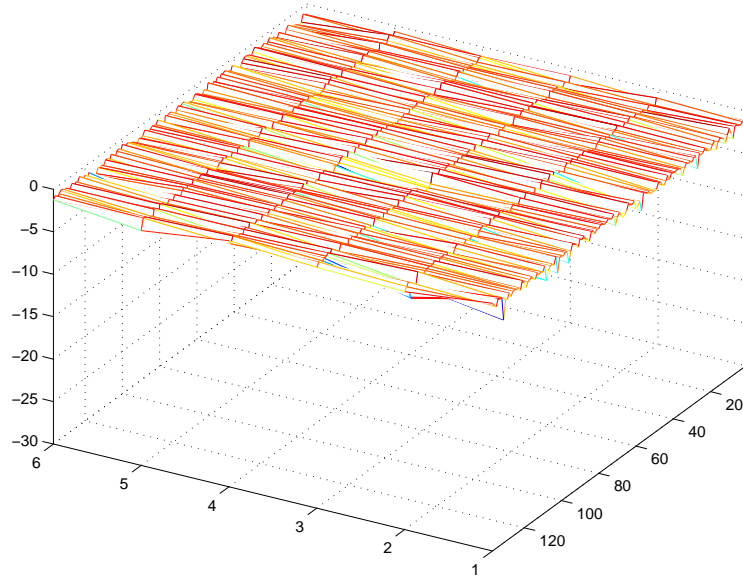
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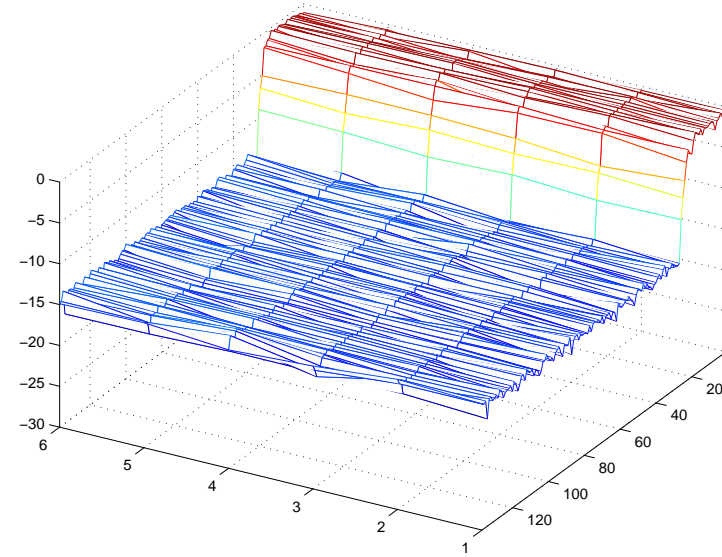
The eigencomponents of the resulting vector \mathbf{v} are close to that of the initial vector \mathbf{z} for all i such that λ_i is close to 0 and relatively much smaller for large enough degree n and all i such that

$$\lambda_i \in [\mu, \lambda_{\max}(\hat{\mathbf{A}})].$$

The two-phase iterative approach



Eigencomponents of the starting set of orthonormal vectors (6 vectors, randomly generated, and orthonormalized).



Eigencomponents of this set of vectors after 51 Chebyshev iterations (the resulting 6 vectors have also been reorthonormalized).

- The eigenvectors of \mathbf{A} are indexed on the X-axis (from 1 to 136) in increasing order of their corresponding eigenvalue.
- The indexes (from 1 to 6) of the vectors in the current set are indicated on the Y-axis.
- The Z-axis indicates the logarithm of the absolute values of the eigencomponents in each of the 6 vectors.

The two-phase iterative approach

We can interpret the use of Chebyshev polynomials as a *filtering* tool that increases the degree of colinearity with some selected eigenvectors. Then, after “*filtering*” the initial starting vectors, we obtain a set of s vectors with eigencomponents below a certain level ε for those eigenvalues in the range $[\mu, \lambda_{\max}(\hat{\mathbf{A}})]$, and relatively much bigger eigencomponents linked with the smallest eigenvalues in $\hat{\mathbf{A}}$.

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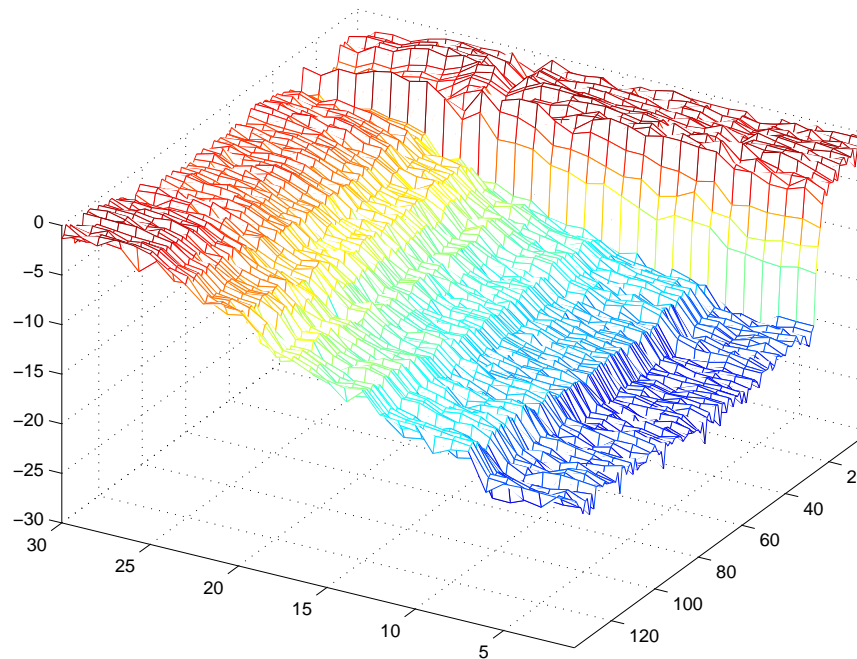
- $k \leq s$, a Ritz decomposition enables us to get the k wanted eigenvectors.
- $k > s$, we use a Block-Lanczos type of approach to build a Krylov basis starting with these filtered vectors and to stop when appropriate.

The two-phase iterative approach

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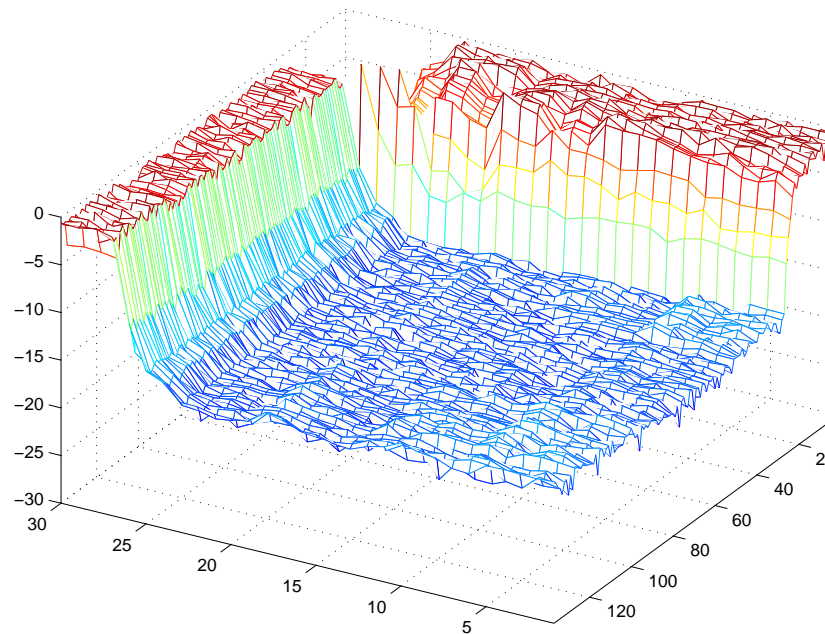
Eigendecomposition of the Krylov basis obtained after 5 block-Lanczos steps (Block Lanczos with block size 6 and full classical Gram-Schmidt reorthogonalization).

Lanczos/Orthodir approach

To maintain the level of the unwanted eigenfrequencies in the orthonormal block Krylov basis under ε , perform, at each Block-Lanczos iteration, a few extra Chebyshev iterations on the newly generated Block Lanczos vectors $\mathbf{V}^{(k+1)}$.

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Eigendecomposition of the Krylov basis obtained after 5 block-Lanczos/Orthodir steps with additional Chebyshev filtering at each Lanczos iteration

$$\mathbf{Z} = \text{Chebyshev_Filter}(\mathbf{Y}, \varepsilon, [\mu, \lambda_{\max}], \hat{\mathbf{A}})$$

is the application of a Chebyshev polynomial in $\hat{\mathbf{A}}$ to \mathbf{Y} , viz.

$$\mathbf{Z} = \mathcal{P}_n(\hat{\mathbf{A}})\mathbf{Y},$$

where \mathcal{P}_n has a degree such that its L_∞ norm over the interval $[\mu, \lambda_{\max}]$ is less than ε .

Fixing the block size to s , the cut-off eigenvalue μ ,

$\lambda_{\min}(\hat{\mathbf{A}}) < \mu < \lambda_{\max}(\hat{\mathbf{A}})$, and the filtering level $\varepsilon \ll 1$:

Partial Spectral Factorization phase

$$\mathbf{P}^{(0)} = \text{random}(n, s); \quad \text{and } \mathbf{Q}^{(0)} = \text{orthonormalize}(\mathbf{P}^{(0)})$$

$$\mathbf{Z}^{(0)} = \text{Chebyshev_Filter}(\mathbf{Q}^{(0)}, \varepsilon, [\mu, \lambda_{\max}], \hat{\mathbf{A}})$$

$$[\mathbf{Y}^{(0)}, \boldsymbol{\Sigma}_1^{(0)}, \mathbf{W}] = \text{SVD}(\mathbf{Z}^{(0)}, 0); \quad \text{and } \delta_0 = \sigma_{\min}(\boldsymbol{\Sigma}_1^{(0)})$$

$$\hat{\mathbf{Z}}^{(0)} = \text{Chebyshev_Filter}(\mathbf{Y}^{(0)}, \delta_0, [\mu, \lambda_{\max}], \hat{\mathbf{A}}); \quad \text{and } \mathbf{V}^{(0)} = \text{orthonormalize}(\hat{\mathbf{Z}}^{(0)})$$

$$\mathbf{V} = \mathbf{V}^{(0)}; \quad \text{and set } \delta_2 = 1$$

for $k = 0, 1, 2, \dots$, until convergence do :

$$\mathbf{P}^{(k+1)} = \hat{\mathbf{A}}\mathbf{V}^{(k)} - \mathbf{V}\mathbf{V}^T\hat{\mathbf{A}}\mathbf{V}^{(k)}; \quad [\mathbf{V}^{(k+1)}, \boldsymbol{\Sigma}_1^{(k+1)}, \mathbf{W}] = \text{SVD}(\mathbf{P}^{(k+1)}, 0);$$

$$\text{set } \delta_1 = \sigma_{\min}(\boldsymbol{\Sigma}_1^{(k+1)})/\lambda_{\max} \text{ and } \delta = \max(\varepsilon, \delta_1 \times \delta_2)$$

for $i = 1, 2$

$$\mathbf{Z}^{(k+1)} = \text{Chebyshev_Filter}(\mathbf{V}^{(k+1)}, \delta, [\mu, \lambda_{\max}], \hat{\mathbf{A}})$$

$$\mathbf{Y}^{(k+1)} = \mathbf{Z}^{(k+1)} - \mathbf{V}\mathbf{V}^T\mathbf{Z}^{(k+1)}$$

$$[\mathbf{V}^{(k+1)}, \boldsymbol{\Sigma}_2^{(k+1)}, \mathbf{W}] = \text{SVD}(\mathbf{Y}^{(k+1)}, 0)$$

$$\delta_2 = \sigma_{\min}(\boldsymbol{\Sigma}_2^{(k+1)}) \text{ and set } \delta = \delta_2$$

end

$$\mathbf{V} = [\mathbf{V}; \mathbf{V}^{(k+1)}]$$

Solution of the system

Once the *near*-invariant subspace linked to the smallest eigenvalues is obtained, we can use it for the computation of further solutions. The idea is to perform an oblique projection of the initial residual ($\hat{\mathbf{r}}_0 = \hat{\mathbf{b}} - \hat{\mathbf{A}}\mathbf{x}_0$) onto this *near* invariant subspace in order to get the eigencomponents in the solution corresponding to the smallest eigenvalues, viz.

$$\hat{\mathbf{r}}_1 = \hat{\mathbf{r}}_0 - \hat{\mathbf{A}}\mathbf{V} \left(\mathbf{V}^T \hat{\mathbf{A}}\mathbf{V} \right)^{-1} \mathbf{V}^T \hat{\mathbf{r}}_0,$$

with

$$\mathbf{x}_1 = \mathbf{x}_0 + \mathbf{V} \left(\mathbf{V}^T \hat{\mathbf{A}}\mathbf{V} \right)^{-1} \mathbf{V}^T \hat{\mathbf{r}}_0.$$

To compute the remaining part of the solution vector $\hat{\mathbf{A}}\mathbf{x}_2 = \hat{\mathbf{r}}_1$, one can then use the classical Chebyshev algorithm with eigenvalue bounds given by μ and $\lambda_{\max}(\hat{\mathbf{A}})$.

Solution phase

$$[\hat{\mathbf{r}}_1, \mathbf{x}_1] = \text{Chebyshev_Solve}(\hat{\mathbf{r}}_0, \mathbf{x}_0, \delta, [\mu, \lambda_{\max}], \hat{\mathbf{A}})$$

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Solution phase

For any right-hand side vector $\hat{\mathbf{b}}$, set \mathbf{x}_0 and $\hat{\mathbf{r}}_0 = \hat{\mathbf{b}} - \hat{\mathbf{A}}\mathbf{x}_0$, and perform the following consecutive steps:

$$[\hat{\mathbf{r}}_1, \mathbf{x}_1] = \text{Chebyshev_Solve}(\hat{\mathbf{r}}_0, \mathbf{x}_0, \varepsilon, [\mu, \lambda_{\max}], \hat{\mathbf{A}})$$

$$\hat{\mathbf{r}} = \hat{\mathbf{r}}_1 - \hat{\mathbf{A}}\mathbf{V} \left(\mathbf{V}^T \hat{\mathbf{A}} \mathbf{V} \right)^{-1} \mathbf{V}^T \hat{\mathbf{r}}_1; \quad \text{and}$$

$$\mathbf{x} = \mathbf{x}_1 + \mathbf{V} \left(\mathbf{V}^T \hat{\mathbf{A}} \mathbf{V} \right)^{-1} \mathbf{V}^T \hat{\mathbf{r}}_1$$

Error Analysis

$$\begin{aligned} \|\hat{\mathbf{r}}\|_{\hat{\mathbf{A}}^{-1}} &= \|\mathbf{x}^* - \mathbf{x}\|_{\hat{\mathbf{A}}} & \mathbf{e}_0 &= \hat{\mathbf{A}}^{-1}\hat{\mathbf{r}}_0 = \mathbf{x}^* - \mathbf{x}_0 \\ \mathbf{v} &= \mathcal{P}_n(\hat{\mathbf{A}})\hat{\mathbf{r}}_0 / \|\mathcal{P}_n(\hat{\mathbf{A}})\mathbf{e}_0\|_2. \end{aligned}$$

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$$\frac{\|\hat{\mathbf{r}}\|_{\hat{\mathbf{A}}^{-1}}}{\|\hat{\mathbf{r}}_0\|_{\hat{\mathbf{A}}^{-1}}} \leq \|\hat{\mathbf{A}}^{\frac{1}{2}}\|_2 \|\hat{\mathbf{A}}^{-\frac{1}{2}}\|_2 \|(\mathbf{I} - \mathbf{V}\mathbf{V}^T)\mathbf{v}\|_2.$$

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Theorem Let $\mathbf{U}_1 \in \mathbb{R}^{n \times m}$ be the matrix of the eigenvectors of $\hat{\mathbf{A}}$ corresponding to Λ_1 and $\mathbf{U}_2 \in \mathbb{R}^{n \times (n-m)}$ be the matrix of the remaining eigenvectors of $\hat{\mathbf{A}}$. Let $\mathbf{V} \in \mathbb{R}^{n \times \ell}$ be the full basis generated by the Algorithm using a filtering level ε and $\mathbf{v} = \mathcal{P}_n(\hat{\mathbf{A}})\hat{\mathbf{r}}_0 / \|\mathcal{P}_n(\hat{\mathbf{A}})\mathbf{e}_0\|_2$. If $m\varepsilon \ll 1$ and $\ell \geq m$ then

$$\|(\mathbf{I} - \mathbf{V}\mathbf{V}^T)\mathbf{v}\|_2 \leq 2\varepsilon\sqrt{m} + 2\varepsilon^2m.$$

Error Analysis

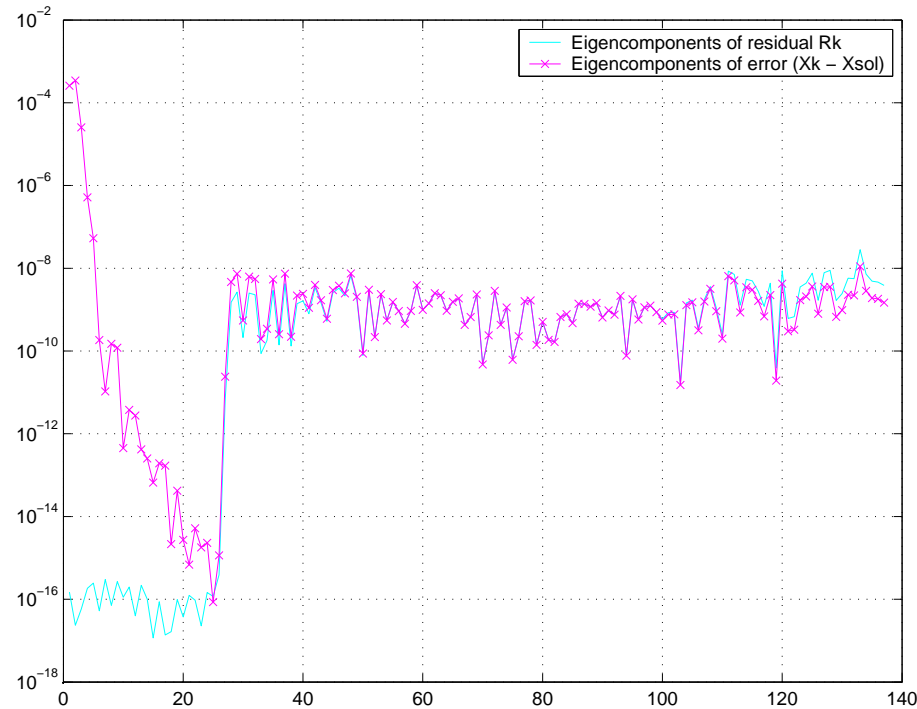
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$$\frac{\|\hat{\mathbf{r}}\|_{\hat{\mathbf{A}}^{-1}}}{\|\hat{\mathbf{r}}_0\|_{\hat{\mathbf{A}}^{-1}}} \leq 4\sqrt{m}\varepsilon \|\hat{\mathbf{A}}^{\frac{1}{2}}\|_2 \|\hat{\mathbf{A}}^{-\frac{1}{2}}\|_2.$$

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Error Analysis



Computation of the solution of a linear system with a right-hand side vector \mathbf{b} corresponding to a given random exact solution vector \mathbf{x}^* .
The filtering level ε has been fixed at 10^{-8} in both phases of the algorithm.

Influence of the different parameters

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$$\frac{\|\hat{\mathbf{r}}\|_{\hat{\mathbf{A}}^{-1}}}{\|\hat{\mathbf{r}}_0\|_{\hat{\mathbf{A}}^{-1}}} \leq \tau,$$
$$\varepsilon = \frac{\tau}{\sqrt{\kappa(\hat{\mathbf{A}})}}.$$

$\kappa(\hat{\mathbf{A}}) = \|\hat{\mathbf{A}}\| \|\hat{\mathbf{A}}^{-1}\|$ “*a posteriori*” good approximation

Influence of the different parameters

		Number of Chebyshev Iterations ($s = 6$)					
		$\mu = \lambda_{\max}/5$		$\mu = \lambda_{\max}/10$		$\mu = \lambda_{\max}/100$	
Block Krylov Iteration	Value of ε		Value of ε		Value of ε		
	10^{-14}	10^{-8}	10^{-14}	10^{-8}	10^{-14}	10^{-8}	
Start	35 + 2	20 + 3	51 + 4	30 + 3	165 + 14	96 + 14	
1	10	9	15	15	59	56	
2	11	11	20	18	88	90	
3	16	15	32	30	165	96	
4	25	20	43	30	-	-	
5	35	20	-	-	-	-	

In the case $\mu = \lambda_{\max}/5$, there are 33 eigenvectors to capture.

In the case $\mu = \lambda_{\max}/10$, there are 26 eigenvectors to capture.

In the case $\mu = \lambda_{\max}/100$, there are 19 eigenvectors to capture.

Back to the starting example

Numerical experiments

$\mu = \lambda_{\max}/\gamma$	Spectral Factorization		Solution phase	
γ	Tot. Chebyshev Iterations	Size \mathbf{V}	Chebyshev Iterations	Error Energy Norm
Jacobi				
1000	1030 (1004)	3	231	$7 \cdot 10^{-3}$ ($2.6 \cdot 10^{-5}$)
500	1101 (1114)	5	163	$6 \cdot 10^{-4}$ ($7.0 \cdot 10^{-6}$)
200	2234 (2615)	1	103	$2.5 \cdot 10^{-4}$ ($4 \cdot 10^{-6}$)
Inc. Cholesky(0)				
100	433 (248)	5 (3)	68	$7.4 \cdot 10^{-3}$ ($1.8 \cdot 10^{-5}$)
50	462 (503)	9	48	$3 \cdot 10^{-3}$ ($1.3 \cdot 10^{-5}$)
Inc. Cholesky(10^{-2})				
10	55 (70)	3	19	$8.2 \cdot 10^{-3}$ ($3.3 \cdot 10^{-6}$)

Summary of the results

THE END