Using Spectral Information to Precondition Saddle-Point Systems

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Outline

The target

Design efficient preconditioners to solve the system:

$$\mathcal{A}u = b \Leftrightarrow \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

with $A = A^T \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{n \times m}$ $(m \leq n)$

Overall goal

Find $\mathcal{P}$ such that $\mathcal{P}^{-1}\mathcal{A}$ has a better eigenvalue clustering and a reduced condition number

$\longrightarrow$ To reduce the number of MINRES iterations

"Ideal" block diagonal preconditioner

$$\mathcal{A}u = b \Leftrightarrow \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

Murphy, Golub and Wathen (2000):

$$\mathcal{P} = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix}$$

where $S = B^T A^{-1} B$ is the Schur complement

Spectral properties

$\mathcal{P}^{-1}\mathcal{A}$ has at most four distinct eigenvalues $0, 1, \frac{1 \pm \sqrt{5}}{2}$

Color code*

As much as possible:

- ■ $\rightarrow$ when related to A
- ■ $\rightarrow$ when related to B
- ■ $\rightarrow$ when related to S (or any combination of A and B)

*Except for the pictures

"Approximate" block diagonal preconditioners

$$\mathcal{P} = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \rightarrow \tilde{\mathcal{P}} = \begin{bmatrix} \tilde{A} & 0 \\ 0 & \tilde{S} \end{bmatrix}$$

- Golub, Greif and Varah (2006):

$$\tilde{A} = A + BWB^T \text{ and } \tilde{S} = B^T(A + BWB^T)^{-1}B$$

  with W symmetric positive semidefinite

- Rees, Dollar and Wathen (2010):

$$\tilde{A} \approx A \text{ and } \tilde{S} \approx S$$

  adapted to PDE-constrained optimization

- Olshanskii and Simoncini (2010) for a spectral-based analysis
- Benzi, Golub and Liesen (2005) for a survey

Assumptions and framework

$$\mathcal{A}u = b \Leftrightarrow \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

- A is symmetric positive definite
- B has full column rank

Additional assumptions

- A has few very small eigenvalues
- These eigenvalues and their associated eigenvectors are available (or good approximations)

In practice

How can we meet these additional assumptions?

- A has few very small eigenvalues

  $\rightarrow$ First-level preconditioner

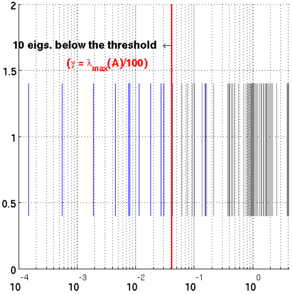
- These eigenvalues and their associated eigenvectors are available (or good approximations)

  $\rightarrow$ Krylov method with Chebyshev filters on $Ax = f$

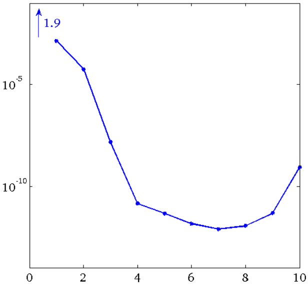
Chebyshev-based Krylov method

$\{\tilde{\lambda}_1, \cdots, \tilde{\lambda}_{10}\}$ and $[\tilde{u}_1 \ \cdots \ \tilde{u}_{10}]$:

obtained using a Conjugate Gradient method preconditioned by Chebyshev polynomials playing the role of spectral filter



$\tilde{\lambda}_i$ (in blue)



$$\frac{\|A\tilde{u}_i - \tilde{\lambda}_i \tilde{u}_i\|}{|\tilde{\lambda}_i|}$$

Golub, Ruiz and Touhami (2007)

SLRU-type spectral approximation of A^{-1}

$$\mathcal{P} = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \rightarrow \tilde{\mathcal{P}} = \begin{bmatrix} \tilde{A} & 0 \\ 0 & \tilde{S} \end{bmatrix} \; ?$$

Consider the low-rank spectral approximation*:

$$A_\gamma^{-1} = \frac{1}{\alpha} I_n + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T$$

- $\lambda_{\min}(A) \leq \gamma \leq \lambda_{\max}(A)$
- $\Lambda_\gamma = \mathrm{diag}\{\lambda_i\}_{i=1}^p$ with $\lambda_i \leq \gamma$
- $U_\gamma \in \mathbb{R}^{n \times p}$ is the set of associated orthonormal eigenvectors
- $\alpha > 0$ is a scaling parameter

*Carpentieri, Duff and Giraud (2003)

Spectral properties of $A_\gamma^{-1}A$

$$A_\gamma^{-1} = \frac{1}{\alpha} I_n + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T$$

The eigenvalues $\{\mu_i\}_{i=1}^n$ of $A_\gamma^{-1}A$ satisfy:

$$\begin{cases} \mu_i = 1 + \frac{\lambda_i}{\alpha} & \text{if} \quad \lambda_i \leq \gamma \quad (p \text{ eigenvalues}) \\ \mu_i = \frac{\lambda_i}{\alpha} & \text{if} \quad \lambda_i > \gamma \quad (n - p \text{ eigenvalues}) \end{cases}$$

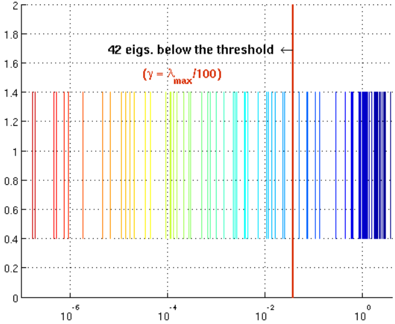
The eigenvalues $\{\mu_i\}_{i=1}^n$ of $A_\gamma^{-1}A$ are bounded within the interval

$$\left[\min\left(\frac{\alpha + \lambda_{\min}(A)}{\alpha}, \frac{\gamma}{\alpha}\right), \max\left(\frac{\alpha + \gamma}{\alpha}, \frac{\lambda_{\max}(A)}{\alpha}\right)\right]$$

$\longrightarrow$ In terms of $\lambda_{\min}(A), \lambda_{\max}(A), \gamma$ and α

Illustration

$$A \in \mathbb{R}^{300\times300},\ \lambda_{\min}(A) \approx 1.7\ 10^{-7},\ \lambda_{\max}(A) \approx 3.8$$



Spectrum of A

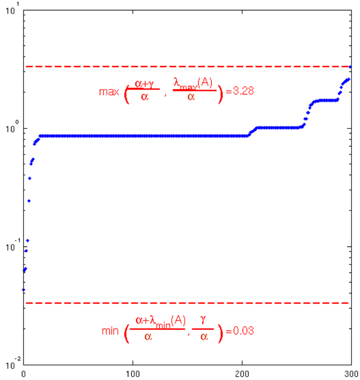
- $\gamma = \dfrac{\lambda_{\max}(A)}{100} \approx 3.8\ 10^{-2}$
- $\Lambda_\gamma = \mathrm{diag}\{\lambda_i\}_{i=1}^{42} \quad (\lambda_i \leq \gamma)$
- $U_\gamma \in \mathbb{R}^{300\times 42}$
- $\alpha = \dfrac{\mathrm{tr}(A)-\mathrm{tr}(\Lambda_\gamma)}{258} = 1.16$

Illustration (continued)

- $A \in \mathbb{R}^{300\times 300}$, $\lambda_{\min}(A) \approx 1.7\ 10^{-7}$, $\lambda_{\max}(A) \approx 3.8$
- $A_\gamma \in \mathbb{R}^{300\times 300}$, $\lambda_{\min}(A_\gamma) \approx 1.7\ 10^{-7}$, $\lambda_{\max}(A_\gamma) \approx 1.2$
- $A_\gamma^{-1} A \in \mathbb{R}^{300\times 300}$, $\mu_{\min} \approx 4.3\,10^{-2}$, $\mu_{\max} \approx 3.3$

The eigenvalues of $A_\gamma^{-1} A$ are guaranteed to be in the interval

$$[3.3\,10^{-2}, 3.3]$$



Eigenvalue dist. of $A_\gamma^{-1} A$

Approximation of the Schur complement and of its inverse

$$S_\gamma = B^T A_\gamma^{-1} B = B^T \left(\frac{1}{\alpha} I_n + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T\right) B$$

whose inverse is given by (Sherman-Morrison-Woodbury formula):

$$S_\gamma^{-1} = \alpha (B^T B)^{-\frac{1}{2}} (I_m - K \underbrace{(\tfrac{1}{\alpha} \Lambda_\gamma + K^T K)^{-1}}_{p \times p} K^T)(B^T B)^{-\frac{1}{2}}$$

where $K = (B^T B)^{-\frac{1}{2}} B^T U_\gamma \in \mathbb{R}^{m \times p}$

Approximation of the Schur complement and of its inverse

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where $K = (B^T B)^{-\frac{1}{2}} B^T U_\gamma \in \mathbb{R}^{m \times p}$

Remark: The singular values of K correspond to the cosines of the principal angles between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$

Spectral properties of $S_\gamma^{-1}S$

Main result

The eigenvalues $\{\nu_i\}_{i=1}^m$ of $S_\gamma^{-1}S$ are bounded within the interval

$$\left[\frac{\alpha}{\alpha+\lambda_{\max}(A)+\gamma}, \frac{\alpha+\gamma}{\gamma}\right]$$

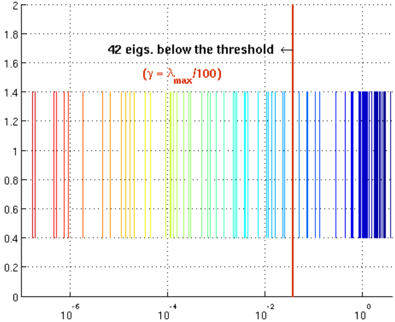
- In terms of $\lambda_{\max}(A), \gamma$ and α
- $\kappa(S_\gamma^{-1}S)$ is fully controlled by the choice of α and γ:

e.g., if $\gamma = \dfrac{\lambda_{\max}(A)}{100}$ and $\alpha = \dfrac{\lambda_{\max}(A)+\gamma}{2}$, then

$$\nu_i \in \left[\frac{1}{3}, \frac{103}{2}\right] \quad \text{and} \quad \kappa(S_\gamma^{-1}S) \leq 154.5$$

Illustration

$$A \in \mathbb{R}^{300\times 300},\ \lambda_{\min}(A) \approx 1.7\ 10^{-7},\ \lambda_{\max}(A) \approx 3.8$$



Spectrum of A

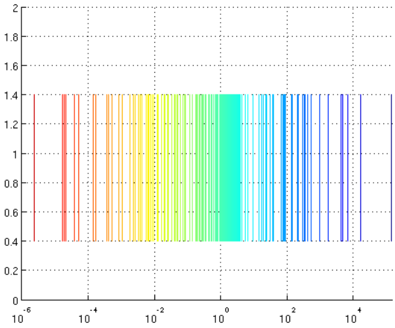
- $\gamma = \frac{\lambda_{\max}(A)}{100} \approx 3.8\ 10^{-2}$
- $\Lambda_\gamma = \mathrm{diag}\{\lambda_i\}_{i=1}^{42} \quad (\lambda_i \le \gamma)$
- $U_\gamma \in \mathbb{R}^{300\times 42}$
- $\alpha = \frac{\mathrm{tr}(A)-\mathrm{tr}(\Lambda_\gamma)}{258} = 1.16$

The eigenvalues of $S_\gamma^{-1} S$ are guaranteed in

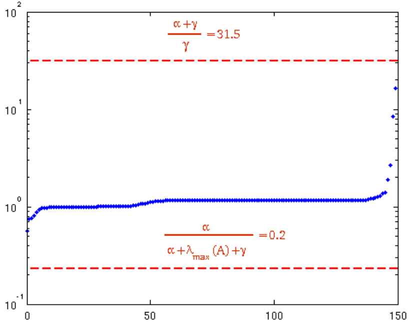
$[0.2, 31.5]$

Illustration (continued)

- $S \in \mathbb{R}^{150\times150}$, $\lambda_{\min}(S) \approx 2.4\ 10^{-6}$, $\lambda_{\max}(S) \approx 1.4\ 10^{5}$
- $S_\gamma \in \mathbb{R}^{150\times150}$, $\lambda_{\min}(S_\gamma) \approx 2.1\ 10^{-6}$, $\lambda_{\max}(S_\gamma) \approx 1.4\ 10^{5}$
- $S_\gamma^{-1} S \in \mathbb{R}^{150\times150}$, $\nu_{\min} \approx 0.56$, $\nu_{\max} \approx 16.28$



Spectrum of S



Eigenvalue dist. of $S_\gamma^{-1} S$

Two alternatives for an efficient spectral preconditioner

$$\mathcal{P}_1 = \begin{bmatrix} A & 0 \\ 0 & S_\gamma \end{bmatrix}$$

$$\mathcal{P}_2 = \begin{bmatrix} A_\gamma & 0 \\ 0 & S_\gamma \end{bmatrix}$$

with

$$A_\gamma^{-1} = \frac{1}{\alpha} I_n + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T$$

$$S_\gamma^{-1} = \alpha (B^T B)^{-\frac{1}{2}} (I_m - K(\frac{1}{\alpha}\Lambda_\gamma + K^T K)^{-1} K^T)(B^T B)^{-\frac{1}{2}}$$

where $K = (B^T B)^{-\frac{1}{2}} B^T U_\gamma$

Spectral properties of $\mathcal{A}$

$$\mathcal{A} = \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix}$$

- A is symmetric positive definite, with eigenvalues $\{\lambda_i\}_{i=1}^n$
- B has full column rank, with singular values $\{\sigma_i\}_{i=1}^m$

Rusten and Winther (1992)

The eigenvalues of $\mathcal{A}$ are bounded within $I^- \cup I^+$ with

$$I^- = \left[\frac{\lambda_{\min} - \sqrt{\lambda_{\min}^2 + 4\sigma_{\max}^2}}{2}, \frac{\lambda_{\max} - \sqrt{\lambda_{\max}^2 + 4\sigma_{\min}^2}}{2} \right]$$

$$I^+ = \left[\lambda_{\min}, \frac{\lambda_{\max} + \sqrt{\lambda_{\max}^2 + 4\sigma_{\max}^2}}{2} \right]$$

For our illustration: $\mathrm{Spec}(\mathcal{A})$ in $[-2, -2.4\,10^{-7}] \cup [1.7\,10^{-7}, 4.7]$ and $\kappa(\mathcal{A}) \leq 2.\,10^7$

Spectral properties of $\mathcal{P}_1^{-1}\mathcal{A}$

$$\mathcal{A} = \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \text{ preconditioned by } \boxed{\mathcal{P}_1 = \begin{bmatrix} A & 0 \\ 0 & S_\gamma \end{bmatrix}}$$

With Rusten and Winther, applied on

$$\mathcal{P}_1^{-1/2}\mathcal{A}\mathcal{P}_1^{-1/2} = \begin{bmatrix} I_n & Q_1 \\ Q_1^T & 0 \end{bmatrix},$$

where $Q_1 = A^{-1/2}BS_\gamma^{-1/2}$ satisfies $Q_1^TQ_1 = S_\gamma^{-1/2}SS_\gamma^{-1/2} \sim S_\gamma^{-1}S$

$$\boxed{\Longrightarrow \ \lambda_i(I_n) = 1 \quad \text{and} \quad \sigma_i^2(Q_1) = \lambda_i(S_\gamma^{-1}S) = \nu_i}$$

Spectral properties of $\mathcal{P}_1^{-1}\mathcal{A}$ (Rusten and Winther)

The eigenvalues of $\mathcal{P}_1^{-1}\mathcal{A}$ are bounded within the intervals

$$\left[\frac{1-\sqrt{1+4\nu_{\max}}}{2}, \frac{1-\sqrt{1+4\nu_{\min}}}{2}\right] \bigcup \left[1, \frac{1+\sqrt{1+4\nu_{\max}}}{2}\right]$$

where

$$\nu_{\min} \text{ and } \nu_{\max} \in \left[\frac{\alpha}{\alpha+\lambda_{\max}(A)+\gamma}, \frac{\alpha+\gamma}{\gamma}\right]$$

(eigenvalues of $S_\gamma^{-1}S$)

$\longrightarrow$ In terms of $\lambda_{\max}(A), \gamma$ and α

Spectral properties of $\mathcal{P}_1^{-1}\mathcal{A}$ (direct proof)

The eigenvalues of $\mathcal{P}_1^{-1}\mathcal{A}$ are bounded within the (refined) intervals

$$\left[\frac{1-\sqrt{1+4\nu_{\text{max}}}}{2}, \frac{1-\sqrt{1+4\nu_{\text{min}}}}{2}\right] \bigcup \{1\} \bigcup \left[\frac{1+\sqrt{1+4\nu_{\text{min}}}}{2}, \frac{1+\sqrt{1+4\nu_{\text{max}}}}{2}\right]$$

where

$$\nu_{\text{min}} \text{ and } \nu_{\text{max}} \in \left[\frac{\alpha}{\alpha+\lambda_{\text{max}}(A)+\gamma}, \frac{\alpha+\gamma}{\gamma}\right]$$

(eigenvalues of $S_\gamma^{-1}S$)

$\longrightarrow$ In terms of $\lambda_{\text{max}}(A), \gamma$ and α

Spectral properties of $\mathcal{P}_2^{-1}\mathcal{A}$

$$\mathcal{A} = \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \text{ preconditioned by } \boxed{\mathcal{P}_2 = \begin{bmatrix} A_\gamma & 0 \\ 0 & S_\gamma \end{bmatrix}}$$

With Rusten and Winther, applied on

$$\mathcal{P}_2^{-1/2}\mathcal{A}\mathcal{P}_2^{-1/2} = \begin{bmatrix} A_\gamma^{-1/2} A A_\gamma^{-1/2} & Q_2 \\ Q_2^T & 0 \end{bmatrix},$$

where $Q_2 = A_\gamma^{-1/2} B S_\gamma^{-1/2}$ satisfies $Q_2^T Q_2 = S_\gamma^{-1/2} S_\gamma S_\gamma^{-1/2} = I_m$

$$\Longrightarrow \ \lambda_i(A_\gamma^{-1/2} A A_\gamma^{-1/2}) = \lambda_i(A_\gamma^{-1} A) = \mu_i \quad \text{and} \quad \sigma_i^2(Q_2) = 1$$

Spectral properties of $\mathcal{P}_2^{-1}\mathcal{A}$ (Rusten and Winther)

The eigenvalues of $\mathcal{P}_2^{-1}\mathcal{A}$ are bounded within the intervals

$$\left[\frac{\mu_{\mathsf{min}} - \sqrt{\mu_{\mathsf{min}}^2 + 4}}{2}, \frac{\mu_{\mathsf{max}} - \sqrt{\mu_{\mathsf{max}}^2 + 4}}{2}\right] \bigcup \left[\mu_{\mathsf{min}}, \frac{\mu_{\mathsf{max}} + \sqrt{\mu_{\mathsf{max}}^2 + 4}}{2}\right]$$

where

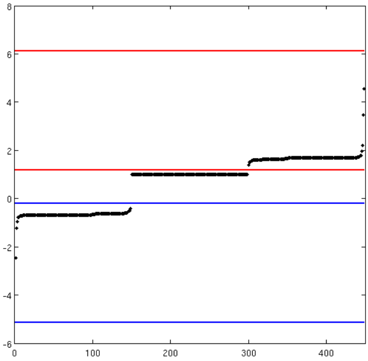
$$\mu_{\mathsf{min}} = \min\left(\frac{\alpha + \lambda_{\mathsf{min}}(A)}{\alpha}, \frac{\gamma}{\alpha}\right) \quad \text{and} \quad \mu_{\mathsf{max}} = \max\left(\frac{\alpha + \gamma}{\alpha}, \frac{\lambda_{\mathsf{max}}(A)}{\alpha}\right)$$

(eigenvalues of $A_\gamma^{-1}A$)

$\longrightarrow$ In terms of $\lambda_{\mathsf{min}}(A), \lambda_{\mathsf{max}}(A), \gamma$ and α

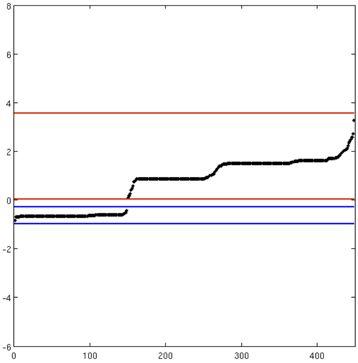
$\mathcal{P}_1^{-1}\mathcal{A}$ versus $\mathcal{P}_2^{-1}\mathcal{A}$ (Intervals in terms of $\lambda_{\max}(A), \lambda_{\min}(A), \gamma$ and α)

$[-5.13, -0.19] \cup \{1\} \cup [1.19, 6.13]$



$\boxed{\kappa(\mathcal{P}_1^{-1}\mathcal{A}) \leq 32.3}$

$[-0.98, -0.28] \cup [0.03, 3.56]$



$\boxed{\kappa(\mathcal{P}_2^{-1}\mathcal{A}) \leq 119}$

$\longrightarrow$ Reduced condition numbers in both cases

Varying γ ("True" intervals)

γ	$\lvert\{\lambda_i \le \gamma\}\rvert$	$\mathrm{Spec}(\mathcal{P}_1^{-1}\mathcal{A})$	$\kappa(\mathcal{P}_1^{-1}\mathcal{A})$
$\frac{\lambda_{\max}(A)}{100}$	42	$[-3.57, -0.40] \cup [1, 4.57]$	11.43
$\frac{\lambda_{\max}(A)}{1000}$	33	$[-12.12, -0.39] \cup [1, 13.12]$	33.64
$\frac{\lambda_{\max}(A)}{10000}$	23	$[-27.20, -0.38] \cup [1, 28.20]$	74.21

γ	$\lvert\{\lambda_i \le \gamma\}\rvert$	$\mathrm{Spec}(\mathcal{P}_2^{-1}\mathcal{A})$	$\kappa(\mathcal{P}_2^{-1}\mathcal{A})$
$\frac{\lambda_{\max}(A)}{100}$	42	$[-0.90, -0.45] \cup [9.7\,10^{-2}, 3.28]$	33.81
$\frac{\lambda_{\max}(A)}{1000}$	33	$[-0.98, -0.43] \cup [1.1\,10^{-2}, 3.40]$	309.09
$\frac{\lambda_{\max}(A)}{10000}$	23	$[-0.99, -0.42] \cup [2.5\,10^{-3}, 3.52]$	1408.00

Convergence bound of preconditioned MINRES

Assume that $\mathrm{Spec}(\mathcal{P}^{-1}\mathcal{A}) \subset [-a, -b] \cup [c, d]$, with $a, b, c, d > 0$

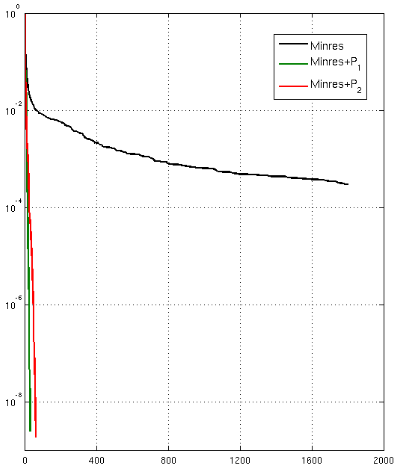
The iteration residual $r^{2k} = b - \mathcal{A}u^{2k}$ satisfies the bound

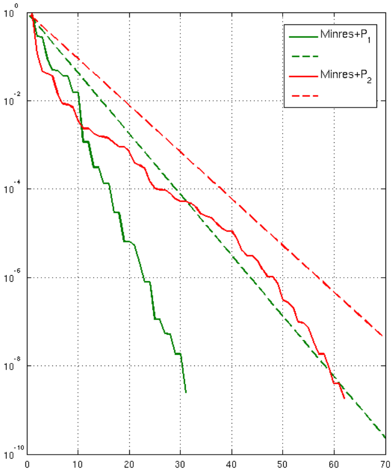
$$\frac{\|r^{2k}\|_{\mathcal{P}^{-1}}}{\|r^0\|_{\mathcal{P}^{-1}}} \leq 2 \left(\underbrace{\frac{\sqrt{ad} - \sqrt{bc}}{\sqrt{ad} + \sqrt{bc}}}_{\to \text{ slope}} \right)^k$$

$\to$ Illustration on our example for various γ's

$$\left(\text{Stopping criterion in MINRES: } \frac{\|r^k\|_2}{\|r^0\|_2} \leq 10^{-8} \right)$$

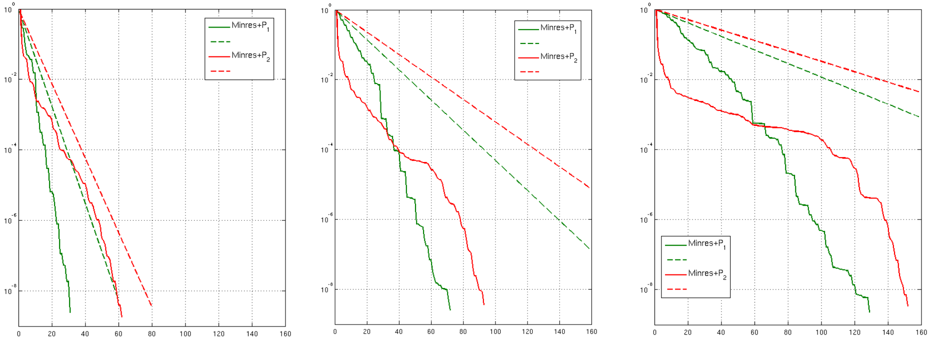
MINRES for $\gamma = \frac{\lambda_{max}(A)}{100}$





Convergence curves ($\mathcal{P}_1^{-1}$-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

MINRES for $\gamma = \frac{\lambda_{max}(A)}{100}$, $\gamma = \frac{\lambda_{max}(A)}{1000}$ and $\gamma = \frac{\lambda_{max}(A)}{10000}$



Convergence curves ($\mathcal{P}_1^{-1}$-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

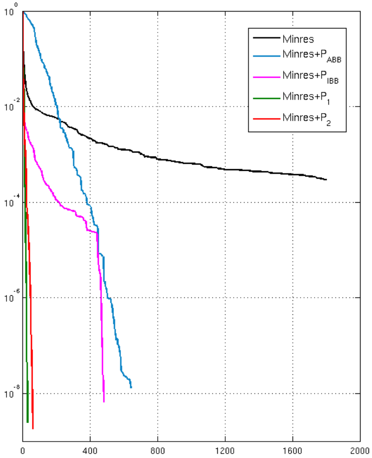
Further comparisons (“True” intervals, $\gamma = \frac{\lambda_{max}(A)}{100}$)

$$\mathcal{P}_1 = \begin{bmatrix} A & 0 \\ 0 & S_\gamma \end{bmatrix} \qquad \mathcal{P}_{IBB} = \begin{bmatrix} I_n & 0 \\ 0 & B^T B \end{bmatrix}$$

$$\mathcal{P}_2 = \begin{bmatrix} A_\gamma & 0 \\ 0 & S_\gamma \end{bmatrix} \qquad \mathcal{P}_{ABB} = \begin{bmatrix} A & 0 \\ 0 & B^T B \end{bmatrix}$$

$\mathcal{P}$	Spec($\mathcal{P}^{-1}\mathcal{A}$)			$\kappa(\mathcal{P}^{-1}\mathcal{A})$
	$[-1.6, -2.4\,10^{-6}]$	$\cup$	$[2.3\,10^{-5}, 3.8]$	$1.6\,10^{6}$
$\mathcal{P}_1$	$[-3.6, -0.4]$	$\cup$	$[1.0, 4.6]$	11.4
$\mathcal{P}_2$	$[-0.9, -0.5]$	$\cup$	$[9.7\,10^{-2}, 3.3]$	33.8
$\mathcal{P}_{IBB}$	$[-1.0, -0.4]$	$\cup$	$[3.0\,10^{-5}, 3.8]$	$1.3\,10^{5}$
$\mathcal{P}_{ABB}$	$[-8.9\,10^{2}, -0.4]$	$\cup$	$[1.0, 8.9\,10^{2}]$	$2.5\,10^{3}$

MINRES for $\gamma = \frac{\lambda_{max}(A)}{100}$



Convergence curves ($\mathcal{P}^{-1}$-norm of relative residuals)

First-level preconditioner

Preconditioner on A:
$M = R^T R$

Preconditioner on B:
$N = W^T W$

$$\Downarrow$$

$$\mathcal{P}_{Init} = \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix}$$

A $\mathcal{P}_2$-type preconditioner applied to $\mathcal{P}_{Init}^{-1}\mathcal{A}$ amounts to

$\mathcal{A} = \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix}$ preconditioned by $\tilde{\mathcal{P}}_2 = \begin{bmatrix} \tilde{A}_\gamma & 0 \\ 0 & \tilde{S}_\gamma \end{bmatrix}$

Two levels of preconditioner in one

where

$$\tilde{A}_\gamma^{-1} = \frac{1}{\alpha} M^{-1} + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T$$

$$\tilde{S}_\gamma^{-1} = \alpha (B^T M^{-1} B)^{-\frac{1}{2}} (I_m - K(\tfrac{1}{\alpha}\Lambda_\gamma + K^T K)^{-1} K^T)(B^T M^{-1} B)^{-\frac{1}{2}}$$

$$K = (B^T M^{-1} B)^{-\frac{1}{2}} B^T U_\gamma$$

and

- $\lambda_{\min}(M^{-1}A) \leq \gamma \leq \lambda_{\max}(M^{-1}A)$
- $\Lambda_\gamma = \mathrm{diag}\{\lambda_i(M^{-1}A)\}_{i=1}^p$ with $\lambda_i \leq \gamma$
- $U_\gamma \in \mathbb{R}^{n \times p}$ is the set of associated orthonormal eigenvectors
- $\alpha > 0$ is a scaling parameter

Construction of $\tilde{A}_\gamma^{-1}$ and $\tilde{S}_\gamma^{-1}$

$$\tilde{A}_\gamma^{-1} = \frac{1}{\alpha} M^{-1} + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T$$

$$\tilde{S}_\gamma^{-1} = \alpha (B^T M^{-1} B)^{-\frac{1}{2}} (I_m - K(\tfrac{1}{\alpha}\Lambda_\gamma + K^T K)^{-1} K^T)(B^T M^{-1} B)^{-\frac{1}{2}}$$

$$K = (B^T M^{-1} B)^{-\frac{1}{2}} B^T U_\gamma$$

1. Extract U_γ and Λ_γ:
   - Chebyshev-based Krylov method on $AU_\gamma = MU_\gamma\Lambda_\gamma$
2. $(B^T M^{-1} B)^{-1} v$

$$\hookrightarrow \begin{bmatrix} M & B \\ B^T & 0 \end{bmatrix} \quad \cdots$$

Interaction between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$

Recombination issue

$$S_\gamma^{-1} = \alpha(B^TB)^{-\frac{1}{2}}(I_m - K\underbrace{(\tfrac{1}{\alpha}\Lambda_\gamma + K^TK)^{-1}}_{\text{Key part}}K^T)(B^TB)^{-\frac{1}{2}}$$

where $K = (B^TB)^{-\frac{1}{2}}B^TU_\gamma = Q^TU_\gamma$, with

- Q: orthonormal basis of $\mathcal{I}m(B)$
- U_γ: orthonormal basis of $\mathcal{I}m(U_\gamma)$

$\longrightarrow$ The singular values of K correspond to the cosines of the principal angles between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$

Interaction between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$ (continued)

Consider the Singular Value Decomposition of $K = Q^T U_\gamma$:

$$Y^T K Z = \underbrace{Y^T Q^T}_{\substack{\text{Princ. vec.} \\ \text{in } \mathcal{I}m(B) \\ (p \text{ first lines})}} \quad \underbrace{U_\gamma Z}_{\substack{\text{Princ. vec.} \\ \text{in } \mathcal{I}m(U_\gamma)}} = \begin{array}{|c|} \hline C_\gamma \\ \hline 0 \\ \hline \end{array}$$

where

- $Y \in \mathbb{R}^{m \times m}$ and $Z \in \mathbb{R}^{p \times p}$ are orthogonal matrices
- $C_\gamma = \mathrm{diag}\{\cos\theta_i\}_{i=1}^p$ (that we assume nonsingular)
- $\{\theta_i\}_{i=1}^p \in \; [0, \pi/2[$ are the principal angles

Interaction between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$ (continued)

$$S_\gamma^{-1} = \alpha(B^T B)^{-\frac{1}{2}}(I_m - K\underbrace{(\tfrac{1}{\alpha}\Lambda_\gamma + K^T K)}_{\text{Key part}}{}^{-1}K^T)(B^T B)^{-\frac{1}{2}}$$

becomes, using $Y_\gamma = Y(:,1{:}p)$ and $V_\gamma = U_\gamma Z$ (princ. vec.),

$$S_\gamma^{-1} = \alpha(B^T B)^{-\frac{1}{2}}(I_m - Y_\gamma\underbrace{(\tfrac{1}{\alpha}C_\gamma^{-1}(V_\gamma^T A V_\gamma)C_\gamma^{-1} + I_p)}_{\text{Key part}}{}^{-1}Y_\gamma^T)(B^T B)^{-\frac{1}{2}}$$

where $V_\gamma^T A V_\gamma = Z^T U_\gamma^T A U_\gamma Z = Z^T \Lambda_\gamma Z$

Interaction between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$ (continued)

$$S_\gamma^{-1} = \alpha(B^TB)^{-\frac{1}{2}}(I_m - Y_\gamma\underbrace{(\tfrac{1}{\alpha}C_\gamma^{-1}(V_\gamma^TAV_\gamma)C_\gamma^{-1} + I_p)}_{\text{Key part}}{}^{-1}Y_\gamma^T)(B^TB)^{-\frac{1}{2}}$$

where $V_\gamma^TAV_\gamma = Z^TU_\gamma^TAU_\gamma Z = Z^T\Lambda_\gamma Z$

Observing that:

$$\frac{1}{\alpha}\|C_\gamma^{-1}(V_\gamma^TAV_\gamma)C_\gamma^{-1}\|_2 \leq \frac{1}{\alpha}\,\frac{\max\{\lambda_i\}_{i=1}^p}{\min\{\cos^2\theta_i\}_{i=1}^p} \leq \frac{1}{\alpha}\,\frac{\gamma}{\min\{\cos^2\theta_i\}_{i=1}^p},$$

roughly speaking, small eigenvalues "have an impact" on S_γ^{-1} when:

$$\boxed{\min\{\cos^2\theta_i\}_{i=1}^p \lesssim \mathcal{O}(\gamma/\alpha)}$$

Interaction between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$ (continued)

$$S_\gamma^{-1} = \alpha(B^TB)^{-\frac{1}{2}}(I_m - Y_\gamma\underbrace{(\tfrac{1}{\alpha}C_\gamma^{-1}(V_\gamma^T A V_\gamma)C_\gamma^{-1} + I_p)^{-1}}_{\text{Key part}}Y_\gamma^T)(B^TB)^{-\frac{1}{2}}$$

with $\displaystyle \frac{1}{\alpha}\|C_\gamma^{-1}(V_\gamma^T A V_\gamma)C_\gamma^{-1}\|_2 \leq \frac{1}{\alpha}\frac{\gamma}{\min\{\cos^2\theta_i\}_{i=1}^p}$

that is, if

$$\frac{1}{\alpha}\frac{\gamma}{\min\{\cos^2\theta_i\}_{i=1}^p} \ll 1, \quad \text{or equivalently,} \quad \min\{\cos^2\theta_i\}_{i=1}^p \gg \frac{\gamma}{\alpha},$$

the spectral information contained in $V_\gamma^T A V_\gamma$ is inhibited
($\rightarrow$ problem dependent)

Illustration on a toy example

- $A \in \mathbb{R}^{500\times 500}$ is a diagonal matrix with entries in $]0,1]$ and s.t.:
  - $p = 5 \quad (\gamma = 10^{-1}$ and $\alpha = 1)$
  - $\Lambda_\gamma = A(1{:}5,1{:}5)$
  - $U_\gamma = I_{500}(:,1{:}5)$
- $B \in \mathbb{R}^{500\times 200}$ is set to $B = \begin{bmatrix} C_\gamma & 0 \\ B_1 S_\gamma & B_2 \end{bmatrix}$, where
  - $C_\gamma = \mathrm{diag}\{\cos\theta_i\}_{i=1}^5$ and $S_\gamma = \mathrm{diag}\{\sin\theta_i\}_{i=1}^5$
  - $Q = \begin{bmatrix} B_1 & B_2 \end{bmatrix} \in \mathbb{R}^{495\times 200}$ with $Q^T Q = I_{200}$

Ensuring that

- B has othonormal columns
- $(B^T B)^{-\frac{1}{2}} B^T U_\gamma = B^T U_\gamma = \boxed{\begin{array}{c} C_\gamma \\ \hline 0 \end{array}}$

Illustration on a toy example (continued)

Implies a one to one match

- Eigenvectors versus principal vectors:

$$V_\gamma = U_\gamma$$

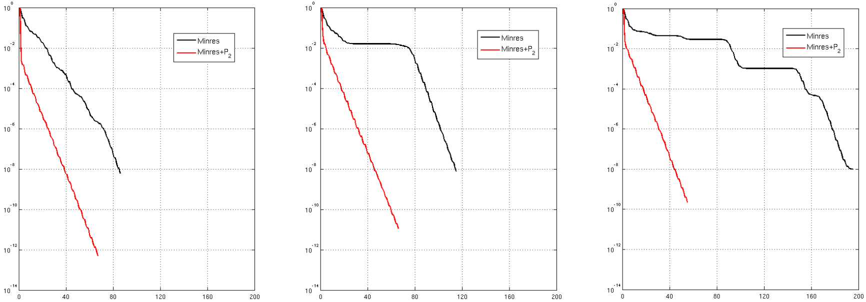
- Eigenvalues versus cosines of principal angles:

$$\text{Key part} = C_\gamma^{-1} \Lambda_\gamma C_\gamma^{-1} + I_5$$

Illustration on a toy example (continued)

$\Lambda_\gamma = \mathrm{diag}(10^{-8}, 10^{-6}, 10^{-4}, 10^{-2}, 10^{-1})$ and $C_\gamma = \mathrm{diag}\{\cos\theta_i\}_{i=1}^{5}$, where:

$$\begin{cases} \cos\theta_1 = 0.3 \\ \cos\theta_2 = 0.3 \\ \cos\theta_3 = 0.3 \\ \cos\theta_4 = 0.3 \\ \cos\theta_5 = 0.3 \end{cases} \qquad \begin{cases} \cos\theta_1 = 0.3 \\ \cos\theta_2 = 10^{-3} \\ \cos\theta_3 = 0.3 \\ \cos\theta_4 = 0.3 \\ \cos\theta_5 = 0.3 \end{cases} \qquad \begin{cases} \cos\theta_1 = 10^{-6} \\ \cos\theta_2 = 10^{-5} \\ \cos\theta_3 = 10^{-4} \\ \cos\theta_4 = 10^{-3} \\ \cos\theta_5 = 0.3 \end{cases}$$



Convergence curves (2-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

Interaction between $\mathcal{I}m(B)$ and $\mathcal{I}m(U_\gamma)$ (continued)

From these observations, we can extrapolate (bet?) that:

The bad conditioning contained in the smallest eigenvalues of A (if any)
will impact and spoil the convergence of MINRES
if (some of) the principal angles between $\mathcal{I}m(B)$
and the associated invariant subspace $\mathcal{I}m(U_\gamma)$, are close to $\pi/2$

because

the key part: $\frac{1}{\alpha} C_\gamma^{-1} (V_\gamma^T A V_\gamma) C_\gamma^{-1} + I_p$ reveals that
the square of the inverse of the cosines of these principal angles
push the corresponding bad conditioning of A
to "show up" in the Schur complement inverse

Short recap

$\Lambda_\gamma = \mathrm{diag}\{\lambda_i \leq \gamma\}_{i=1}^{p}$ and U_γ contains the orthonormal eigenvectors

$$\text{(SLRU)} \quad A_\gamma^{-1} = \frac{1}{\alpha} I_n + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T$$

$$S_\gamma^{-1} = B^T A_\gamma^{-1} B = \alpha (B^T B)^{-\frac{1}{2}} (I_m - \underbrace{K(\tfrac{1}{\alpha}\Lambda_\gamma + K^T K)^{-1} K^T}_{\text{Key part}}) (B^T B)^{-\frac{1}{2}}$$

where $K = (B^T B)^{-\frac{1}{2}} B^T U_\gamma = Q^T U_\gamma$ such that

$$\text{(SVD)} \quad Y^T K Z = \underbrace{Y^T Q^T}_{\substack{\text{Princ. vec.} \\ \text{in } \mathcal{I}m(B)}} \quad \underbrace{U_\gamma Z}_{\substack{\text{Princ. vec.} \\ \text{in } \mathcal{I}m(U_\gamma)}} = \begin{array}{|c|} \hline C_\gamma \\ \hline 0 \\ \hline \end{array}$$

$C_\gamma = \mathrm{diag}\{\cos\theta_i\}_{i=1}^{p}$ $(\{\theta_i\}_{i=1}^{p} \in [0, \pi/2[$ the principal angles$)$

Short recap (continued) and a question

$$S_\gamma^{-1} = \alpha(B^TB)^{-\frac{1}{2}}(I_m - Y_\gamma\underbrace{(\tfrac{1}{\alpha}C_\gamma^{-1}(V_\gamma^T A V_\gamma)C_\gamma^{-1} + I_p)^{-1}}_{\text{Key part}}Y_\gamma^T)(B^TB)^{-\frac{1}{2}}$$

where $V_\gamma = U_\gamma Z$ are the principal vectors in $\mathcal{I}m(U_\gamma)$ and where the smaller the associated cosines are, the "greater" the impact may be

A question:

Among the "available" information (Λ_γ, U_γ, V_γ and C_γ),
which one is the most relevant to accelerate the convergence of MINRES
between
a subset of smallest eigenvalues and their associated eigenvectors and
a subset of smallest cosines and their associated principal vectors in $\mathcal{I}m(U_\gamma)$?

"Smart" selection of principal vectors in $\mathcal{I}m(U_\gamma)$

$$S_\gamma^{-1} = \alpha(B^TB)^{-\frac{1}{2}}(I_m - Y_\gamma(\tfrac{1}{\alpha}C_\gamma^{-1}(V_\gamma^T A V_\gamma)C_\gamma^{-1} + I_p)^{-1}Y_\gamma^T)(B^TB)^{-\frac{1}{2}}$$

Select the principal vectors $V_\gamma = U_\gamma Z$ whose associated principal angles satisfy (let ℓ be the number of such vectors):

$$\cos^2\theta_i \le c\,\frac{\gamma}{\alpha}, \qquad c \in \left[\frac{1}{4}, 4\right]$$

i.e., select the appropriate columns in Z (yielding $Z_\theta \in \mathbb{R}^{p\times\ell}$), and "restrict" S_γ^{-1} accordingly:

$$S_\theta^{-1} = \alpha(B^TB)^{-\frac{1}{2}}(I_m - Y_\theta(\tfrac{1}{\alpha}C_\theta^{-1}(V_\theta^T A V_\theta)C_\theta^{-1} + I_\ell)^{-1}Y_\theta^T)(B^TB)^{-\frac{1}{2}}$$

where $V_\theta = U_\gamma Z_\theta \in \mathbb{R}^{n\times\ell}$, $C_\theta \in \mathbb{R}^{\ell\times\ell}$ and $Y_\theta \in \mathbb{R}^{m\times\ell}$

A "smarter" $\mathcal{P}_2$

In practice, this amounts to use the preconditioner:

$$\mathcal{P}_\theta = \begin{bmatrix} A_\theta & 0 \\ 0 & S_\theta \end{bmatrix}$$

where

$$A_\theta^{-1} = \frac{1}{\alpha} I_n + V_\theta (V_\theta^T A V_\theta)^{-1} V_\theta^T$$

$$S_\theta^{-1} = \alpha (B^T B)^{-\frac{1}{2}} \left(I_m - K_\theta \left(\frac{1}{\alpha} V_\theta^T A V_\theta + K_\theta^T K_\theta\right)^{-1} K_\theta^T \right) (B^T B)^{-\frac{1}{2}}$$

with $K_\theta = (B^T B)^{-\frac{1}{2}} B^T V_\theta$

$\mathcal{P}_2$ versus $\mathcal{P}_\theta$

$$\mathcal{P}_2 = \begin{bmatrix} A_\gamma & 0 \\ 0 & S_\gamma \end{bmatrix} \qquad \mathcal{P}_\theta = \begin{bmatrix} A_\theta & 0 \\ 0 & S_\theta \end{bmatrix}$$

with

$$A_\gamma^{-1} = \frac{1}{\alpha} I_n + U_\gamma \Lambda_\gamma^{-1} U_\gamma^T$$

$$S_\gamma^{-1} = \alpha (B^T B)^{-\frac{1}{2}} \left(I_m - K(\tfrac{1}{\alpha}\Lambda_\gamma + K^T K)^{-1} K^T \right) (B^T B)^{-\frac{1}{2}}$$

$$K = (B^T B)^{-\frac{1}{2}} B^T U_\gamma$$

$$A_\theta^{-1} = \frac{1}{\alpha} I_n + V_\theta (V_\theta^T A V_\theta)^{-1} V_\theta^T$$

$$S_\theta^{-1} = \alpha (B^T B)^{-\frac{1}{2}} \left(I_m - K_\theta(\tfrac{1}{\alpha} V_\theta^T A V_\theta + K_\theta^T K_\theta)^{-1} K_\theta^T \right) (B^T B)^{-\frac{1}{2}}$$

$$K_\theta = (B^T B)^{-\frac{1}{2}} B^T V_\theta$$

$\mathcal{P}_2$ versus $\mathcal{P}_\theta$ on our example

- $\gamma = \frac{\lambda_{max}(A)}{100} \approx 3.8\ 10^{-2}$ $\longrightarrow$ $p = 42$
- $\cos^2\theta_i \leq 4\,\frac{\gamma}{\alpha}$ $(c = 4)$ $\longrightarrow$ $\ell = 22$

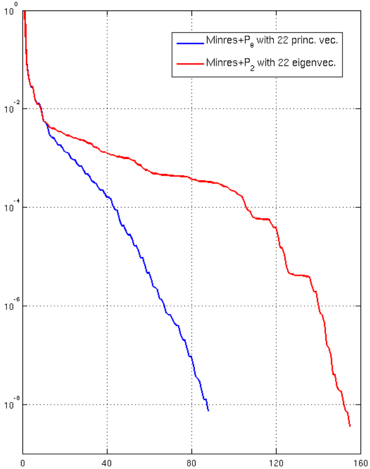
Comparison on Minres preconditioned by:

$\mathcal{P}_2$ built with $\ell = 22$ eigenvectors
corresponding to the ℓ smallest eigenvalues λ_i's
(among the p ones below γ)

versus

$\mathcal{P}_\theta$ built with $\ell = 22$ principal vectors
corresponding to the ℓ smallest $\cos\theta_i$'s
(among the p ones)

MINRES preconditioned using $\mathcal{P}_2$ versus $\mathcal{P}_\theta$ ($\ell = 22$)



Convergence curves ($\mathcal{P}_\theta^{-1}$-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

MINRES preconditioned using $\mathcal{P}_2$ versus $\mathcal{P}_\theta$ (for various ℓ)

Comparison on Minres preconditioned by:

$\mathcal{P}_2$ built with ℓ eigenvectors
corresponding to the ℓ smallest eigenvalues λ_i's
(among the p ones below γ)

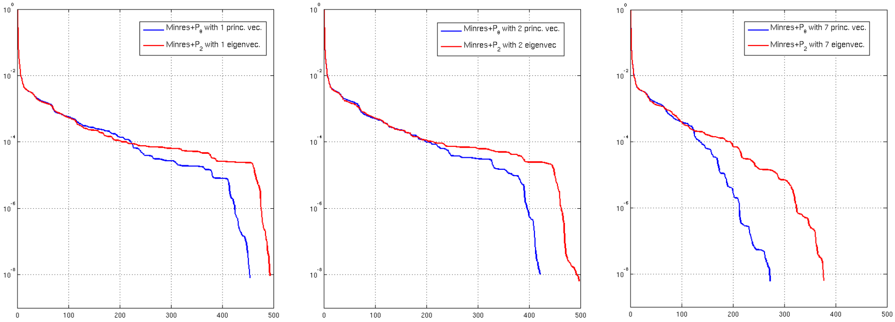
versus

$\mathcal{P}_\theta$ built with ℓ principal vectors
corresponding to the ℓ smallest $\cos\theta_i$'s
(among the p ones)

where

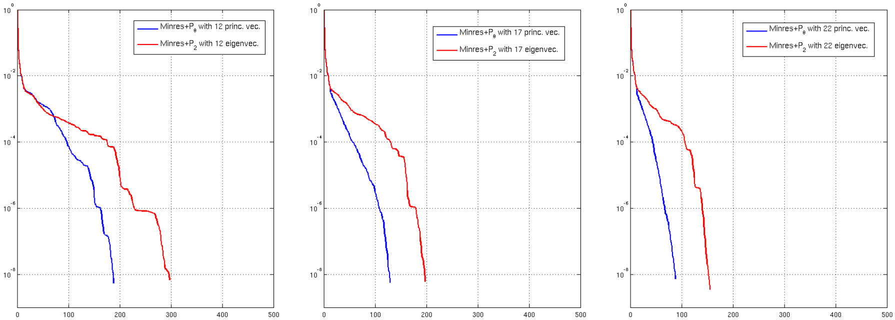
$$\ell = 1, 2, 7, 12, 17, 22, 27, 32, 37, 42$$

MINRES preconditioned using $\mathcal{P}_2$ versus $\mathcal{P}_\theta$ (for $\ell = 1, 2, 7$)



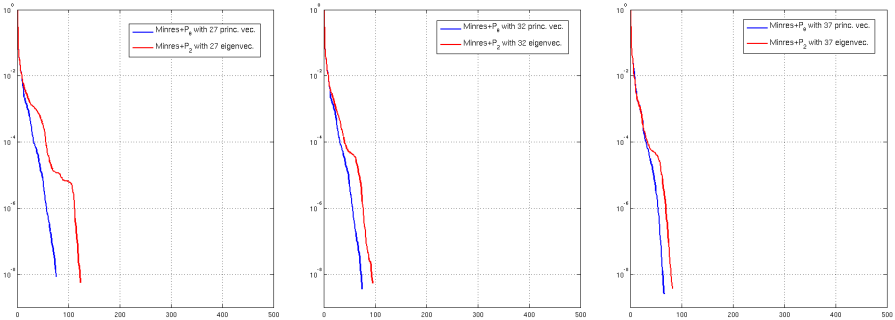
Convergence curves ($\mathcal{P}_\theta^{-1}$-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

MINRES preconditioned using $\mathcal{P}_2$ versus $\mathcal{P}_\theta$ (for $\ell = 12, 17, 22$)



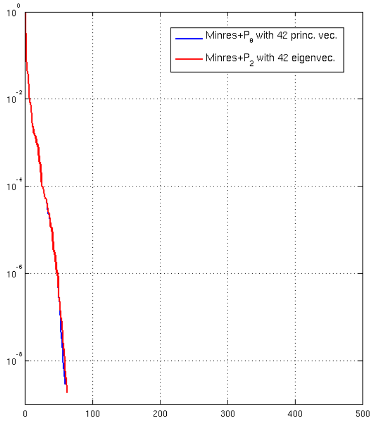
Convergence curves ($\mathcal{P}_\theta^{-1}$-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

MINRES preconditioned using $\mathcal{P}_2$ versus $\mathcal{P}_\theta$ (for $\ell = 27, 32, 37$)



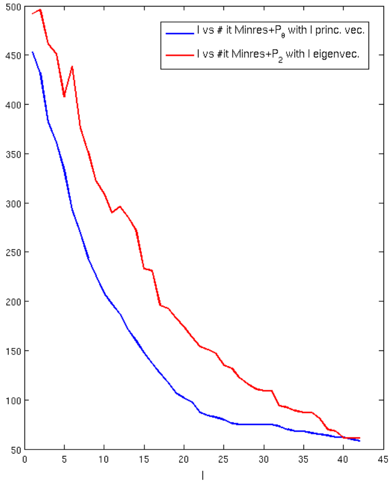
Convergence curves ($\mathcal{P}_\theta^{-1}$-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

MINRES preconditioned using $\mathcal{P}_2$ versus $\mathcal{P}_\theta$ (for $\ell = 42$)

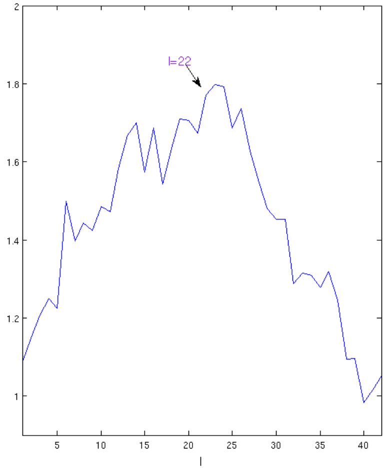


Convergence curves ($\mathcal{P}_\theta^{-1}$-norm and $\mathcal{P}_2^{-1}$-norm of relative residuals)

MINRES preconditioned using $\mathcal{P}_2$ versus $\mathcal{P}_\theta$ (overall picture)



ℓ versus # MINRES it.



ℓ versus $\dfrac{\#\text{MINRES } +\mathcal{P}_2 \text{ it.}}{\#\text{MINRES } +\mathcal{P}_\theta \text{ it.}}$

Conclusion

- Address the (bad) conditioning of A and that of B separately

  $\rightarrow$ Using a low-rank spectral approximation

- Recombine this spectral information appropriately to build an efficient block diagonal preconditioner

  $\rightarrow$ Through the Schur complement approximation

- Get some insight on the recombination issue between A and B

  $\rightarrow$ Through some analytic dissection ☺ and illustrations

Perspectives

- Look deeper into the recombination issue
- Use a similar spectral approach to address the bad conditioning of B
- Analyse the cost and the amortization (multiple r.h.s.)
- Derive practical and efficient implementations
- Perform numerical experiments on academic problems and applications

Thank you for your attention!

Construction of $\tilde{S}_\gamma^{-1}$

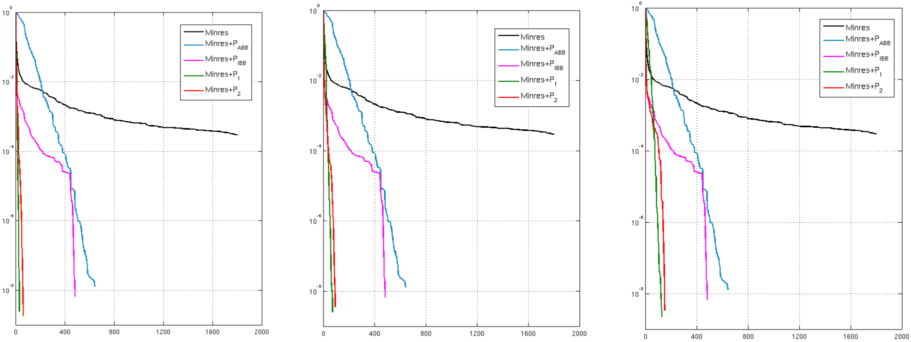
How to deal with $\begin{bmatrix} M & B \\ B^T & 0 \end{bmatrix}$?

1. Using Schilders' factorization, see Dollar and Wathen (2006)

2. Using a preconditioner of the form $\begin{bmatrix} D^{-1} & 0 \\ 0 & (B^T D^{-1} B)^{-1} \end{bmatrix}$ where D is diagonal, see Golub, Greif and Varah (2006)

3. Using a similar spectral approach on $B^T M^{-1} B$. How can we include efficiently spectral information in the Schur complement? $\Rightarrow$ We work on it !

MINRES for $\gamma = \frac{\lambda_{max}(A)}{100}$, $\gamma = \frac{\lambda_{max}(A)}{1000}$ and $\gamma = \frac{\lambda_{max}(A)}{10000}$



Convergence curves ($\mathcal{P}^{-1}$-norm of relative residuals)

Spectrum of $\mathcal{P}_{IBB}$ and $\mathcal{P}_{ABB}$