Spectral analysis of saddle point matrices with indefinite leading blocks

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Joint work with Nick Gould, RAL

The problem

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

- Computational Fluid Dynamics (Elman, Silvester, Wathen 2005)
- Elasticity problems
- Mixed (FE) formulations of II and IV order elliptic PDEs
- Linearly Constrained Programs
- Linear Regression in Statistics
- Image restoration
- ... Survey: Benzi, Golub and Liesen, Acta Num 2005

The problem

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Hypotheses:

- $\star$ $A \in \mathbb{R}^{n \times n}$ symmetric
- $\star$ $B^T \in \mathbb{R}^{n \times m}$ tall, $m \leq n$
- $\star$ C symmetric positive (semi)definite

More hypotheses later...

Why are we interested in spectral bounds?

- To detect “sensitive” blocks in the coeff. matrix

  (guidelines for preconditioning strategies)

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- To "tune" the stabilization parameter (matrix C)

- To predict convergence behavior of the iterative solver

Iterative solver. Convergence considerations.

$$\mathcal{M}x = b$$

$\mathcal{M}$ is symmetric and indefinite $\quad \longrightarrow \quad$ MINRES

$$x_k \in x_0 + K_k(\mathcal{M}, r_0), \quad \text{s.t.} \qquad \min \|b - \mathcal{M}x_k\|$$

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If $\mu(\mathcal{M}) \subset [-a, -b] \cup [c, d]$, with $|b - a| = |d - c|$, then

$$\|b - \mathcal{M}x_{2k}\| \leq 2 \left(\frac{\sqrt{ad} - \sqrt{bc}}{\sqrt{ad} + \sqrt{bc}} \right)^k \|b - \mathcal{M}x_0\|$$

Note: more general but less tractable bounds available

Well-exercised spectral properties

$$\mathcal{M} = \begin{bmatrix} A & B^T \\ B & O \end{bmatrix} \qquad \begin{array}{ll} 0 < \lambda_n \le \cdots \le \lambda_1 & \text{eigs of } A \\ 0 < \sigma_m \le \cdots \le \sigma_1 & \text{sing. vals of } B \end{array}$$

$\mu(\mathcal{M})$ subset of (Rusten & Winther 1992)

$$\left[\frac{1}{2}(\lambda_n - \sqrt{\lambda_n^2 + 4\sigma_1^2}), \frac{1}{2}(\lambda_1 - \sqrt{\lambda_1^2 + 4\sigma_m^2})\right] \quad \cup \quad \left[\lambda_n, \frac{1}{2}(\lambda_1 + \sqrt{\lambda_1^2 + 4\sigma_1^2})\right]$$

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A positive definite

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A semidefinite but $\frac{u^TAu}{u^Tu} > \alpha_0 > 0$, $u \in \text{Ker}(B)$ Perugia & S., '00

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B full rank

Well-exercised spectral properties

$$\mathcal{M} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \qquad \begin{array}{ll} 0 < \lambda_n \leq \cdots \leq \lambda_1 & \text{eigs of } A \\ 0 = \sigma_m \leq \cdots \leq \sigma_1 & \text{sing. vals of } B \end{array}$$

$\mu(\mathcal{M})$ subset of (Silvester & Wathen 1994)

$$\left[\frac{1}{2}(-\gamma_1 + \lambda_n - \sqrt{(\gamma_1 + \lambda_n)^2 + 4\sigma_1^2})\ , \frac{1}{2}(\lambda_1 - \sqrt{\lambda_1^2 + 4\theta})\right] \cup \left[\lambda_n, \frac{1}{2}(\lambda_1 + \sqrt{\lambda_1^2 + 4\sigma_1^2})\right]$$

B rank deficient, but $\theta = \lambda_{\min}(BB^T + C)$ full rank

$\gamma_1 = \lambda_{\max}(C)$

Spectral properties. Interpretation.

$$\mathcal{M} = \begin{bmatrix} A & B^T \\ B & O \end{bmatrix} \qquad \begin{array}{ll} 0 < \lambda_n \leq \cdots \leq \lambda_1 & \text{eigs of } A \\ 0 < \sigma_m \leq \cdots \leq \sigma_1 & \text{sing. vals of } B \end{array}$$

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Good (= slim) spectrum: $\lambda_1 \approx \lambda_n, \quad \sigma_1 \approx \sigma_m$

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e.g.

$$\mathcal{M} = \begin{bmatrix} I & U^T \\ U & O \end{bmatrix}, \quad UU^T = I$$

Block diagonal Preconditioner

⋆ A spd, $C = 0$:

$$\mathcal{P}_0 = \begin{bmatrix} A & 0 \\ 0 & BA^{-1}B^T \end{bmatrix}$$

$$\Rightarrow \qquad \mathcal{P}_0^{-\frac{1}{2}} \mathcal{M} \mathcal{P}_0^{-\frac{1}{2}} = \begin{bmatrix} I & A^{-\frac{1}{2}} B^T (BA^{-1}B^T)^{-\frac{1}{2}} \\ (BA^{-1}B^T)^{-\frac{1}{2}} BA^{-\frac{1}{2}} & 0 \end{bmatrix}$$

MINRES converges in at most 3 iterations. $\mu(\mathcal{P}_0^{-\frac{1}{2}} \mathcal{M} \mathcal{P}_0^{-\frac{1}{2}}) = \{1, 1/2 \pm \sqrt{5}/2\}$

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A more practical choice:

$$\mathcal{P} = \begin{bmatrix} \widetilde{A} & 0 \\ 0 & \widetilde{S} \end{bmatrix} \qquad \text{spd.} \quad \widetilde{A} \approx A \qquad \widetilde{S} \approx BA^{-1}B^T$$

eigs in $\quad [-a, -b] \cup [c, d], \qquad a, b, c, d > 0$

Still an Indefinite Problem, but possibly much easier to solve

Indefinite A

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

$\lambda_n \le \cdots \le \lambda_1$	eigs of A
$0 < \sigma_m \le \cdots \le \sigma_1$	sing. vals of B
A pos.def. on $\mathrm{Ker}(B)$	

$\sigma(\mathcal{M})$ subset of

$$\left[\frac{1}{2}(\lambda_n - \sqrt{\lambda_n^2 + 4\sigma_1^2}), \frac{1}{2}(\lambda_1 - \sqrt{\lambda_1^2 + 4\sigma_m^2})\right] \quad \cup \quad \left[\Gamma, \frac{1}{2}(\lambda_1 + \sqrt{\lambda_1^2 + 4\sigma_1^2})\right]$$

If $m = n$, $\quad \Gamma = \frac{1}{2}(\lambda_n + \sqrt{\lambda_n^2 + 4\sigma_m^2})$

Indefinite A, $C = 0$. Cont'd

$$\left[\frac{1}{2}(\lambda_n - \sqrt{\lambda_n^2 + 4\sigma_1^2}), \frac{1}{2}(\lambda_1 - \sqrt{\lambda_1^2 + 4\sigma_m^2})\right] \quad \cup \quad \left[\Gamma, \frac{1}{2}(\lambda_1 + \sqrt{\lambda_1^2 + 4\sigma_1^2})\right]$$

Letting $\alpha_0 > 0$ be s.t. $\frac{u^T A u}{u^T u} > \alpha_0$, $u \in$ Ker(B)

$$\Gamma \geq \begin{cases} \dfrac{\alpha_0 \sigma_m^2}{|\alpha_0 \lambda_n - \|A\|^2 - \sigma_m^2|} & \text{if } \alpha_0 + \lambda_n \leq 0 \\ \\ \dfrac{\alpha_0 \lambda_n - \|A\|^2 - \sigma_m^2}{2(\alpha_0 + \lambda_n)} + \sqrt{\left(\dfrac{\alpha_0 \lambda_n - \|A\|^2 - \sigma_m^2}{2(\alpha_0 + \lambda_n)}\right)^2 + \dfrac{\alpha_0 \sigma_m^2}{\alpha_0 + \lambda_n}} & \\ & \text{otherwise.} \end{cases}$$

Sharpness of the bounds

Ex.1. $A = \begin{bmatrix} 1 & -3 \\ -3 & 2 \end{bmatrix}$, $B^T = \begin{bmatrix} 0 \\ 0.1 \end{bmatrix}$ $\mu(\mathcal{M}) = \{-1.5441, 0.0014257, 4.5427\}$

Ex.2. $A = \begin{bmatrix} 0.01 & 3 \\ 3 & -0.01 \end{bmatrix}$, $B = [0,\ 3]$ $\mu(\mathcal{M}) = \{-4.2452, 5.0 \cdot 10^{-3}, 4.2402\}$

Ex.3. $A = \begin{bmatrix} 1 & -4 & 0 \\ -4 & -1 & 0 \\ 0 & 0 & 2 \end{bmatrix}$, $B^T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}$, $\mu(\mathcal{M}) =$ $\{-4.3528, \quad -0.22974, \quad 0.22974, \quad 2, \quad 4.3528\}$

case	λ_n	λ_1	α_0	σ_m, σ_1	$\mathcal{I}^-$	$\mathcal{I}^+$
Ex.1	-1.5414	4.5414	1.0	0.1	[-1.5478, -0.0022]	[0.0004, 4.5436]
Ex.2	-3.0000	3.0000	0.01	3	[-4.8541, -1.8541]	[$4.9917 \cdot 10^{-3}$, 4.8541]
Ex.3	-4.1231	4.1231	2.0	1	[-4.3528, -0.22974]	[0.0762, 4.3528]

Augmenting the (1,1) block

Equivalent formulation ($C = 0$):

$$\begin{bmatrix} A + \tau B^T B & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} a + \tau B^T b \\ b \end{bmatrix}, \quad \tau \in \mathbb{R}$$

coefficient matrix: $\mathcal{M}(\tau)$

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Condition on τ for definiteness of $A + \tau B^T B$:

$$\tau > \frac{1}{\sigma_m^2} \left(\frac{\|A\|^2}{\alpha_0} - \lambda_n \right)$$

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$\frac{1}{\sigma_m^2} \left(\frac{\|A\|^2}{\alpha_0} - \lambda_n \right) = 100.33$

for $\tau = 100 \rightarrow A + \tau B^T B$ is indefinite

Augmenting the (1,1) block

Assume "good" τ is taken.

$$\begin{bmatrix} A + \tau B^T B & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} a + \tau B^T b \\ b \end{bmatrix}, \quad \tau \in \mathbb{R}$$

Spectral intervals for (1,1) spd may be obtained

“Stabilized” problem

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} a + \tau B^T b \\ b \end{bmatrix}, \qquad \tau \in \mathbb{R}$$

Coefficient matrix: $\mathcal{M}_C$

Warning: for A indefinite, conditions on C required:

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \qquad \text{singular!}$$

Note: Perturbation results yield spectral bounds assuming $\lambda_{\max}^C < \Gamma$

“Stabilized” problem

More accurate result:

If $\lambda_{\max}^{C} < \frac{\alpha_0 \sigma_m^2}{\|A\|^2 - \lambda_n \alpha_0}$, then $\mu(\mathcal{M}_C) \subset \mathcal{I}^- \cup \mathcal{I}^+$ with

$$\mathcal{I}^- = \left[\frac{1}{2}\left(\lambda_n - \lambda_{\max}^C - \sqrt{(\lambda_n + \lambda_{\max}^C)^2 + 4\sigma_1^2}\right), \frac{1}{2}\left(\lambda_1 - \sqrt{(\lambda_1)^2 + 4\sigma_m^2}\right)\right] \subset \mathbb{R}^-$$

$$\mathcal{I}^+ = \left[\Gamma_C, \frac{1}{2}\left(\lambda_1 + \sqrt{(\lambda_1)^2 + 4\sigma_1^2}\right)\right] \subset \mathbb{R}^+,$$

For $m = n$, $\quad \Gamma_C = \frac{1}{2}\left(\lambda_n - \lambda_{\max}^C + \sqrt{(\lambda_n + \lambda_{\max}^C)^2 + 4\sigma_m^2}\right)$

more complicated (but explicit!) estimate for $m < n$

“Stabilized” problem

An example:

$$\mathcal{M}_C = \begin{bmatrix} \lambda_n & 0 & \sigma \\ 0 & \lambda_1 & 0 \\ \sigma & 0 & -\gamma^C \end{bmatrix},$$

with $\lambda_n < 0, \lambda_1 > 0, \sigma > 0$. If $\gamma^C = -\sigma^2/\lambda_n$ then $\mathcal{M}_C$ is singular.

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Our estimate requires: $0 \le \gamma^C \le \frac{1}{2} \; \frac{-\sigma^2}{\lambda_n}$

(half the value from singularity!)

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Related result: Bai, Ng, Wang (tech.rep.2008) qualitatively similar bound based on $B^T C^{-1} B$, $A + B^T C^{-1} B$
(no full rank assumption on B)

Full rank assumption of B

In some optimization problems:

$$B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} C_1 & 0 \\ 0 & 0 \end{bmatrix},$$

with positive definite C_1

Natural assumption: $A + B_1^T C_1^{-1} B_1$ definite on the null space of the full-rank B_2. In this case,

$$\mathcal{M}_C = \begin{bmatrix} \begin{pmatrix} A & B_1^T \\ B_1 & -C_1 \end{pmatrix} & \begin{pmatrix} B_2^T \\ 0 \end{pmatrix} \\ \begin{pmatrix} B_2 & 0 \end{pmatrix} & 0 \end{bmatrix}.$$

Spectral analysis: Use Bai, Ng, Wang result to get spectral intervals for the "(1,1)" block, and then apply our bounds for $\mathcal{M}_C$

Application to ideal block diagonal preconditioners

Indefinite preconditioner, $C = 0$:

1. Let $\mathcal{P}_+ = \mathrm{blkdiag}(A, BA^{-1}B^T)$. Then

$$\mu(\mathcal{P}_+^{-1}\mathcal{M}) \subset \left\{1, \frac{1}{2}(1+\sqrt{5}), \frac{1}{2}(1-\sqrt{5})\right\} \subset \mathbb{R};$$

2. Let $\mathcal{P}_- = \mathrm{blkdiag}(A, -BA^{-1}B^T)$. Then

$$\mu(\mathcal{P}_-^{-1}\mathcal{M}) \subset \left\{1, \frac{1}{2}(1+i\sqrt{3}), \frac{1}{2}(1-i\sqrt{3})\right\} \subset \mathbb{C}^+.$$

Application to **practical** block diagonal preconditioners

Indefinite preconditioner, $C = 0$:

Let $\mathcal{P}_\pm = \mathrm{blkdiag}(A, \pm\widetilde{S})$ with A, $\widetilde{S}$ nonsingular. Then

$$\mu(\mathcal{P}_\pm^{-1}\mathcal{M}) \subset \left\{1, \frac{1}{2}(1+\sqrt{1+4\xi}), \frac{1}{2}(1-\sqrt{1+4\xi})\right\} \subset \mathbb{C},$$

ξ : (possibly complex) eigenvalues of $(BA^{-1}B^T, \pm\widetilde{S})$

Application to ideal block diagonal preconditioners

Indefinite preconditioner, $C \neq 0$:

Let $\mathcal{P}_+ = \mathrm{blkdiag}(A, C + BA^{-1}B^T)$. Then

$$\mu(\mathcal{P}_+^{-1}\mathcal{M}) \subset \left\{1, \frac{1}{2}(1 \pm \sqrt{5}), \frac{1}{2\theta}(\theta - 1 \pm \sqrt{(1-\theta)^2 + 4\theta^2})\right\} \subset \mathbb{R}.$$

θ finite eigs of $(C + BA^{-1}B^T, C)$

Similar results for $\mathcal{P}_- = \mathrm{blkdiag}(A, -C - BA^{-1}B^T)$

Application to ideal block diagonal preconditioners

Definite preconditioner, $C = 0$:

$$\mathcal{P}(\tau) = \begin{bmatrix} P_A & \\ & P_C \end{bmatrix}, \qquad \begin{array}{l} P_A \approx P_A(\tau) = A + \tau B^T B \\ P_C \approx P_C(\tau) = B(A + \tau B^T B)^{-1} B^T \end{array}$$

- Definite preconditioner on definite problem:

$\mathcal{P}(\tau)^{-1}\mathcal{M}(\tau)$ has eigenvalues

$$1,\ \tfrac{1}{2}(1+\sqrt{5}),\ \tfrac{1}{2}(1-\sqrt{5})$$

with multiplicity $n-m$, m and m, respectively.

Application to ideal block diagonal preconditioners

• Definite preconditioner on indefinite (original) problem:

Suppose that $B(Y\ Z) = (L\ 0)$ is of full rank and that $Z^T AZ$ and $P_A(\tau)$ are positive definite. Then $\mathcal{P}(\tau)^{-1}\mathcal{M}$ has eigenvalues

$i)$ 1, of multiplicity $n - m + Nullity(A)$;

$ii)$ -1, of multiplicity $Nullity(A)$;

$iii)$ $(\mu_i \pm \sqrt{\mu_i^2 + 4})/2$, $i = 1, \dots, m - Nullity(A)$, where $\mu_i = \omega_i/(\omega_i + \tau)$ and ω_i are the eigenvalues of $L^{-T}(Y^T AY - Y^T AZ(Z^T AZ)^{-1} Z^T AY)L^{-1}$

(cf. also Golub, Greif, Varah '06)

Note: as τ increases the eigenvalues of $\mathcal{P}(\tau)^{-1}\mathcal{M}$ cluster around the two values ± 1.

Spectral intervals for $\mathcal{P}(\tau)^{-1}\mathcal{M}$ using the new bounds

Final considerations and outlook

- Sharp bounds obtained for indefinite (1,1) block
- Estimates also for the Augmented formulation
- Spectral bounds for ideal block diagonal preconditioners

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- Sharp bounds obtained for indefinite (1,1) block
- Estimates also for the Augmented formulation
- Spectral bounds for ideal block diagonal preconditioners
- Future work: exploit this knowledge to devise and analyze effective preconditioners