Acquired clustering properties of certain saddle point systems and applications

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The problem

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \qquad \mathcal{M}x = b$$

- 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 and registration
- ... Survey: Benzi, Golub and Liesen, Acta Num 2005

The problem

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \qquad \mathcal{M}x = b$$

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 on specific problems...

Outline

- Approximating the Schur complement
- Facing a spectral difficulty
- Fix during the iterative solve
- Application to
  - A Stokes type problem
  - A PDE-constrained problem

Iterative solver. Convergence considerations.

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

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

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

$r_k = b - \mathcal{M}x_k$, $k = 0, 1, \ldots$, x_0 starting guess

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

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

Note: more general but less tractable bounds available

Spectral properties

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

$\mathrm{spec}(\mathcal{M})$ 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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$\mathrm{spec}(\mathcal{M})$ 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

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

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

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

some extremes still valid for $\lambda_n = 0$

Block diagonal Preconditioner

⋆ A nonsing., $C = 0$:

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

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

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

A more practical choice:

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

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

Approximating the Schur complement

$$\widetilde{S} \approx BA^{-1}B^T$$

$\widetilde{S}$ optimal[a] approximation when spec$(BA^{-1}B^T\widetilde{S}^{-1})$ well clustered

Typical choices for $\widetilde{S}$:

- Incomplete Cholesky fact. of $BA^{-1}B^T$
- Algebraic/Geometric Multigrid method
- Operator-based approximation
- ...

[a] With some abuse of language

A quasi-optimal approximate Schur complement

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For certain operators, the approximate Schur complement $\widetilde{S}$ is quasi-optimal:

spec($BA^{-1}B^T\widetilde{S}^{-1}$) well clustered except for few eigenvalues

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Possibly: well clustered eigs are mesh-independent

Questions

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- Do these spectral properties influence the convergence of MINRES on $\mathcal{M}\mathcal{P}^{-1}$?

- Can we eliminate this influence?

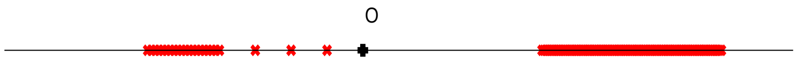
All answers in the affirmative...

The role of $\widetilde{S}$

Claim:

The presence of outliers in $BA^{-1}B^T\widetilde{S}^{-1}$ is accurately inherited by the preconditioned matrix $\mathcal{M}\mathcal{P}^{-1}$

spec($BA^{-1}B^T\widetilde{S}^{-1}$)



spec($\mathcal{M}\mathcal{P}^{-1}$)

Spectral intervals of preconditioned problem

spec$(A\widetilde{A}^{-1})$: $\quad 0 < \gamma_1 \leq \cdots \leq \gamma_n$

spec$(BA^{-1}B^T\widetilde{S}^{-1})$: $\quad 0 < \mu_1 \leq \cdots \leq \mu_m$

Assume that for some $\ell \ll m$:

$$0 < \mu_1 \leq \cdots \leq \mu_\ell \ \leq \ \ \varepsilon_0 \ \ \ll \ \ c_0 \ \ < \mu_{\ell+1} \leq \cdots \leq \mu_m$$

for some ε_0, c_0.

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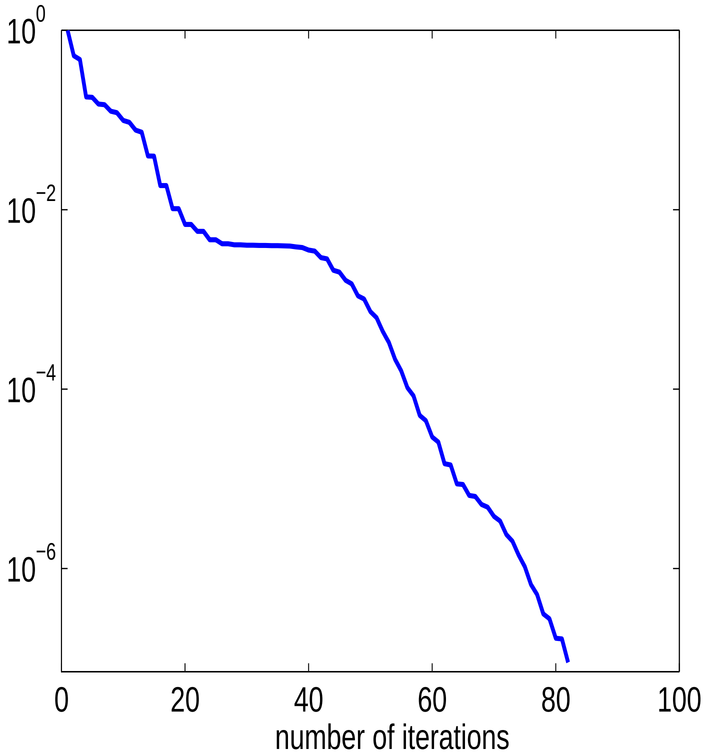
for some ε_0, c_0. Then $\mathrm{spec}(\mathcal{MP}^{-1})$ is contained in:

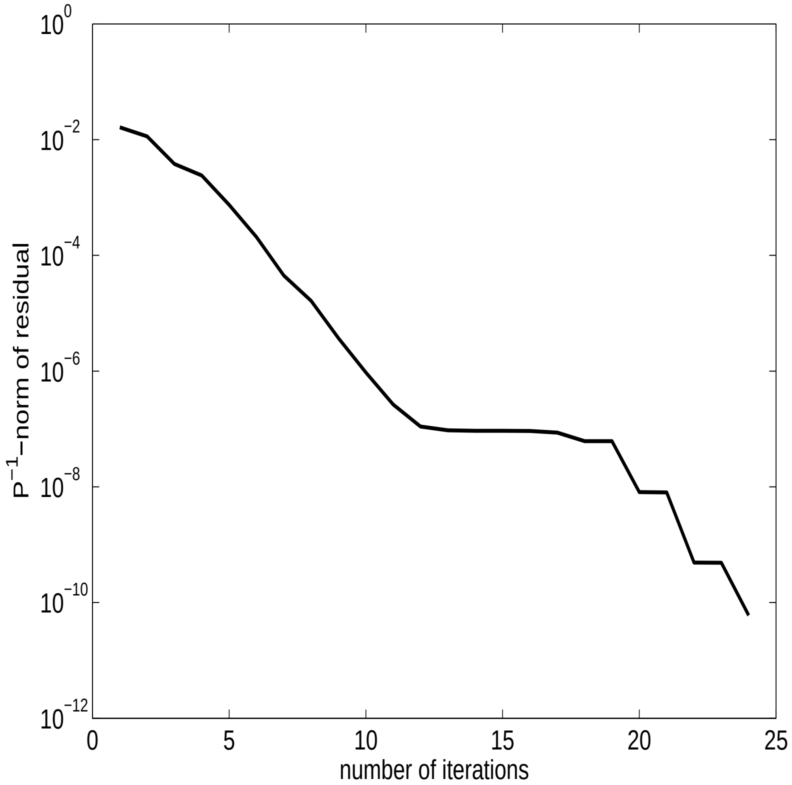
$$\left[\frac{1}{2}\left(\gamma_1 - \sqrt{\gamma_1^2 + 4\gamma_n\mu_m}\right), \frac{1}{2}\left(\gamma_n - \sqrt{\gamma_n^2 + 4\gamma_1\mu_{\ell+1}}\right) + \sqrt{\varepsilon_0\gamma_n}\right]$$

$$\bigcup \left[\gamma_1, \frac{1}{2}\left(\gamma_n + \sqrt{\gamma_n^2 + 4\gamma_n\mu_m}\right)\right] \bigcup \underbrace{\left[-\sqrt{\varepsilon_0\gamma_n},\; \gamma_n - \sqrt{\gamma_n^2 + 4\gamma_1\mu_1}\right]}_{I_\varepsilon}$$

For sufficiently small ε_0 at most ℓ eigenvalues of $\mathcal{MP}^{-1}$ are in I_ε

Effect on MINRES convergence





Stokes-type problem

Monge-Kantorovich problem

Eliminating the stagnation phase: “Deflated” MINRES

Consider $\underbrace{L^{-1}\mathcal{M}L^{-T}}_{\widehat{\mathcal{M}}}\hat{u} = \hat{b}, \quad \mathcal{P} = LL^T$

Let Y be an approximate eigenbasis of $\widehat{\mathcal{M}}$.

* Approximation space: Augmented Lanczos sequence

$$v_{j+1} \perp \mathrm{span}\{Y, v_1, v_2, ..., v_j\}, \qquad \|v_{j+1}\| = 1$$

obtained by standard Lanczos method with coeff.matrix

$$\mathcal{G} := \widehat{\mathcal{M}} - \widehat{\mathcal{M}}Y(Y^T\widehat{\mathcal{M}}Y)^{-1}Y^T\widehat{\mathcal{M}}, \qquad \text{giving} \quad K_j(\widehat{\mathcal{M}}, Y, v_1)$$

* MINimal RESidual method:

$$r_j = \hat{b} - \widehat{\mathcal{M}}\hat{u}_j \;\perp\; \mathcal{G}K_j(\widehat{\mathcal{M}}, Y, v_1)$$

$\Rightarrow$ $\hat{u}_j$ obtained with a short-term recurrence

Augmented MINRES ("Stanford" style)

Given $\mathcal{M}, b$, maxit, tol, $\mathcal{P}$, and Y with orthonormal columns

$\mathbf{u} = \mathbf{Y}(\mathbf{Y^T}\mathcal{M}\mathbf{Y})^{-\mathbf{1}}\mathbf{Y^T}\mathbf{b}$ starting approx, $\ r = b - \mathcal{M}u, \ \ r_1 = r, \ \ y = \mathcal{P}^{-1}r$, etc

while ($i <$ maxit)

$i = i + 1 \qquad v = y/\beta;$

$\mathbf{y} = \mathcal{M}\mathbf{v} - \mathcal{M}\mathbf{Y}(\mathbf{Y^T}\mathcal{M}\mathbf{Y})^{-\mathbf{1}}\mathbf{Y^T}\mathcal{M}\mathbf{v}$

if $i \geq 2$, $y = y - (\beta/\beta_0)r_1$

$\alpha = v^T y, \qquad y = y - r_2\alpha/\beta$

$r_1 = r_2, \qquad r_2 = y$

$y = \mathcal{P}^{-1}r_2$

$\beta_0 = \beta, \qquad \beta = \sqrt{r_2^T y}$

$e_0 = e, \qquad \delta = c\bar{d} + s\alpha \qquad \bar{g} = s\bar{d} - c\alpha \qquad e = s\beta \qquad \bar{d} = -c\beta$

$\gamma = \|[\bar{g}, \beta]\| \qquad c = \bar{g}/\gamma, \qquad s = \beta/\gamma, \qquad \phi = c\bar{\phi}, \qquad \bar{\phi} = s\bar{\phi}$

$w_1 = w_2, \qquad w_2 = w$

$w = (v - e_0 w_1 - \delta w_2)\gamma^{-1}$

$\mathbf{g} = \mathbf{Y}(\mathbf{Y^T}\mathcal{M}\mathbf{Y})^{-\mathbf{1}}\mathbf{Y^T}\mathcal{M}\mathbf{w}\boldsymbol{\phi}$

$u = u - \mathbf{g} + \phi w$

$\zeta = \chi_1/\gamma, \qquad \chi_1 = \chi_2 - \delta z, \qquad \chi_2 = -e\zeta$

Check preconditioned residual norm ($\bar{\phi}$) for convergence

end

Stokes type problem with variable viscosity in $\Omega \subset \mathbb{R}^d$

$$
\begin{aligned}
-\mathbf{div}\nu(\mathbf{x})\mathbf{Du} + \nabla p = \mathbf{f} \quad & \text{in} \quad \Omega, \\
-\operatorname{div} \mathbf{u} = 0 \quad & \text{in} \quad \Omega, \\
\mathbf{u} = 0 \quad & \text{on} \quad \partial\Omega,
\end{aligned}
$$

with $0 < \nu_{\min} \leq \nu(\mathbf{x}) \leq \nu_{\max} < \infty$. (Here, $\nu(\mathbf{x}) = 2\mu + \frac{\tau_s}{\sqrt{\varepsilon^2 + |\mathbf{Du}(\mathbf{x})|^2}}$)

$\mathbf{u}$: velocity vector field $\qquad$ p : pressure

$\mathbf{Du} = \frac{1}{2}(\nabla\mathbf{u} + \nabla^T\mathbf{u})$ rate of deformation tensor;

Prec. S: pressure mass matrix wrto weighted product $(\nu^{-1}\cdot, \cdot)_{L^2(\Omega)}$

Experiments with Bercovier-Engelman model of the Bingham viscoplastic fluid

* One zero pressure mode (eigvec easy to approx)

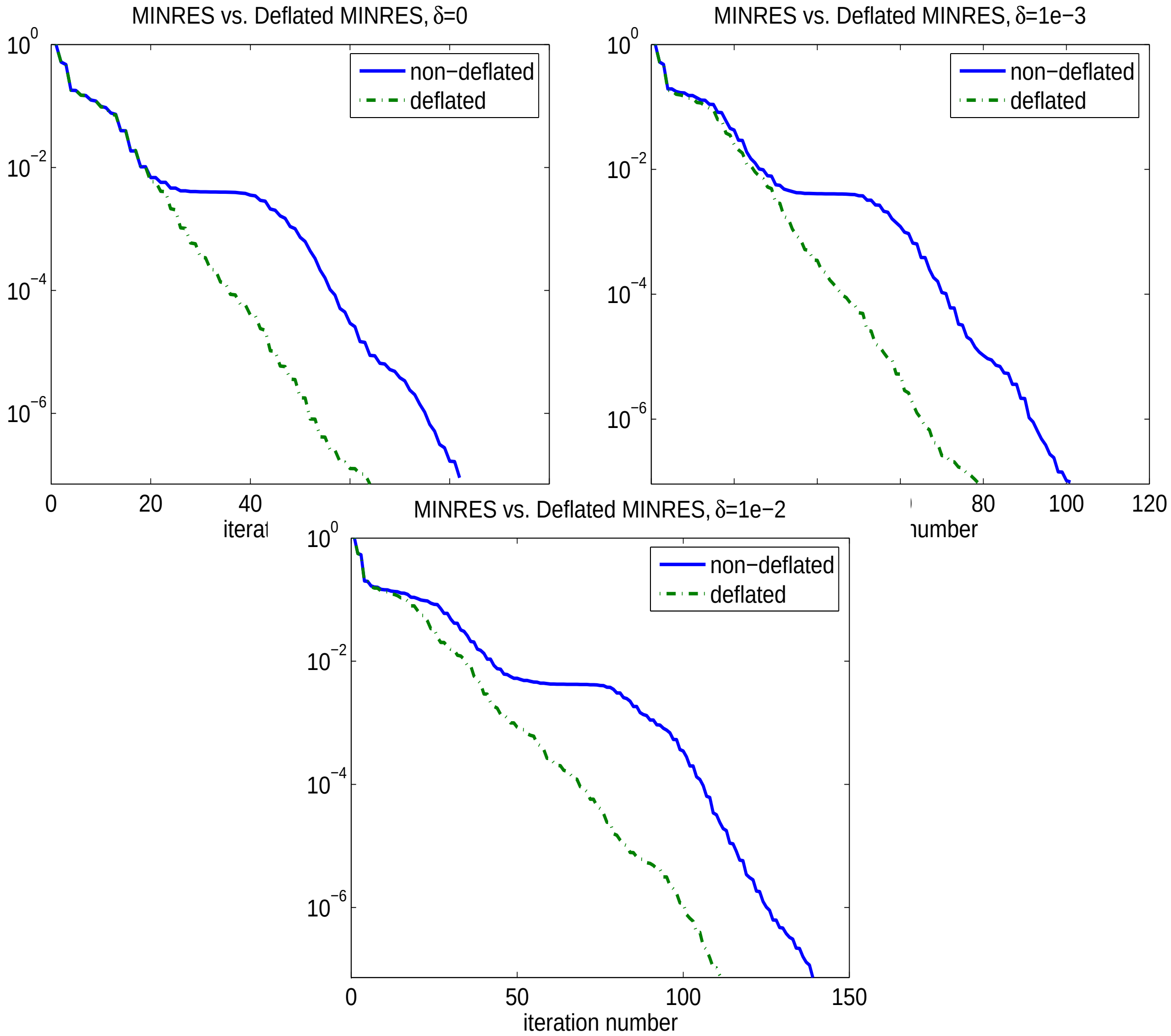
* One small eigenvalue of precon'd Schur Complement

$\Rightarrow$ rough eigvec approximation : $\{\widetilde{u}_2, \widetilde{p}_2\}^T \approx \{u_2, p_2\}^T$

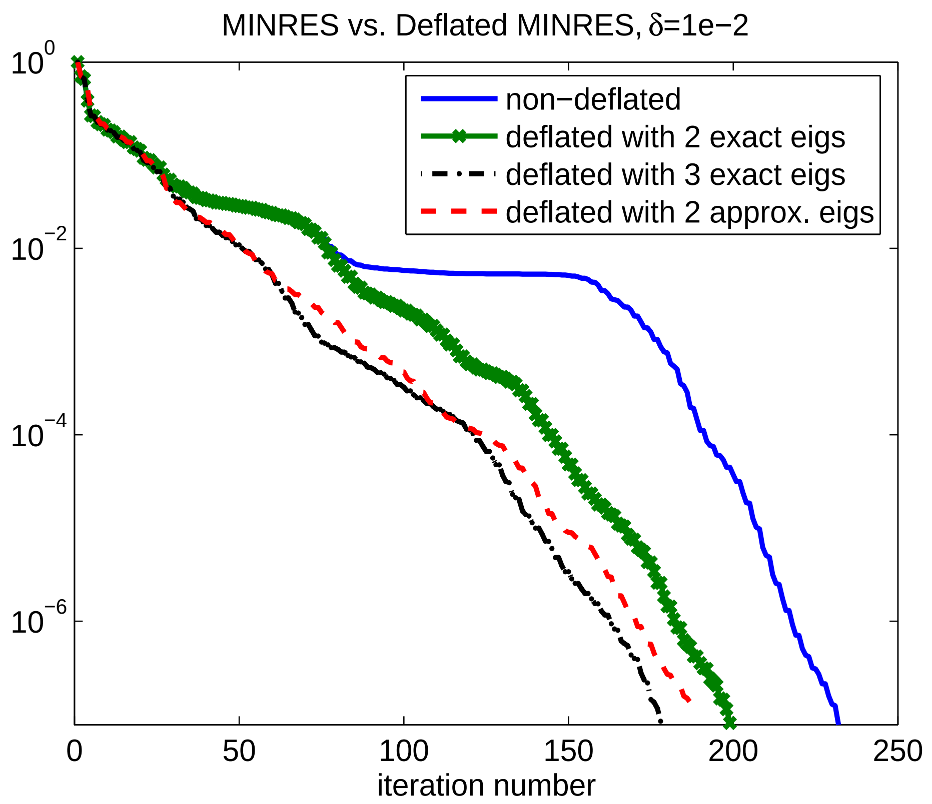
$$\widetilde{p}_2 = \begin{cases} 0 & \text{if } \frac{1}{2} - \tau_s \le y \le \frac{1}{2} + \tau_s, \\ 1 & \text{if } 0 \le y < \frac{1}{2} - \tau_s, \\ -1 & \text{if } 1 \ge y > \frac{1}{2} + \tau_s, \end{cases} \quad \text{and} \quad \widetilde{u}_2 = -\widetilde{A}^{-1} B^T \widetilde{p}_2$$

Bercovier-Engelman model of the Bingham viscoplastic fluid

$$\widetilde{A} = \mathrm{IC}(A, \delta)$$



Exact and approximate eigenvectors



Here $\widetilde{A} = \mathrm{IC}(A, 10^{-2})$ poor approximation $\Rightarrow$ one small positive eig

A parameter identification problem

$$\min_q \frac{1}{2}||F(q) - z||^2 + \alpha \mathcal{J}_{reg}(q) \tag{1}$$

$$\mathcal{B}(q)u \equiv -\nabla \cdot (\sigma \nabla u) = f \tag{2}$$

(2): model for groundflow

u: fluid pressure $\quad\quad$ $\sigma(x)$: (spatially dep.) hydraulic conductivity

$f(x)$: in/out-going fluid (incompressible flows)

Parameter of interest: $\quad q(x) = \log(\sigma(x))$, obs from soln: $u_{obs} = Cu$

(1): $F(q) = C\mathcal{B}(q)^{-1} f$ (parameter-to-obs map, non-linear function)

$\mathcal{J}_{reg}$ regularization functional (e.g. total variation)

PDE-constrained formulation

$$\min_{q,u} \frac{1}{2}||Cu - z||^2 + \alpha \mathcal{J}_{reg}(q)$$
$$\mathcal{B}(q)u - f = 0.$$

Space discretization + inexact Newton method provide linear systems:

$$\begin{bmatrix} H & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} v \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -L_v \\ -L_{\boldsymbol{\lambda}} \end{bmatrix}$$

H: Hessian of the operator

B: Jacobian of the constraint

$v = [q, u]$ variables, $\boldsymbol{\lambda}$: Lagrange multipliers

A similar setting: Monge-Kantorovich mass transfer problem

Pb: Given two density functions u_0 and u_T on the set Ω, find an "optimal" mapping from u_0 to u_T

Formulation (time in $[0, T]$):

$$\min_{u,m} \frac{1}{2}\|u(T, \mathbf{x}) - u_T(\mathbf{x})\|^2 + \frac{1}{2}\alpha T \int_\Omega \int_0^T u\|m\|^2 dt d\mathbf{x}$$

$$s.t. \qquad u_t + \nabla \cdot (um) = 0, \qquad u(0, \mathbf{x}) = u_0$$

$u(t, \mathbf{x})$: density field $\qquad m(t, \mathbf{x})$: velocity field

A preconditioning technique for a class of PDE-constrained optimization problems

M. Benzi, E. Haber and L. Taralli, Adv. in Comput. Math. '10

A similar setting: Monge-Kantorovich mass transfer problem

Time and space discretization + Gauss-Newton approximation on the Lagrangian

Sequence of "Newton step-depending" linear systems:

$$\begin{bmatrix} Q^T Q & 0 & B_1^T \\ 0 & L & B_2^T \\ B_1 & B_2 & 0 \end{bmatrix} \begin{bmatrix} \widetilde{u}_k \\ \widetilde{m}_k \\ \widetilde{p}_k \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

with $Q^T Q$ diagonal and highly singular, $L > 0$ diagonal

B_2 rank deficient

Reduced order problem

$$\begin{bmatrix} Q^TQ & 0 & B_1^T \\ 0 & L & B_2^T \\ B_1 & B_2 & 0 \end{bmatrix} \begin{bmatrix} \widetilde{u}_k \\ \widetilde{m}_k \\ \widetilde{p}_k \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

into

$$\begin{bmatrix} Q^TQ & B_1^T \\ B_1 & -B_2L^{-1}B_2^T \end{bmatrix} \begin{bmatrix} \widetilde{u}_k \\ \widetilde{p}_k \end{bmatrix} = \begin{bmatrix} b_2 \\ \tilde{b}_3 \end{bmatrix}$$

Both Q^TQ, $B_2L^{-1}B_2^T$ pos. semi-definite, B_1 square nonsing.

Augmented Block Diagonal Preconditioning

$$\mathcal{M} = \begin{bmatrix} Q^T Q & B_1^T \\ B_1 & -B_2 L^{-1} B_2^T \end{bmatrix}$$

Both diagonal blocks are singular. Augmented preconditioning:

$$\mathcal{P}_{ad} = \begin{bmatrix} D & 0 \\ 0 & C(D) \end{bmatrix}, \qquad \begin{array}{l} D > 0 \\ C(D) \approx B_2 L^{-1} B_2^T + B_1 D^{-1} B_1^T \end{array}$$

Work in Progress

Exact preconditioner

$$\mathcal{P}_{ad} = \begin{bmatrix} D & 0 \\ 0 & B_2 L^{-1} B_2^T + B_1 D^{-1} B_1^T \end{bmatrix} \qquad \begin{aligned} D &= Q^T Q + \gamma \mathcal{N}(Q^T Q) \\ \gamma &= \|L\| \end{aligned}$$

n_x	n_t	n	#	CPU time	n_x	n_t	n	#	CPU time
20	20	8000	14	8.17	30	10	9000	21	34.16
25	25	15625	15	33.31	40	20	32000	21	376.54
30	30	27000	16	109.25	50	20	50000	-	-
35	35	42875	16	309.97					
40	40	64000	-	-					

Practical preconditioner

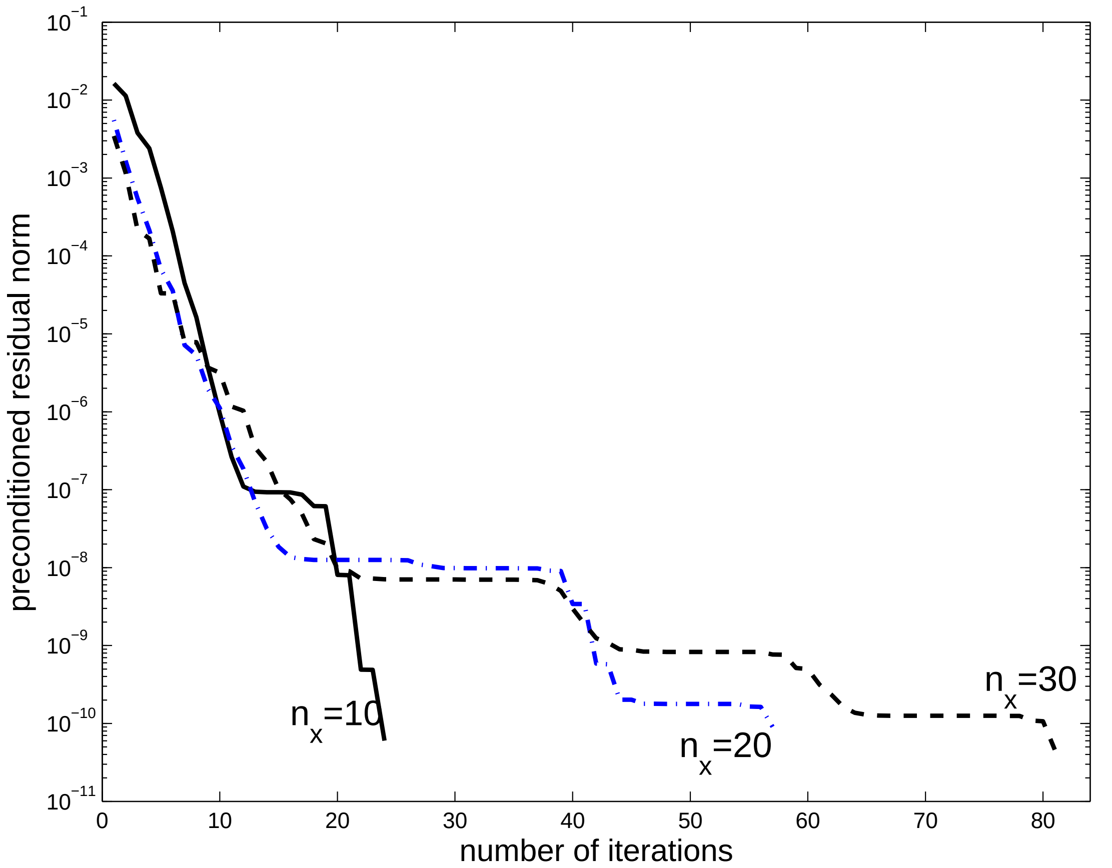
$$\mathcal{P}_{ad} = \begin{bmatrix} D & 0 \\ 0 & C(D) \end{bmatrix}$$

D: $\quad D = Q^T Q + \gamma \mathcal{N}(Q^T Q), \qquad \gamma = \|L\|$

$C(D)$: Algebraic Multigrid of $B_2 L^{-1} B_2^T + B_1 D^{-1} B_1^T$

(routine HSL_MI20)

Numerical results with practical $\mathcal{P}_{ad}$



Approximate smallest eigenvalues

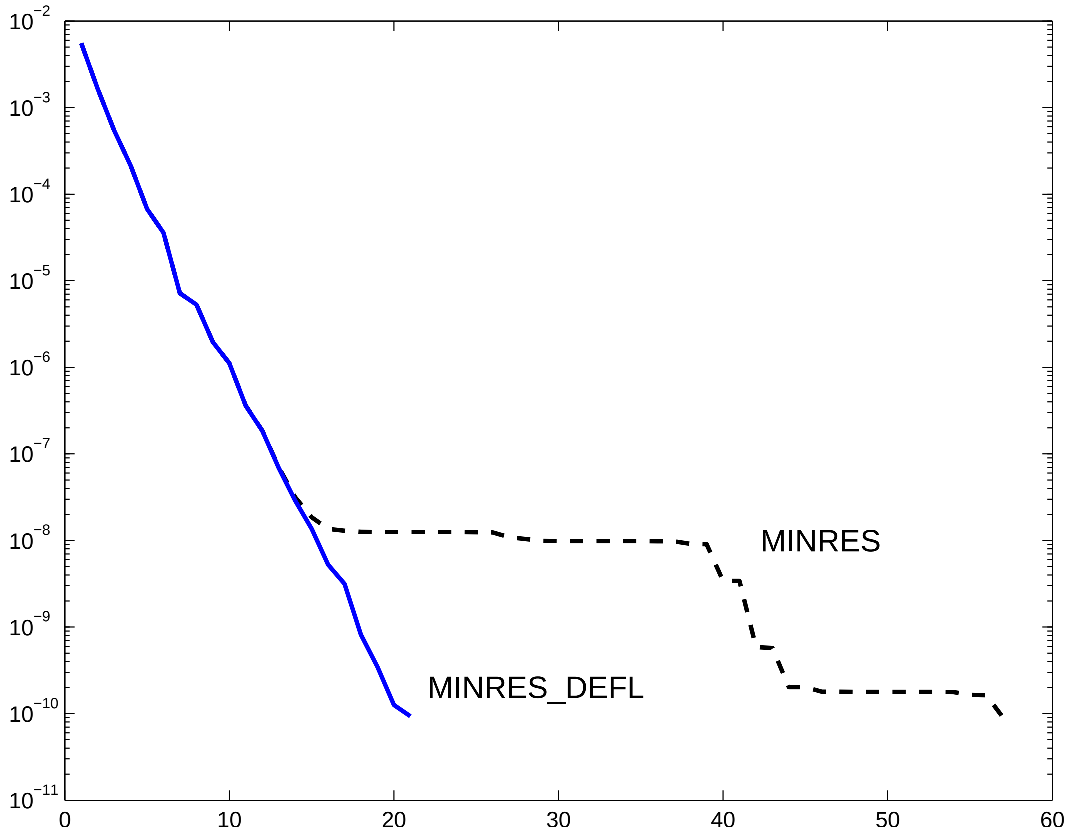
$C(D)$: Algebraic Multigrid of $B_2 L^{-1} B_2^T + B_1 D^{-1} B_1^T$

Eigs of "preconditioned augmented Schur complement"

$$\mathrm{spec}((B_2 L^{-1} B_2^T + B_1 D^{-1} B_1^T) C(D)^{-1})$$

approx λ_i	$n_x = 10$	$n_x = 20$	$n_x = 30$
i=1	**9.4632e-04**	**1.7676e-05**	**1.3247e-05**
i=2	**9.4999e-04**	**1.8274e-05**	**1.3937e-05**
i=3	8.5302e-01	**1.5449e-04**	**4.6116e-05**
i=4	8.5400e-01	**1.5484e-04**	**4.6200e-05**
i=5	8.5722e-01	6.2973e-01	3.7707e-01
i=6	8.5752e-01	6.3079e-01	3.7791e-01
i=7	8.6410e-01	6.6089e-01	3.8408e-01
i=8	8.6825e-01	6.6091e-01	3.8409e-01
i=9	8.7875e-01	6.6557e-01	4.0425e-01
i=10	8.8097e-01	6.6674e-01	4.0514e-01

Augmented/Deflated MINRES



Approximation:

50 its of Arnoldi method of precon'd Schur complement

(at first Newton step)

Complete timings

n	$\mathcal{P}_{ad}$		$\mathcal{P}_{ad}$ w/AMG		$\mathcal{P}_{ad}$ w/AMG+DEFL		
	# its	time	# its	time	# its	time	
1000	12	0.19	24	0.29	17	0.26	+ 0.52, 2 eigs
3375	13	1.28	52	1.43	25	0.80	+ 1.53, 5 eigs
8000	14	8.17	57	4.64	21	1.95	+ 4.51, 4 eigs
15625	15	33.31	85	14.64	36	6.68	+ 9.57, 5 eigs
27000	16	109.25	81	28.37	28	10.61	+19.03, 4 eigs
42875	16	309.97	122	65.82	47	27.33	+29.82, 5 eigs
64000	-		90	88.63	37	37.82	+52.23, 4 eigs

Conclusions

- Construction of Schur complement type preconditioner is spectrally crucial
- An effective way to overcome an “isolated” difficulty

Bibliography:

Acquired clustering properties and solution of certain saddle point systems,

Maxim A. Olshanskii and V. Simoncini

To appear in SIAM J. Matrix Analysis and Appl.

see also `www.dm.unibo.it://~ simoncin`