Inexact inverse iteration for the generalised nonsymmetric eigenproblem

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Outline

Problem and Inverse Iteration

- Find an eigenvalue and eigenvector of:

$$Ax = \lambda Mx, \quad \lambda \in \mathbb{C}, x \in \mathbb{C}^n$$

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- A and M are large, sparse, nonsymmetric, and M possibly singular
- Inverse iteration with preconditioned iterative solves

Inverse Iteration

Choose $x^{(0)}$
for $i = 1, \dots$ **do**
Choose $\sigma^{(i)}$ and $\tau^{(i)}$
Solve

$$\|(A - \sigma^{(i)} M) y^{(i)} - M x^{(i)}\| \leq \tau^{(i)},$$

Update $x^{(i+1)} = y^{(i)} / \phi(y^{(i)})$,
Set $\lambda^{(i+1)} = \rho(x^{(i+1)})$
Evaluate $r^{(i+1)} = (A - \lambda^{(i+1)} M) x^{(i+1)}$,
Test for convergence.
end for

Outline

Schur decomposition and block factorisation I

Theorem (Generalised Schur Decomposition)

There exist unitary matrices Q *and* Z *such that* $Q^H AZ = T$ *and* $Q^H MZ = S$ *are upper triangular. If for some* j, t_{jj} *and* s_{jj} *are both zero, then* $\lambda(A, M) = \mathbb{C}$. *If* $s_{jj} \neq 0$ *then* $\lambda(A, M) = \{t_{jj}/s_{jj}\}$, *otherwise, the* j*th eigenvalue is infinite.*

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Theorem (Generalised Schur Decomposition)

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Partitioning the eigenproblem

$$Q^H AZ = \begin{bmatrix} t_{11} & t_{12}^H \\ 0 & T_{22} \end{bmatrix} \quad \text{and} \quad Q^H MZ = \begin{bmatrix} s_{11} & s_{12}^H \\ 0 & S_{22} \end{bmatrix},$$

if λ_1, the desired eigenvalue, is finite, then $s_{11} \neq 0$ and $\lambda_1 = t_{11}/s_{11}$.

Schur decomposition and block factorisation II

A linear transformation

If $\lambda_1 = \dfrac{t_{11}}{s_{11}} \notin \lambda(T_{22}, S_{22})$ then

$$G = \begin{bmatrix} 1 & g_{12}^H \\ \mathbf{0} & I_{n-1} \end{bmatrix} \quad \text{and} \quad H = \begin{bmatrix} 1 & h_{12}^H \\ 0 & I_{n-1} \end{bmatrix}$$

$G^{-1}TH = \mathrm{diag}(t_{11}, T_{22})$ and $G^{-1}SH = \mathrm{diag}(s_{11}, S_{22})$.

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Lemma

Define $U = QG$ and $X = ZH$. Then both U and X are nonsingular and we can block-factorise $A - \lambda M$ as

$$U^{-1}(A - \lambda M)X = \begin{bmatrix} t_{11} & 0^H \\ 0 & T_{22} \end{bmatrix} - \lambda \begin{bmatrix} s_{11} & 0^H \\ 0 & S_{22} \end{bmatrix}.$$

A new convergence measure

Splitting

$$x^{(i)} = \alpha^{(i)}(x_1 q^{(i)} + X_2 p^{(i)}),$$

where $\alpha^{(i)} := \|U^{-1}Mx^{(i)}\|$.

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A generalised tangent

$$1 = \frac{\|U^{-1}Mx^{(i)}\|}{\alpha^{(i)}} = \|s_{11}q^{(i)}e_1 + \bar{I}_{n-1}S_{22}p^{(i)}\| = ((s_{11}q^{(i)})^2 + \|S_{22}p^{(i)}\|^2)^{\frac{1}{2}}$$

Define

$$T^{(i)} := \frac{\|S_{22}p^{(i)}\|}{|s_{11}q^{(i)}|}.$$

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Convergence rate

Theorem (One step bound)

With $\beta \in (0,1)$ *and* $\tau^{(i)} \leq \beta|\alpha^{(i)} s_{11} q^{(i)}|/\|u_1\|$ *small enough, we have*

$$T^{(i+1)} = \frac{\|S_{22}p^{(i+1)}\|}{|s_{11}q^{(i+1)}|} \leq \frac{|\lambda_1 - \sigma^{(i)}|\|S_{22}\|}{\|(T_{22} - \sigma^{(i)} S_{22})^{-1}\|^{-1}} \frac{\left(\|\alpha^{(i)} S_{22} p^{(i)}\| + \|d^{(i)}\|\right)}{(1-\beta)|\alpha^{(i)} s_{11} q^{(i)}|}.$$

$\|(T_{22} - \sigma^{(i)} S_{22})^{-1}\|^{-1} =: sep(\sigma^{(i)}, (T_{22}, S_{22}))$.

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Lemma (Convergence rate)

We have

- *Fixed shift: decreasing tolerance $\tau^{(i)} = C_1\|r^{(i)}\| \Rightarrow$ linear convergence*

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$\|(T_{22} - \sigma^{(i)} S_{22})^{-1}\|^{-1} =: sep(\sigma^{(i)}, (T_{22}, S_{22}))$.

Lemma (Convergence rate)

We have

- *Fixed shift: decreasing tolerance* $\tau^{(i)} = C_1\|r^{(i)}\| \Rightarrow$ *linear convergence*
- *Rayleigh quotient shift: decreasing tolerance* $\tau^{(i)} = C_1\|r^{(i)}\| \Rightarrow$ *quadratic convergence*

Nuclear Reactor problem

$$
\begin{aligned}
-\mathrm{div}(K_1 \nabla u_1) + (\Sigma_{a,1} + \Sigma_s) u_1 &= \frac{1}{\mu_1}(\Sigma_{f,1} u_1 + \Sigma_{f,2} u_2) \\
-\mathrm{div}(K_2 \nabla u_2) + \Sigma_{a,2} u_1 - \Sigma_s u_2 &= 0,
\end{aligned}
$$

where u_1 and u_2 are defined on $[0,1] \times [0,1]$ density distributions of fast and thermic neutrons respectively. K_1 and K_2 are diffusion coefficients and $\Sigma_{a,1}, \Sigma_{a,2}, \Sigma_s, \Sigma_{f,1}$ and $\Sigma_{f,2}$ measure interaction probabilities taking piecewise constant values; μ_1 measures criticality of the reactor

$$
Ax = \lambda M x,
$$

A, M nonsymmetric, M singular.

Convergence rates

Table: Convergence history *fixed shift* $\sigma = 0.9$ and *variable shift*

	Decreasing tolerance $\tau^{(i)}$		Fixed tolIerance $\tau^{(0)}$
Outer it	*Fixed shift* $\sigma = 0.9$	*Generalised RQ shift*	*Generalised RQ shift*
1	1.2982e+00	1.2982e+00	1.2982e+00
2	1.9999e-02	1.3774e-01	2.6776e-01
3	4.3867e-03	2.7952e-03	9.5850e-02
4	1.3979e-03	2.2022e-07	3.9744e-02
5	5.7163e-04	3.9086e-14	1.4304e-02
6	2.9952e-04	3.6824e-15	6.4409e-03
7	1.6427e-04		2.2448e-03
8	9.1590e-05		8.1950e-04
9	5.1170e-05		2.5762e-04
10	2.8924e-05		9.7647e-05
11	1.6374e-05		3.4961e-05

Jacobi-Davidson method

(1) Given an approximate eigenpair (x, θ), look for correction s such that

$$A(x+s) = \lambda M(x+s).$$

Rewrite

$$(A-\lambda M)s = (\lambda - \theta)Mx - r,$$

Multiplying by $I - \dfrac{Mxx^HM^H}{x^HM^HMx}$, using $r \perp Mx$ and $s \perp M^HMx$:

Correction equation

$$(I - \frac{Mxx^HM^H}{x^HM^HMx})(A-\lambda M)(I - \frac{xx^HM^HM}{x^HM^HMx})s = -r, \quad \text{where} \quad s \perp M^HMx.$$

(2) The given subspace that contains x is then expanded by s.
(3) Simplified version: no subspace expansion but update as normalised version of $x+s$

Exact solves

Lemma (Equivalence to Inverse iteration)

Suppose the correction equation has unique solution $\hat{\mathbf{s}}$. *Then the simplified Jacobi-Davidson solution* $x_{JD} = x + \hat{s}$ *satisfies*

$$(A - \sigma M)\tilde{x} = Mx, \quad \textit{where}$$

$$\tilde{x} = \frac{1}{\gamma} x_{JD} \quad \textit{with} \quad \gamma = \frac{x^H M^H M x}{x^H M^H M (A - \sigma M)^{-1} M x}.$$

Inexact solves

Inexact Inverse Iteration

$$(A - \sigma^{(i)} M) y^{(i)} = M x^{(i)} - d_I^{(i)}, \quad \text{where} \quad \|d_I^{(i)}\| \leq \tau_I^{(i)} \|M x^{(i)}\|$$

with $\tau_I^{(i)} < 1$

Inexact solves

Inexact Inverse Iteration

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Inexact Jacobi-Davidson

$$\left(I - \frac{Mx^{(i)}{x^{(i)}}^H M^H}{\|Mx^{(i)}\|^2}\right)(A-\sigma^{(i)}M)\left(I - \frac{x^{(i)}{x^{(i)}}^H M^H M}{\|Mx^{(i)}\|^2}\right)s^{(i)} = -r^{(i)} + d_{JD}^{(i)}$$

$$s^{(i)} \perp M^H M x^{(i)}, \quad \text{where} \quad \|d_{JD}^{(i)}\| \leq \tau_{JD}^{(i)}\|r^{(i)}\|, \quad \text{and} \quad \tau_{JD}^{(i)} < 1.$$

Inexact solves

Lemma (Connection between IJD and III)

If $\tau_{JD}^{(i)}$ is chosen such that

$$\tau_{JD}^{(i)} = \frac{\tau_I^{(i)}}{1+\tau_I^{(i)}} \frac{\|Mx^{(i)}\|}{\|M(A-\sigma^{(i)}M)^{-1}\|\|r^{(i)}\|}, \quad \textit{then}$$

$$\frac{\|d_{JD}^{(i)}\|}{|\gamma^{(i)}|} \leq \tau_I^{(i)}\|Mx^{(i)}\|.$$

holds, and simplified inexact JD converges at least as fast as inexact II.

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For $\sigma^{(i)} := \rho(x^{(i)})$ we have

$$C \frac{\tau_I^{(i)}}{1+\tau_I^{(i)}} \leq \tau_{JD}^{(i)} \leq \frac{\tau_I^{(i)}}{1+\tau_I^{(i)}},$$

where C is independent of i.

Outline

The inner system

GMRES convergence

$$(A - \sigma^{(i)} M) y^{(i)} = M x^{(i)}, \quad \text{or} \quad Bz = b$$

GMRES convergence bound is given by

$$\|b - Bz_k\| \leq \min_{p_{k-1} \in \Pi_{k-1}} \|p_k(B) b\|.$$

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A more detailed analysis

$$\|b - Bz_k\| \leq c \frac{\|C - \mu_1 I\|}{|\mu_1|} \min_{p_{k-1} \in \Pi_{k-1}} \|p_{k-1}(C)\| \|\mathcal{P} b\|,$$

where C is a matrix that arises after block-diagonalisation of B

$$B = \begin{bmatrix} w_1 & W_2 \end{bmatrix} \begin{bmatrix} \mu_1 & 0^H \\ 0 & C \end{bmatrix} \begin{bmatrix} v_1^H \\ V_2^H \end{bmatrix},$$

and $\mathcal{P} = I - w_1 v_1^H$ is an oblique projector that projects onto $\mathcal{R}(W_2)$.

Idea of the proof

Introduce special polynomial

$$\hat{p}_k(z) = p_{k-1}(z)\left(1 - \frac{z}{\mu_1}\right)$$

$$\begin{aligned} \|b - Bz_k\| &= \min_{p_k \in \Pi_k} \|p_k(B)\mathcal{P}b + p_k(B)(I-\mathcal{P})b\| \\ &\leq \min_{\hat{p}_k \in \Pi_k} \|\hat{p}_k(B)\mathcal{P}b + \hat{p}_k(B)(I-\mathcal{P})b\| \\ &= \min_{p_{k-1} \in \Pi_{k-1}} \|p_{k-1}(B)\left(I - \frac{B}{\mu_1}\right)\mathcal{P}b + p_{k-1}(B)\left(I - \frac{B}{\mu_1}\right)(I-\mathcal{P})b\|. \end{aligned}$$

Idea of the proof

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$$\begin{aligned}
\|b - Bz_k\| &= \min_{p_k \in \Pi_k} \|p_k(B)\mathcal{P}b + p_k(B)(I-\mathcal{P})b\| \\
&\leq \min_{\hat{p}_k \in \Pi_k} \|\hat{p}_k(B)\mathcal{P}b + \hat{p}_k(B)(I-\mathcal{P})b\| \\
&= \min_{p_{k-1} \in \Pi_{k-1}} \|p_{k-1}(B)\left(I - \frac{B}{\mu_1}\right)\mathcal{P}b\| \\
&\leq c \min_{p_{k-1} \in \Pi_{k-1}} \|p_{k-1}(C)\| \frac{\|\mu_1 I - C\|}{|\mu_1|} \|\mathcal{P}b.\|.
\end{aligned}$$

Bounding $\min_{p_{k-1}\in\Pi_{k-1}} \|p_{k-1}(C)\|$

Definition (ε-pseudospectrum $\Lambda_\varepsilon(C)$ of a matrix C)

$$\Lambda_\varepsilon(C) := \{z \in \mathbb{C} : \|(zI - C)^{-1}\|_2 \geq \varepsilon^{-1}\}.$$

Theorem (Convergence of GMRES)

E: convex closed bounded set in the complex plane with $0 \notin E$ and $\Lambda_\varepsilon(C) \subset E$. Ψ: conformal mapping that carries the exterior of E onto the exterior of the unit circle $\{|w| > 1\}$ and that takes ∞ to ∞. Then

$$\min_{p_{k-1}\in\Pi_{k-1}} \|p_{k-1}(C)\| \leq S \left(\frac{1}{|\Psi(0)|}\right)^{k-1}, \quad \textit{where} \quad S = \frac{3\mathcal{L}(\Gamma_\varepsilon)}{2\pi\varepsilon}$$

and $|\Psi(0)| > 1$ and hence

$$\|b - Bz_k\| \leq c \left(\frac{1}{|\Psi(0)|}\right)^{k-1} \frac{\|\mu_1 I - C\|}{|\mu_1|} \|\mathcal{P}b\|.$$

The number of inner iterations

Theorem (Number of inner iterations)

Let z_k be the approximate solution of $Bz = b$ obtained after k iterations of GMRES with starting value $z_0 = 0$. If the number of inner iterations satisfies

$$k \geq 1 + \frac{1}{\log|\Psi(0)|} c \left(\log \frac{S\|\mu_1 I - C\|}{|\mu_1|} + \log \frac{\|\mathcal{P}\mathbf{b}\|}{\tau} \right),$$

then $\|b - Bz_k\| \leq \tau$.

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$$k^{(i)} \geq 1 + \frac{1}{\log|\Psi(0)|}\left(c + \log \frac{\|\mathcal{P}b^{(i)}\|}{\tau^{(i)}}\right),$$

then $\|b^{(i)} - Bz_k^{(i)}\| \leq \tau^{(i)}$.

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then $\|b^{(i)} - Bz_k^{(i)}\| \leq \tau^{(i)}$.

If $\|\mathcal{P}b^{(i)}\|$ is of the same order as $\tau^{(i)}$ the iteration numbers bounded independent of i.

The right hand side is crucial in inner eigenvalue solvers

- The standard eigenproblem

$$(A - \sigma^{(i)} I) y^{(i)} = x^{(i)}$$

The right hand side is crucial in inner eigenvalue solvers

- The generalised eigenproblem

$$(A - \sigma^{(i)} M) y^{(i)} = M x^{(i)} \quad \text{trouble}$$

The right hand side is crucial in inner eigenvalue solvers

- The preconditioned generalised eigenproblem

$$(A - \sigma^{(i)} M) P^{-1} \tilde{y}^{(i)} = M x^{(i)}, \quad P^{-1} \tilde{y}^{(i)} = y^{(i)} \quad \text{trouble.}$$

Tuning strategies II

Tuning for the generalised eigenproblem

The generalised eigenproblem $(A - \sigma^{(i)} M)y^{(i)} = Mx^{(i)}$:

$$(A - \sigma^{(i)} M)\mathbb{T}_i^{-1}\tilde{y}^{(i)} = Mx^{(i)} \quad \mathbb{T}_i^{-1}\tilde{y}^{(i)} = y^{(i)}.$$

where $\mathbb{T}_i x^{(i)} = Mx^{(i)}$.

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where $\mathbb{T}_i x^{(i)} = Mx^{(i)}$.

Tuning preconditioner the generalised eigenproblem

The generalised eigenproblem
$(A-\sigma^{(i)}M)P^{-1}\tilde{y}^{(i)} = Mx^{(i)}, \quad P^{-1}\tilde{y}^{(i)} = y^{(i)}$:

$$(A-\sigma^{(i)}M)\mathbb{P}_i^{-1}\tilde{y}^{(i)} = Mx^{(i)} \quad \mathbb{P}_i^{-1}\tilde{y}^{(i)} = y^{(i)}.$$

where $\mathbb{P}_i x^{(i)} = Ax^{(i)}$.

Implementation

Lemma

Let $\mathbf{x}^{(i)}$ *be the approximate eigenvector* $u^{(i)} = Ax^{(i)} - Px^{(i)}$, *where* P *is a standard preconditioner for* A. *Then*

$$\mathbb{P}_i = P + u^{(i)} x^{(i)} {x^{(i)}}^H$$

assures $\mathbb{P}_i x^{(i)} = Ax^{(i)}$.

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assures $\mathbb{P}_i x^{(i)} = Ax^{(i)}$.

Advantages

- convergence rate of exact solve is retained
- cheap inner solves
- only one extra back solve for each inner iteration

Problem formulation

Consider

$$Ax = \lambda x,$$

where $\mathbf{A}$ is the finite difference discretisation on 32×32 grid of the eigenvalue problem of the convection-diffusion operator

$$-\Delta u + 5u_x + 5u_y = \lambda u \quad \text{on} \quad (0,1)^2, \tag{1}$$

with homogeneous Dirichlet boundary conditions.
Consider the generalised eigenvalue problem

$$Ax = \lambda M x,$$

derived by discretising (1) using a Galerkin-FEM on regular triangular elements with piecewise linear functions. We use a 32×32

Results (no preconditioner)

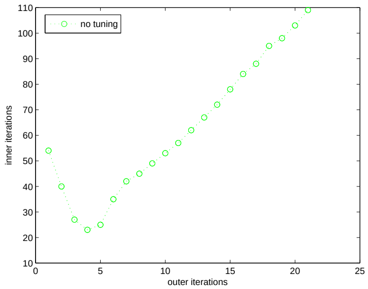


Figure: Inner iterations vs outer iterations for standard/generalised eigenproblem with/without tuning

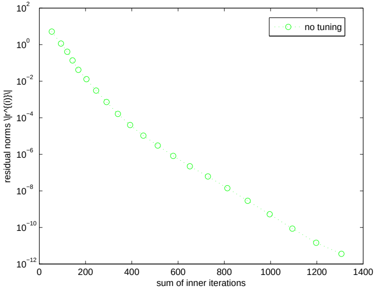
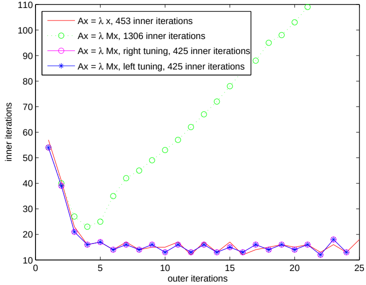


Figure: Residual norms vs the total number of inner iterations with/without tuning

Results



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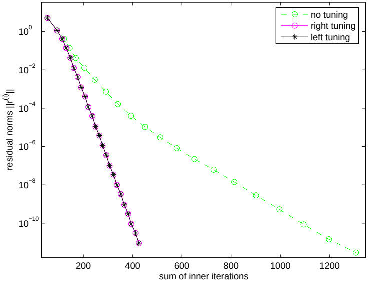

Figure: Residual norms vs total number of inner iterations with/without tuning

More results (preconditioner)

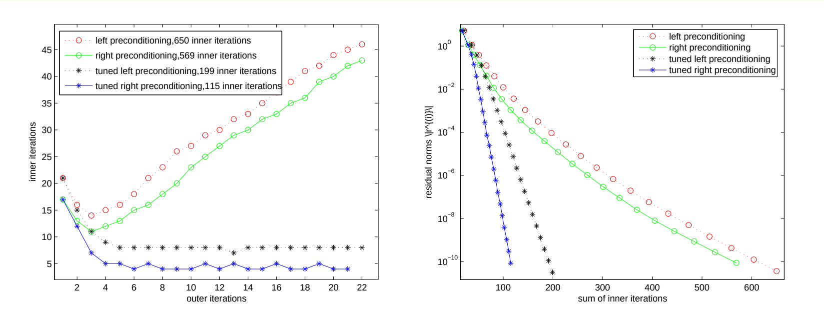

Figure: Inner iterations vs outer iterations with standard and tuned preconditioning

Figure: Residual norms vs total number of inner iterations with standard and tuned preconditioning

More results

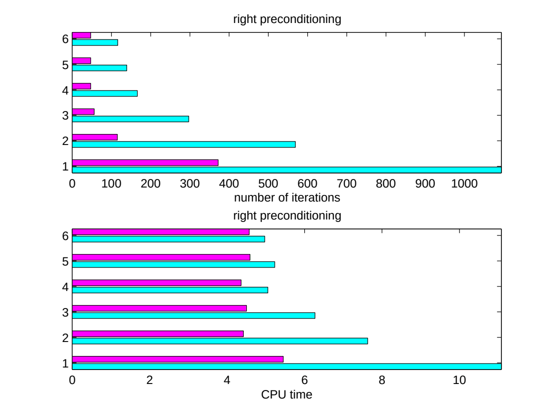

Figure: Comparison of total number of inner iterations and CPU times for different drop tolerances of the preconditioner

More examples

	Matrix name/s	size n	Description
1	`stiff.mtx/mass.mtx`	961	Convection-Diffusion operator
2	`dwa512.mtx/dwb512.mtx`	512	Square Dielectric Waveguide
3	`bcsstk08.mtx/bcsstm08.mtx`	1074	BCS Structural Engineering Matrix
4	`rdb1250l.mtx`	1250	Reaction-Diffusion Brusselator Model $L = 1.0$
5	`cdde1.mtx`	961	Model 2D Convection-Diffusion operator $p_1 = 1$, $p_2 = 2$, $p_3 = 30$
6	`olm2000.mtx`	2000	Olmstead Model

Table: Set of test matrices from the collection Matrix Market

	Matrix name/s	droptol	shift σ	eigenvalue	$\tau^{(0)}$	final $r^{(i)}$
1	`stiff.mtx/mass.mtx`	1	85	91.6223	0.01	10e-11
2	`dwa512.mtx/dwb512.mtx`	0.001	0.001	1.3957e-3	0.001	10e-8
3	`bcsstk08.mtx/bcsstm08.mtx`	0.01	10	6.90070	0.01	10e-11
4	`rdb1250l.mtx`	0.1	-0.325	-3.20983e-1	0.1	10e-11
5	`cdde1.mtx`	0.1	0.001	-5.17244e-3	0.1	10e-15
6	`olm2000.mtx`	0.1	4.3	4.51010	0.1	10e-9

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And even more results

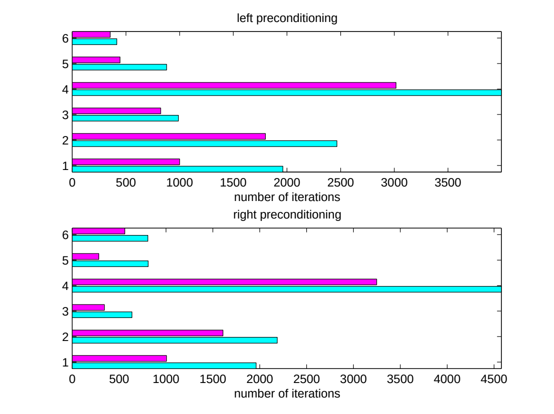

Figure: Total number of inner iterations for left preconditioning with and without tuning (left plot) and for right preconditioning with and without tuning (right plot).

And even more results

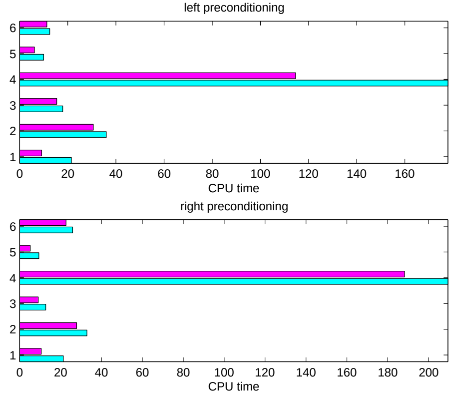

Figure: Total CPU times for left preconditioning with and without tuning (left plot) and for right preconditioning with and without tuning (right plot).

Outline

Symmetric case

Symmetric JD $A = A^T$

Consider Jacobi-Davidson correction equation

$$\underbrace{(I - xx^H)}_{\pi}(A - \rho(x)I)(I - xx^H)s = -r, \quad \text{where} \quad s \perp x.$$

Inverse iteration inner solve

$$(A - \rho(x)I)y = x$$

then

$$\text{span}(x, Ax, A^2x, \ldots, A^kx) = \text{span}(x, r, (\pi A\pi)r, (\pi A\pi)^2r, \ldots, (\pi A\pi)^{k-1}r)$$

Symmetric case - right tuning with $\mathbb{P}x = x$

Symmetric JD $A = A^T$

Consider Jacobi-Davidson correction equation

$$(I - xx^H)(A - \rho(x)I)(I - xx^H)\mathbb{P}^\dagger \tilde{s} = -r, \quad \text{where} \quad s \perp x.$$

Inverse iteration inner solve

$$(A - \rho(x)I)\mathbb{P}^{-1}\tilde{y} = x$$

then

$$\text{span}(x, A\mathbb{P}^{-1}x, (A\mathbb{P}^{-1})^2 x, \ldots, (A\mathbb{P}^{-1})^k x)$$

equals

$$\text{span}(x, r, (\pi A \pi \mathbb{P}^{-1})r, (\pi A \pi \mathbb{P}^{-1})^2 r, \ldots, (\pi A \pi \mathbb{P}^{-1})^{k-1} r)$$

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Generalised eigenproblem

This result also holds for the generalised eigenproblem $Ax = \lambda M x$.

Symmetric case - right tuning with $\mathbb{P}x = x$

Symmetric JD $A = A^T$

Consider Jacobi-Davidson correction equation

$$(I - xx^H)(A - \rho(x)I)(I - xx^H)\mathbb{P}^\dagger \tilde{s} = -r, \quad \text{where} \quad s \perp x.$$

Inverse iteration inner solve

$$(A - \rho(x)I)\mathbb{P}^{-1}\tilde{y} = x$$

then the approximate solutions s_k and y_k obtained by applying a Galerkin-Krylov method are such that

$$y_k = \gamma(x + s_k).$$

Symmetric case - right tuning with $\mathbb{P}x = x$

Symmetric JD $A = A^T$

Consider Jacobi-Davidson correction equation

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Inverse iteration inner solve

$$(A - \rho(x)I)\mathbb{P}^{-1}\tilde{y} = x$$

then the approximate solutions s_k and y_k obtained by applying a Galerkin-Krylov method are such that

$$y_k = \gamma(x + s_k).$$

Generalised eigenproblem

Some weaker result holds for the generalised eigenproblem $Ax = \lambda Mx$.

M. A. Freitag and A. Spence, *Convergence rates for inexact inverse iteration with application to preconditioned iterative solves*, 2006.
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