Inexact inverse iteration with preconditioning

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Computational Methods with Applications
Harrachov, Czech Republic
24th August 2007

(joint work with M. Robbé and M. Sadkane (Brest))

Outline

Introduction

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

- seek λ near a given shift σ.
- A is large, sparse, nonsymmetric (discretised PDE: $Ax = \lambda Mx$)

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- Inverse Iteration: $(A - \sigma I)y = x$
- Preconditioned iterative solves
- Extensions
    - Inverse Subspace Iteration
    - Jacobi-Davidson method
    - Shift-invert Arnoldi method (Melina Freitag)

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- Iterative solves (e.g. GMRES) of

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- $\|x^{(i)} - (A - \sigma I)y_k\| \leq \tau^{(i)}$, ($\tau^{(i)}$: solve tolerance)
- Rescale y_k to get $x^{(i+1)}$

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- Rescale y_k to get $x^{(i+1)}$
- (Right-) preconditioned solves
  - P^{-1} "known"
  - $(A - \sigma I)P^{-1}\tilde{y} = x^{(i)}$, $P^{-1}\tilde{y} = y$.

Convergence of inexact inverse iteration

- Given $x^{(i)}$ and $\lambda^{(i)}$

$$r^{(i)} = Ax^{(i)} - \lambda^{(i)} x^{(i)} \quad \text{Eigenvalue residual}$$

Theorem (Convergence)

If the solve tolerance, $\tau^{(i)}$, is chosen to reduce proportional to the norm of the eigenvalue residual $\|r^{(i)}\|$ then we recover the rate of convergence achieved when using direct solves.

- other options/strategies possible.

Literature

- Ruhe/Wiberg (1972)
- Lai/Lin/Lin (1997)
- Smit/Paardekooper (1999)
- Golub/Ye (2000)
- Simoncini/Eldén (2002)
- Notay (2003), Notay/Hochstenbach (2007)
- Berns-Müller/Graham/Sp. (2006), Freitag/Sp. (2006), ...

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- Shift-Invert Arnoldi (Melina Freitag - this afternoon)
- Always assume decreasing tolerance: $\tau^{(i)} = C\|Ax^{(i)} - \lambda^{(i)}x^{(i)}\|$
- Example →

Convection-Diffusion problem

Finite difference discretisation on a 32×32 grid of the convection-diffusion operator

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

with homogeneous Dirichlet boundary conditions (961×961 matrix).

- smallest eigenvalue: $\lambda_1 \approx 32.18560954$,
- Preconditioned GMRES with tolerance $\tau^{(i)} = 0.01\|r^{(i)}\|$,
- ILU based preconditioners.

Convection-Diffusion problem: No Preconditioning - $\|Ay_k - x^{(i)}\| \leq \tau^{(i)}$

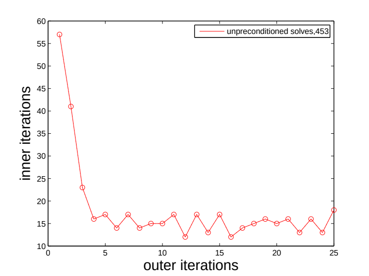


Figure: Inner iterations vs outer iterations

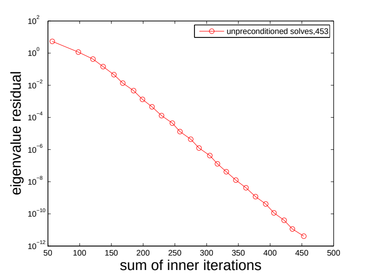
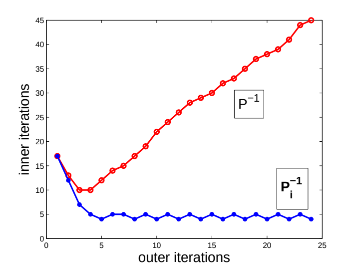


Figure: Eigenvalue residual norms vs total number of inner iterations

Question

Why is there no increase in inner iterations as i increases?

Convection-Diffusion problem: Preconditioning - $\|AP^{-1}\tilde{y}_k - x^{(i)}\| \leq \tau^{(i)}$



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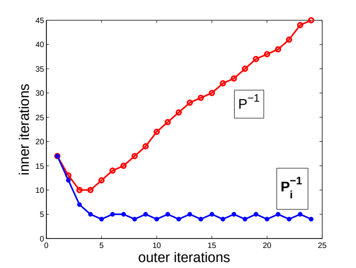

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Question

Why is $\mathbb{P}_i^{-1}$ better than P^{-1}?

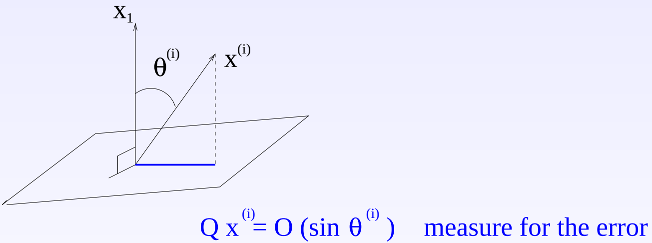
Also

$\mathbb{P}_i$ is a rank-one change to P, "tuned" to the eigenproblem!

Outline

Theory: Unpreconditioned solves to find λ_1, x_1

- $x^{(i)}$ is approximation to x_1



- $x^{(i)} = \cos\theta^{(i)} x_1 + \sin\theta^{(i)} x_\perp$

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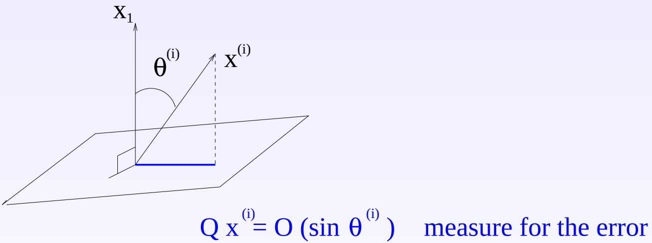

- $x^{(i)} = \cos\theta^{(i)} x_1 + \sin\theta^{(i)} x_\perp$
- $r^{(i)} = Ax^{(i)} - \lambda^{(i)} x^{(i)}, \quad \|r^{(i)}\| \leq C\|\sin\theta^{(i)}\|$
- Parlett (1998) - ideas extend to nonsymmetric problems.

GMRES applied to $Ay = x^{(i)}$

- y_k after k steps
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- $k \geq 1 + C_1 \left(\log C_2 + \log \frac{\sin\theta^{(i)}}{\tau^{(i)}}\right)$
- bound on k does not increase with i.
- Reason: $x^{(i)} = \cos\theta^{(i)}x_1 + \sin\theta^{(i)}x_\perp$

$$x^{(i)} = \boxed{\text{eigenvector of } A \quad + \quad \text{“term”} \quad \to 0}$$

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GMRES applied to $AP^{-1}\tilde{y} = x^{(i)}$

- $AP^{-1}u_1 = \mu_1 u_1$: (μ_1, u_1) eigenpair nearest zero of AP^{-1}
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- BUT $\sin\tilde{\theta}^{(i)} \to 0$ only if $u_1 \in \text{span}\{x_1\}$ generally won't hold
- $\sin\tilde{\theta}^{(i)} \not\to 0$
- inner iteration costs increase with i.
- Reason: $x^{(i)} = \cos\tilde{\theta}^{(i)} u_1 + \sin\tilde{\theta}^{(i)} u_\perp$

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New "tuned" preconditioner $\mathbb{P}_i$

- Idea: recreate the good relationship between the right hand side and the iteration matrix
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- $Ax^{(i)} = \mathbb{P}_i x^{(i)}$

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- $Ax^{(i)} = \mathbb{P}_i x^{(i)}$
- Hence
$$A\mathbb{P}_i^{-1}(Ax^{(i)}) = Ax^{(i)}$$
- $Ax^{(i)}$ is an eigenvector of $A\mathbb{P}_i^{-1}$

GMRES with the tuned preconditioner

Recall

- $A\mathbb{P}_i^{-1}\tilde{y} = x^{(i)}$
- $A\mathbb{P}_i^{-1}Ax^{(i)} = Ax^{(i)}$

Is $x^{(i)}$ a “nice” RHS for $A\mathbb{P}^{-1}$?

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- No increase in inner iterations as i increases
- Explains the numerical results earlier

Theory for tuned preconditioner

- As before

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- Now introduce

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  - $\Rightarrow$ proof of independence of i

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  - $\Rightarrow$ proof of independence of i
- Subspace (block) version (Robbé/Sadkane/Sp.).

Outline

Numerical Example

- same PDE example as before ($5 \to 10$)
- $n = 2025$, $nz = 9945$
- ILU preconditioner, drop tolerance 0.1
- subspace dimension 6
- seek first 4 eigenvalues (stop when residual $\leq 10^{-8}$)

Unpreconditioned Block-GMRES

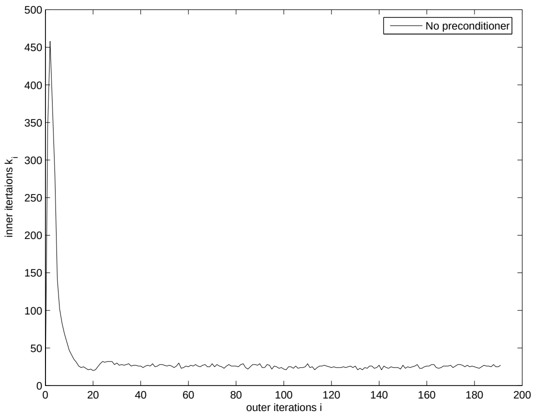

Figure: Inner iterations vs outer iterations

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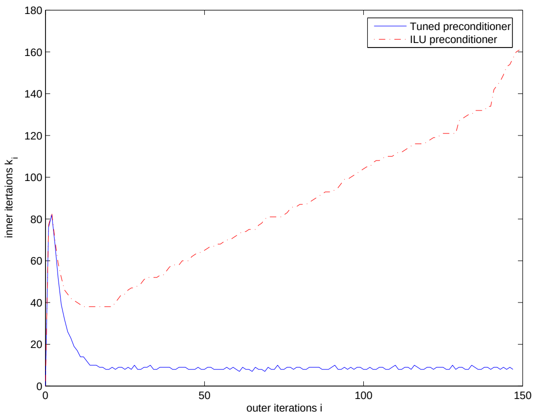

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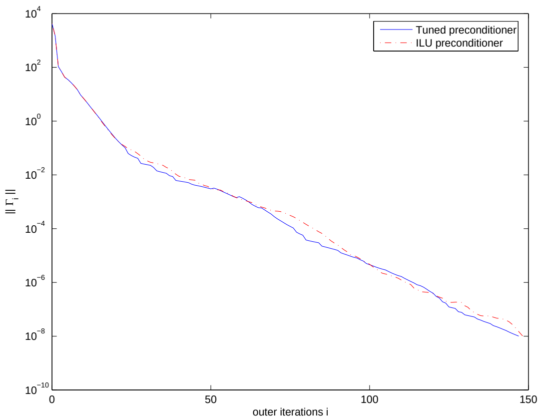

Figure: Residual norms vs outer iterations

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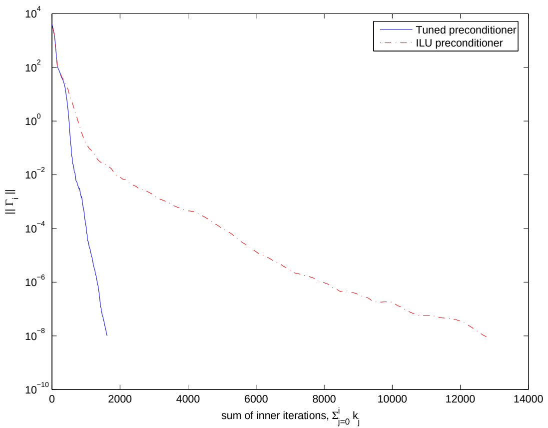
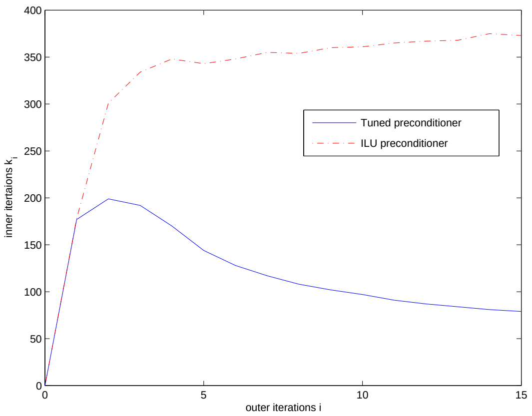


Figure: Residual norms vs total number of iterations

Numerical Example

- matrix market library `qc2534`
- complex symmetric (non-Hermitian)
- $n = 2534$, $nz = 463360$
- ILU preconditioner
- subspace dimension 16
- seek first 10 eigenvalues

Preconditioned GMRES



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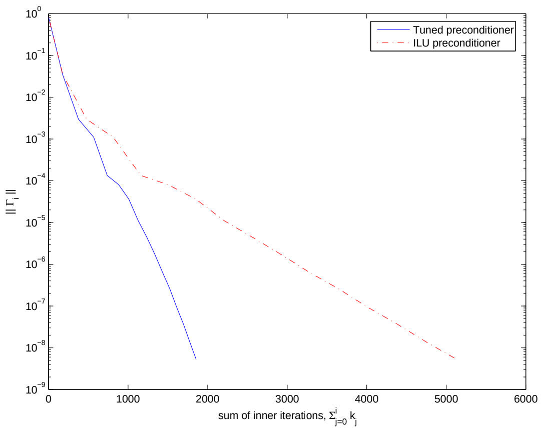

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RQI and J-D: Exact solves

Rayleigh quotient iteration

At each iteration a system of the form

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has to be solved.

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Jacobi-Davidson method

At each iteration a system of the form

$$(I - xx^H)(A - \rho(x)I)(I - xx^H)s = -r$$

has to be solved, where $r = (A - \rho(x)I)x$ is the eigenvalue residual and $s \perp x$.

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Exact solves

Sleijpen and van der Vorst (1996):

$$y = \alpha(x + s)$$

for some constant α

RQI and J-D: Inexact solves

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Galerkin-Krylov Solver

- Simoncini and Eldén (2002), (Hochstenbach and Sleijpen (2003) for two-sided RQ iteration):

$$y_{k+1} = \beta(x + s_k)$$

for some constant β if both systems are solved using a Galerkin-Krylov subspace method

RQI and J-D: Preconditioned Solves

Preconditioning for RQ iteration

At each iteration a system of the form

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

(with $y = P^{-1}\tilde{y}$) has to be solved.

RQI and J-D: Preconditioned Solves

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At each iteration a system of the form

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Preconditioning for JD method

At each iteration a system of the form

$$(I - xx^H)(A - \rho(x)I)(I - xx^H)\tilde{P}^{\dagger}\tilde{s} = -r$$

(with $s = \tilde{P}^{\dagger}\tilde{s}$) has to be solved. Note the restricted preconditioner

$$\tilde{P} := (I - xx^H)P(I - xx^H).$$

Equivalence does not hold!

Example: `sherman5.mtx`

fixed shift; (preconditioned) FOM as inner solver

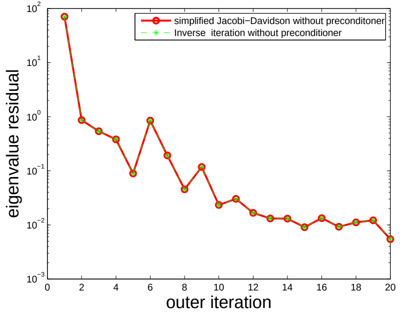

Figure: Convergence history of the eigenvalue residuals; no preconditioner

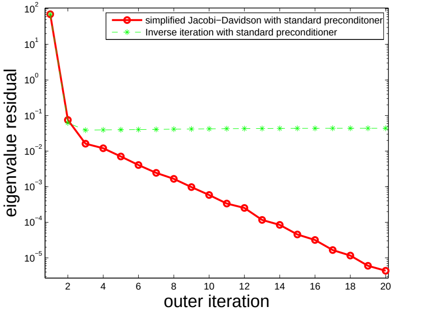

Figure: Convergence history of the eigenvalue residuals; standard preconditioner

Preconditioned Solves

Tuned RQI $\equiv$ preconditioned JD

$$\mathbb{P}x = x$$

Preconditioning for RQ iteration

Inner solves in RQ iteration builds Krylov space

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

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Preconditioning for JD method

Inner solves in JD method builds Krylov space

$$\text{span}\{r, \Pi_1(A - \rho(x)I)\Pi_2^P P^{-1}r, (\Pi_1(A - \rho(x)I)\Pi_2^P P^{-1})^2 r, \ldots\}$$

where $(I - xx^H)$ and $\Pi_2^P = I - \dfrac{P^{-1}xx^H}{x^H P^{-1}x}$.

Consider subspaces

$$A \leftarrow A - \rho(x)I$$

Lemma

The subspaces

$$\mathcal{K}_k = span\{x, A\mathbb{P}^{-1}x, (A\mathbb{P}^{-1})^2x, \ldots, (A\mathbb{P}^{-1})^k x\}$$

and

$$\mathcal{L}_k = span\{x, r, \Pi_1 A \Pi_2^P P^{-1} r, (\Pi_1 A \Pi_2^P P^{-1})^2 r, \ldots, (\Pi_1 A \Pi_2^P P^{-1})^{k-1} r\}$$

are equivalent.

Proof.

Based on Stathopoulos and Saad (1998). □

Equivalence for inexact solves

Theorem

Let both

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

and

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

be solved with the same Galerkin-Krylov method. Then

$$y_{k+1}^{RQ} = \gamma(x + s_k^{JD}).$$

Proof.

Based on Simoncini and Eldén (2002). □

Heuristic Explanation of RQI + $\mathbb{P} \equiv$ JD + P

- $\mathbb{P}x = x$
- $\mathbb{P} = P + (I - P)xx^H$
- $\mathbb{P} = xx^H + P(I - xx^H)$

Example: `sherman5.mtx`

fixed shift; (preconditioned) FOM as inner solver

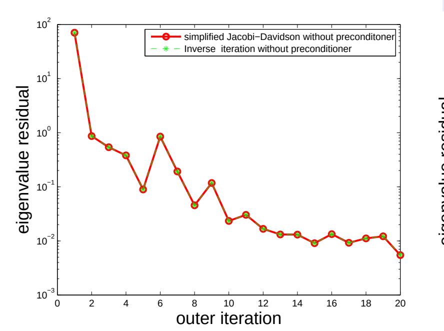

Figure: Convergence history of the eigenvalue residuals; no preconditioner

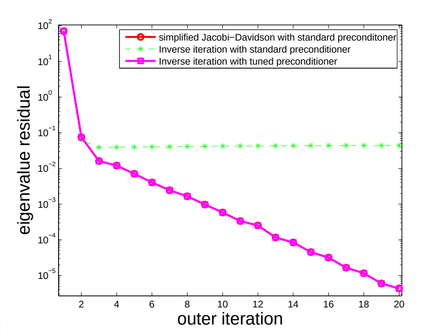

Figure: standard preconditioner for JD, tuned preconditioner for II

Outline

Conclusions

- When using Krylov solvers for shifted systems $(A - \sigma I)y = x^{(i)}$ in eigenvalue computations then it is best if the iteration matrix has a "good relationship" with the right hand side,
- For any preconditioner the "good relationship" is achieved by a small rank change called "tuning",
- essentially no extra costs,
- Numerical results on eigenvalue problems obtained from Mixed FEM Navier-Stokes with DD preconditioner show the same gains.

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