A Tuned Preconditioner for Inexact Inverse Iteration Applied to Hermitian Eigenvalue Problems

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Problem and Inverse Iteration

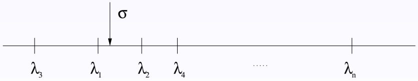
- Find an eigenvalue and eigenvector of s.p.d. A:

$$Ax = \lambda x,$$

- Inverse Iteration:

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

  A large, sparse.



Inexact Inverse Iteration

for $i = 1$ to $\dots$ **do**

choose $\tau^{(i)}$

solve

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

Rescale $x^{(i+1)} = \frac{y^{(i)}}{\|y^{(i)}\|}$,

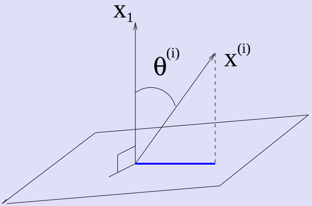
Update $\lambda^{(i+1)} = x^{(i+1)^T} A x^{(i+1)}$,

Eigenvalue residual $r^{(i+1)} = (A - \lambda^{(i+1)} I)x^{(i+1)}$.

end for

Error indicator

Error indicator (orthogonal decomposition, Parlett)



$P_{\perp} x^{(i)} = O(\sin \theta^{(i)})$ measure for the error

Eigenvalue residual

$$C|\sin\theta^{(i)}| \leq \|r^{(i)}\| \leq C'|\sin\theta^{(i)}|$$

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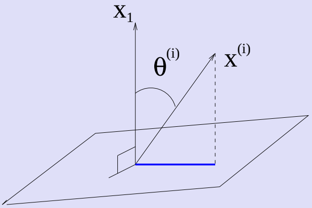

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Convergence rates of inexact inverse iteration

Decreasing tolerance $\tau^{(i)} \leq C\|r^{(i)}\| = \mathcal{O}(\sin\theta^{(i)})$

1. For decreasing tolerance $\tau^{(i)} \leq C\|r^{(i)}\| = \mathcal{O}(\sin\theta^{(i)})$ the inexact method recovers the rate of convergence achieved by exact solves.
2. Fixed shift σ: linear convergence. [see Golub/Ye 2000, Berns-Müller/Graham/Spence 2005]
3. Rayleigh quotient shift $\sigma^{(i)} = \rho(x^{(i)}) = \frac{x^{(i)T}Ax^{(i)}}{x^{(i)T}x^{(i)}}$: cubic convergence. [see Smit/Paardekooper 1999, Berns-Müller/Graham/Spence 2005]

Unpreconditioned solves with MINRES

Convergence rates for solves with MINRES for simple eigenvalue

If A is positive definite and has a simple eigenvalue then

$$\|x^{(i)} - (A - \sigma I)y_k^{(i)}\|_2 \leq 2\frac{|\lambda_1 - \lambda_n|}{|\lambda_1 - \sigma|}\left(\sqrt{\frac{\kappa_1 - 1}{\kappa_1 + 1}}\right)^{k-1} \|\mathcal{P}_1^{\perp} x^{(i)}\|_2.$$

Number of inner solves for each i

$$k^{(i)} \geq C_1 + C_2 \log\left(\frac{\|\mathcal{P}_1^{\perp} x^{(i)}\|_2}{|\lambda_1 - \sigma|\tau^{(i)}}\right)$$

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Example

For fixed shift σ, and $\tau^{(i)} \leq C \|r^{(i)}\| = \mathcal{O}(\sin \theta^{(i)})$ the number of inner solves $k^{(i)}$ for each i does not increase with i

Preconditioning

Incomplete Cholesky preconditioning

$$A = LL^T + E$$

symmetric preconditioning of $(A - \sigma I)y^{(i)} = x^{(i)}$:

$$L^{-1}(A - \sigma I)L^{-T}\tilde{y}^{(i)} = L^{-1}x^{(i)}, \quad y^{(i)} = L^{-T}\tilde{y}^{(i)}$$

Remarks

1. changes number of inner iterations

$$k^{(i)} \geq C_1 + C_2 \log\left(\frac{\|L^{-1}\|}{|\lambda_1 - \sigma|\tau^{(i)}}\right)$$

2. $k^{(i)}$ increases with i for $\tau^{(i)} \leq C\|r^{(i)}\|$.

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Derivation

Aims

1. modify $L \longrightarrow \mathbb{L}$

$$\mathbb{L}^{-1}(A - \sigma I)\mathbb{L}^{-T}\tilde{y}^{(i)} = \mathbb{L}^{-1}x^{(i)}, \quad y^{(i)} = \mathbb{L}^{-T}\tilde{y}^{(i)}$$

2. minor extra computation cost for $\mathbb{L}$
3. "nice" RHS $\mathbb{L}^{-1}x^{(i)}$ (same behaviour as unpreconditioned solves, e.g. for fixed shifts $k^{(i)}$ does not increase with i)

Condition

$$\mathbb{L}^{-T}\mathbb{L}^{-1}x^{(i)} = x^{(i)} \quad \text{or} \quad \mathbb{L}\mathbb{L}^{T}x^{(i)} = Ax^{(i)}$$

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Choice of $\mathbb{L}$

Theorem

With $e^{(i)} = Ax^{(i)} - LL^T x^{(i)}$ (known) and $\mathbb{L}$ chosen such that

$$\mathbb{L} = L + \alpha^{(i)} e^{(i)} e^{(i)^T} L^{-T}$$

with $\alpha^{(i)}$ root of quadratic function we get $\mathbb{L}\mathbb{L}^T x^{(i)} = Ax^{(i)}$.

$\mathbb{L}$ is a rank-one update of L.

Convergence rates

The tuned preconditioner

1. retains outer convergence rates
2. provides cheap inner solves

$$k^{(i)} \geq C_1 + C_2 \log\left(\gamma \frac{|\sin \theta^{(i)}|}{|\lambda_1 - \sigma|\tau^{(i)}}\right)$$

3. only a single extra back substitution with L per outer iteration needed

Fixed shift solves

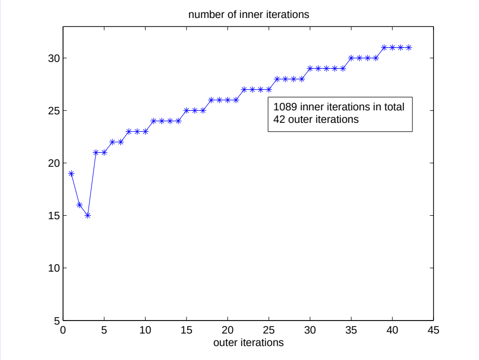
SPD matrix from the Matrix Market library `bscsstk10.mtx`

`Setup:`

- `decreasing tolerance` $\tau^{(i)}$,
- `drop tolerance` 10^{-3},
- `stopping condition:` $\|r^{(i)}\| \leq 10^{-10}$.

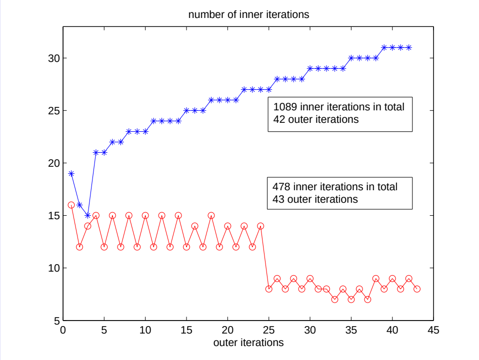
Fixed shift solves

Preconditioning with standard incomplete Cholesky



Fixed shift solves

Preconditioning with tuned incomplete Cholesky



Solves with Rayleigh quotient shifts

Central finite difference approximation of the self-adjoint elliptic operator

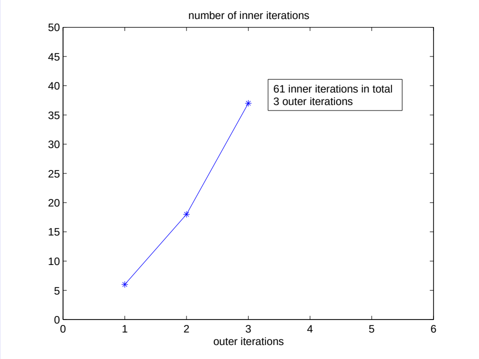
$$\mathcal{A}(t)u = ((1+tx)u_x)_x + ((1+ty)u_y)_y$$

on an equidistant grid on the unit square with Dirichlet boundary conditions and 50 nodes in each dimension. Setup:

- decreasing tolerance $\tau^{(i)}$,
- drop tolerance 10^{-2},
- stopping condition: $\|r^{(i)}\| \leq 10^{-14}$.

Solves with Rayleigh quotient shifts

Preconditioning with standard incomplete Cholesky



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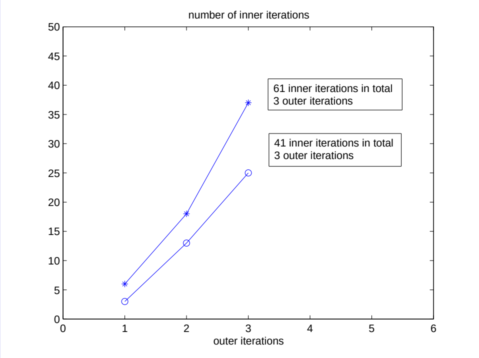
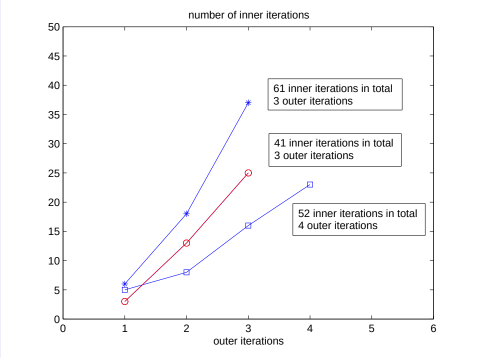


Solves with Rayleigh quotient shifts

Preconditioning with Simoncini & Eldén incomplete Cholesky



Solves with Rayleigh quotient shifts

Iteration numbers and error $\|Ax^{(i)} - \lambda^{(i)}x^{(i)}\|_2$

	Incompl. Cholesky		*Tuned precond.*		*Simoncini & Eldén*	
	Drop Tolerances					
	It.		It.		It.	
		1.0e-2		1.0e-2		1.0e-2
1	6	1.2e-3	3	2.8e-3	5	2.1e-3
2	18	1.9e-6	13	1.9e-6	8	2.5e-5
3	37	8.6e-15	25	5.1e-15	16	2.6e-9
4					23	2.6e-15
total	61		41		52	

M. A. Freitag and A. Spence, *Convergence rates for inexact inverse iteration with application to preconditioned iterative solves*, 2005.
Submitted to BIT.

———, *A tuned preconditioner for inexact inverse iteration applied to Hermitian eigenvalue problems*, 2005.
In preparation.