Rayleigh Quotient iteration and simplified Jacobi-Davidson method with preconditioned iterative solves

Melina Freitag

Department of Mathematical Sciences
University of Bath

10th Copper Mountain Conference on Iterative Methods, 2008
Copper Mountain, Colorado
10th April 2008

joint work with Alastair Spence (Bath)

Problem and iterative methods

Find a small number of eigenvalues close to a shift σ and corresponding eigenvectors of:

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

- A is large, sparse, nonsymmetric

Problem and iterative methods

Find a small number of eigenvalues close to a shift σ and corresponding eigenvectors of:

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

- A is large, sparse, nonsymmetric
- Iterative solves (e.g. Power method)

Problem and iterative methods

Find a small number of eigenvalues close to a shift σ and corresponding eigenvectors of:

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

- A is large, sparse, nonsymmetric
- Iterative solves (e.g. Power method)
- Problem becomes
$$(A - \sigma I)^{-1} x = \frac{1}{\lambda - \sigma} x$$
- each step of the iterative method involves repeated application of $(A - \sigma I)^{-1}$ to a vector (inverse iteration)

Problem and iterative methods

Find a small number of eigenvalues close to a shift σ and corresponding eigenvectors of:

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

- A is large, sparse, nonsymmetric
- Iterative solves (e.g. Power method)
- Problem becomes
$$(A - \sigma I)^{-1}x = \frac{1}{\lambda - \sigma}x$$
- each step of the iterative method involves repeated application of $(A - \sigma I)^{-1}$ to a vector (inverse iteration)
- Inner iterative solve:
$$(A - \sigma I)y = x$$
using Krylov or Galerkin-Krylov method for linear systems.
- leading to inner-outer iterative method.

Shift-invert strategy

This talk:
Inner Iteration and preconditioning

Comparison of two methods: Inexact Rayleigh quotient iteration and Simplified Jacobi-Davidson method

The algorithms

Inexact Rayleigh quotient iteration

solve

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

inexactly.

Rescale $x^{(i+1)} = \frac{y^{(i)}}{\|y^{(i)}\|}$ and update $\rho(x^{(i+1)}) = x^{(i+1)^H} A x^{(i+1)}$,

Test: eigenvalue residual $r^{(i+1)} = (A - \rho(x^{(i+1)})I)x^{(i+1)}$.

The algorithms

Inexact Rayleigh quotient iteration

solve

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

inexactly.

Rescale $x^{(i+1)} = \frac{y^{(i)}}{\|y^{(i)}\|}$ and update $\rho(x^{(i+1)}) = x^{(i+1)^H} A x^{(i+1)}$,

Test: eigenvalue residual $r^{(i+1)} = (A - \rho(x^{(i+1)})I)x^{(i+1)}$.

Inexact simplified Jacobi-Davidson method (without subspace expansion)

solve

$$(I - x^{(i)}x^{(i)^H})(A - \rho(x^{(i)})I)(I - x^{(i)}x^{(i)^H})s^{(i)} = -r^{(i)},$$

Rescale $x^{(i+1)} = \frac{x^{(i)} + s^{(i)}}{\|x^{(i)} + s^{(i)}\|}$ and update $\rho(x^{(i+1)}) = x^{(i+1)^H} A x^{(i+1)}$,

Test: eigenvalue residual $r^{(i+1)} = (A - \rho(x^{(i+1)})I)x^{(i+1)}$.

An experiment

Matrix **sherman5.mtx** Rayleigh quotient shift; FOM as inner solver

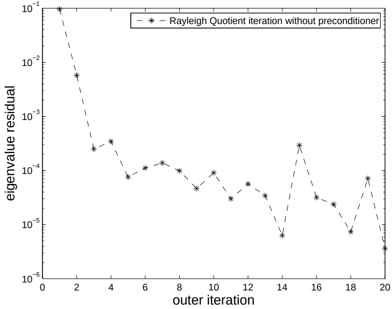

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - without preconditioner

An experiment

Matrix **sherman5.mtx** Rayleigh quotient shift; FOM as inner solver

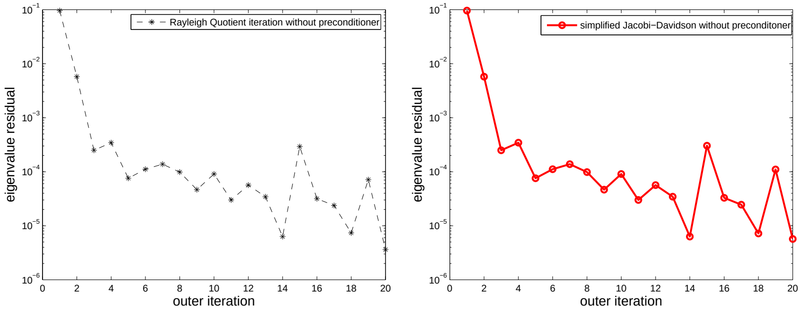

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - without preconditioner

An experiment

Matrix **sherman5.mtx** Rayleigh quotient shift; FOM as inner solver

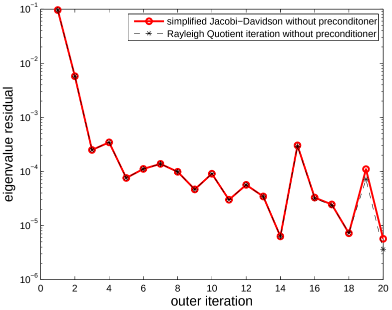

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - without preconditioner

An experiment

Matrix **sherman5.mtx** Rayleigh quotient shift; preconditioned FOM as inner solver

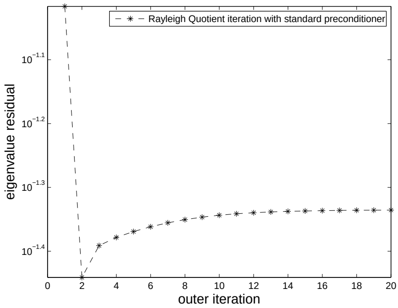

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - with preconditioner P_1

An experiment

Matrix **`sherman5.mtx`** Rayleigh quotient shift; preconditioned FOM as inner solver

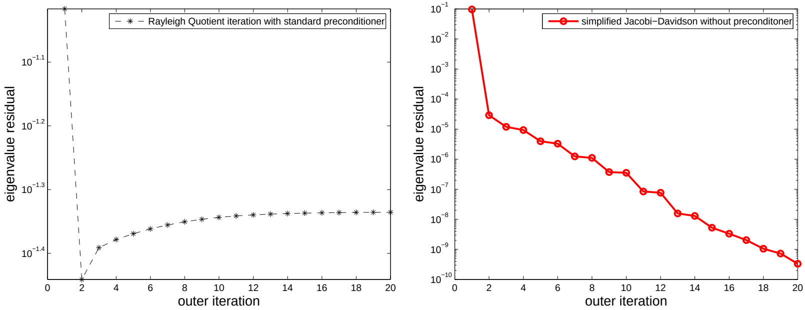

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - with preconditioner P_1

An experiment

Matrix **sherman5.mtx** Rayleigh quotient shift; preconditioned FOM as inner solver

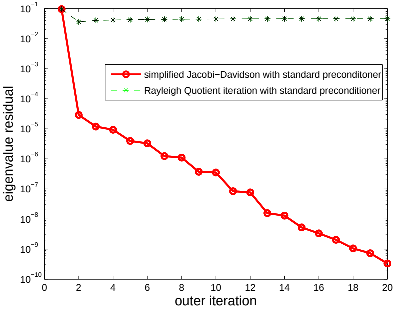

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - with preconditioner P_1

An experiment

Matrix **`sherman5.mtx`** Rayleigh quotient shift; preconditioned FOM as inner solver

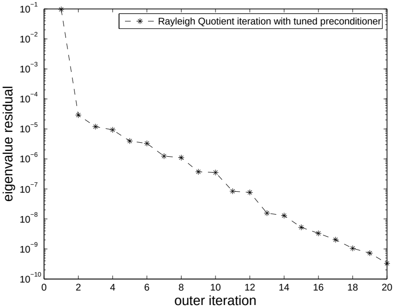

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - with preconditioner P_2

An experiment

Matrix **sherman5.mtx** Rayleigh quotient shift; preconditioned FOM as inner solver

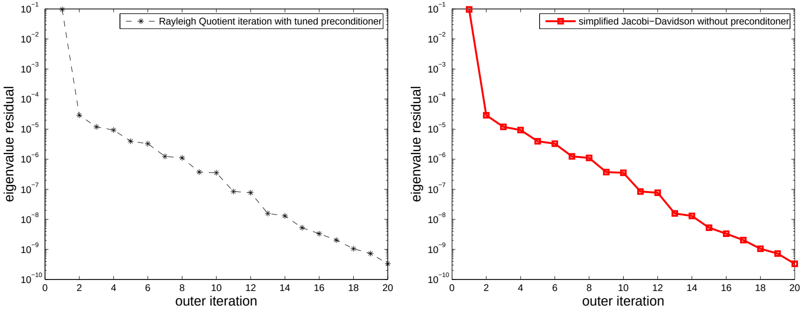

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - with preconditioner P_2

An experiment

Matrix **sherman5.mtx** Rayleigh quotient shift; preconditioned FOM as inner solver

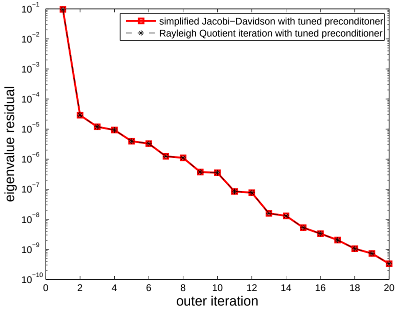

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - with preconditioner P_2

Rayleigh quotient iteration and Jacobi-Davidson: Exact solves

Rayleigh quotient iteration

Solve

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

at each outer iteration.

Rayleigh quotient iteration and Jacobi-Davidson: Exact solves

Rayleigh quotient iteration

Solve

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

at each outer iteration.

Jacobi-Davidson method

Solve

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

at each outer iteration, where $r = (A - \rho(x)I)x$ is the eigenvalue residual and $s \perp x$.

Rayleigh quotient iteration and Jacobi-Davidson: Exact solves

Rayleigh quotient iteration

Solve

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

at each outer iteration.

Jacobi-Davidson method

Solve

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

at each outer iteration, where $r = (A - \rho(x)I)x$ is the eigenvalue residual and $s \perp x$.

Exact solves

Sleijpen and van der Vorst (1996):

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

for some constant α. Solutions are equivalent!

Rayleigh quotient iteration and Jacobi-Davidson: Exact solves

Rayleigh quotient iteration

Solve

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

at each outer iteration.

Jacobi-Davidson method

Solve

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

at each outer iteration, where $r = (A - \rho(x)I)x$ is the eigenvalue residual and $s \perp x$.

Exact solves

Sleijpen and van der Vorst (1996):

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

for some constant α. Solutions are equivalent!

Rayleigh quotient iteration and Jacobi-Davidson: Exact solves

Rayleigh quotient iteration

Solve

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

at each outer iteration.

Jacobi-Davidson method

Solve

$$(A - \rho(x)I)s - \gamma x = -(A - \rho(x)I)x$$

at each outer iteration, where $r = (A - \rho(x)I)x$ is the eigenvalue residual and $s \perp x$.

Exact solves

Sleijpen and van der Vorst (1996):

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

for some constant α. Solutions are equivalent!

Rayleigh quotient iteration and Jacobi-Davidson: Inexact solves

Rayleigh quotient iteration

Solve

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

at each outer iteration.

Jacobi-Davidson method

Solve

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

at each outer iteration, where $r = (A - \rho(x)I)x$ is the eigenvalue residual and $s \perp x$.

Galerkin-Krylov Solver

- Simoncini and Eldén (2002), (Hochstenbach and Sleijpen (2003) for two-sided RQ iteration), based on result by Stathopoulos and Saad (1998)

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

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

An experiment - Inexact solves

Matrix **sherman5.mtx** Rayleigh quotient shift; FOM as inner solver

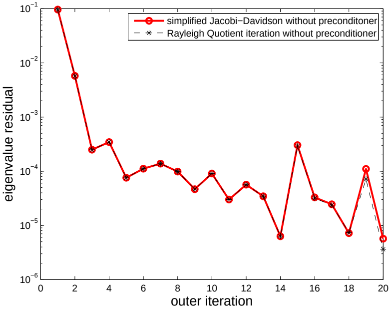

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - without preconditioner

Rayleigh quotient iteration and Jacobi-Davidson: Preconditioned Solves

Preconditioning for RQ iteration

Solve

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

(with $y = P^{-1}\tilde{y}$) at each iteration.

Preconditioning for JD method

Solve

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

(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!

An experiment - with standard preconditioner

Matrix **sherman5.mtx** Rayleigh quotient shift; preconditioned FOM as inner solver

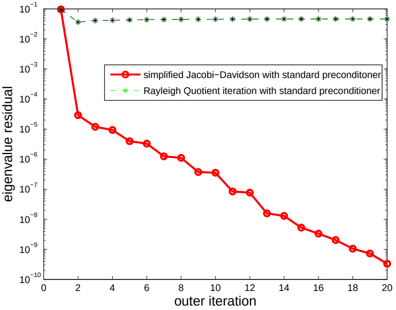

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - with standard preconditioner

Preconditioners

Need a better preconditioner for Rayleigh quotient iteration.

The tuned preconditioner

Advantage of Jacobi-Davidson

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

(with $s = \tilde{P}^\dagger \tilde{s}$). The preconditioner

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

is restricted (to the subspace orthogonal to x).

The tuned preconditioner

Advantage of Jacobi-Davidson

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

(with $s = \tilde{P}^\dagger \tilde{s}$). The preconditioner

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

is restricted (to the subspace orthogonal to x).

The new (tuned) preconditioner for inexact Rayleigh quotient iteration

Use

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

which satisfies

$$\mathbb{P}x = x \quad \text{as well as} \quad \mathbb{P}^{-1}x = x$$

The tuned preconditioner

Implementation

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

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

The tuned preconditioner

Implementation

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

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

minor modification and minor extra computational cost

$$\mathbb{P}^{-1} = P^{-1} - \frac{(P^{-1}x - x)x^H P^{-1}}{x^H P^{-1} x}$$

Preconditioned Solves for inexact Rayleigh Quotient iteration and inexact Jacobi-Davidson

Tuned preconditioner in RQI $\equiv$ preconditioned JD

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

RQ iteration with preconditioner $\mathbb{P}$: $(A - \rho(x)I)\mathbb{P}^{-1}\mathbf{y} = \mathbf{x}$

Inner solves in RQ iteration build Krylov space

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

Preconditioned Solves for inexact Rayleigh Quotient iteration and inexact Jacobi-Davidson

Tuned preconditioner in RQI ≡ preconditioned JD

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

RQ iteration with preconditioner $\mathbb{P}$: $(A-\rho(x)I)\mathbb{P}^{-1}\mathbf{y} = \mathbf{x}$

Inner solves in RQ iteration build Krylov space

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

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

Inner solves in JD method build Krylov space

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

where $\Pi_1 = (I-xx^H)$ and $\Pi_2^P = I - \dfrac{P^{-1}xx^H}{x^HP^{-1}x}$.

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.

Extension of result by 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.

Extension of result by Simoncini and Eldén (2002). □

Example

`sherman5.mtx`; Rayleigh quotient shift; preconditioned FOM as inner solver

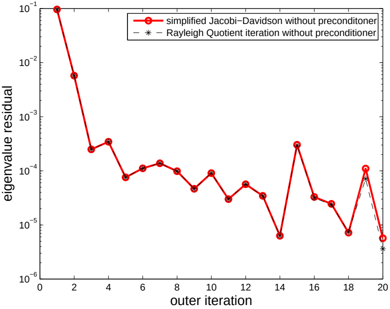

Figure: Convergence history of the eigenvalue residuals; no preconditioner.

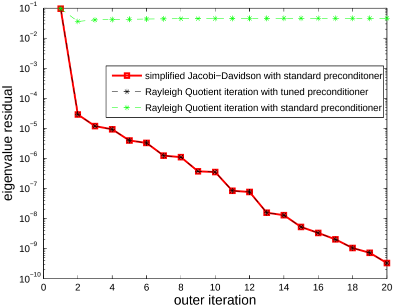

Figure: standard preconditioner for JD, tuned preconditioner for RQ Iteration $P_2 = \mathbb{P}$.

Equivalence between preconditioned JD and preconditioned RQI

Technique applies to *any* preconditioner for linear systems.

Fixed shifts

Matrix **sherman5.mtx** Fixed shift; preconditioned FOM as inner solver

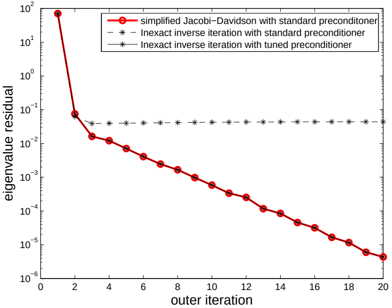

Figure: Inexact inverse iteration and Jacobi-Davidson method - standard and tuned preconditioner

Petrov-Galerkin method (GMRES)

$$\|r_k^{FOM}\| = \frac{\|r_k^{GMRES}\|}{\sqrt{1-(\|r_k^{GMRES}\|/\|r_{k-1}^{GMRES}\|)^2}}.$$

Matrix **sherman5.mtx** Fixed shift; preconditioned GMRES as inner solver

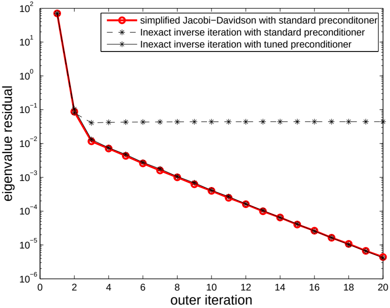

Figure: Inexact inverse iteration and Jacobi-Davidson method - standard and tuned preconditioner

Petrov-Galerkin method (GMRES)

$$\|r_k^{FOM}\| = \frac{\|r_k^{GMRES}\|}{\sqrt{1-(\|r_k^{GMRES}\|/\|r_{k-1}^{GMRES}\|)^2}}.$$

Matrix `sherman5.mtx` Fixed shift; preconditioned GMRES as inner solver

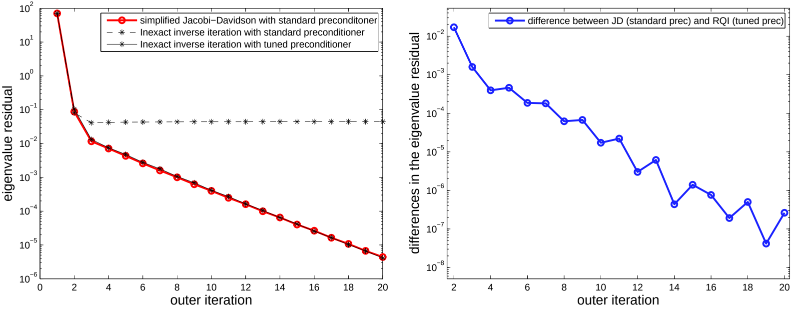

Figure: Inexact inverse iteration and Jacobi-Davidson method - standard and tuned preconditioner

Improvement $\mathbb{P}x = Ax$

The tuned preconditoner $\mathbb{P}x = Ax$

Instead of

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

use

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

which satisfies $\mathbb{P}x = Ax$

Improvement $\mathbb{P}x = Ax$

The tuned preconditoner $\mathbb{P}x = Ax$

Instead of

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

use

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

which satisfies $\mathbb{P}x = Ax$

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

minor modification and minor extra computational cost

$$\mathbb{P}^{-1} = P^{-1} - \frac{(P^{-1}Ax - x)x^H P^{-1}}{x^H P^{-1} Ax}$$

Tuning with $\mathbb{P}x = Ax$

Matrix **sherman5.mtx** Rayleigh quotient shift; preconditioned FOM as inner solver

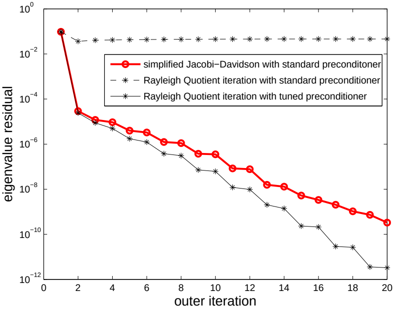

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - standard and tuned preconditioner

Generalised eigenproblem $Ax = \lambda Mx$

Solving

$$(A - \rho(\mathbf{x})M)\mathbb{P}^{-1}\tilde{y} = Mx, \quad \text{with} \quad y = \mathbb{P}^{-1}\tilde{y},$$

and

$$(I - \frac{Mxx^H M^H}{x^H M^H Mx})(A - \rho(\mathbf{x})M)(I - xu^H)\tilde{P}^\dagger \tilde{s} = -\mathbf{r}, \quad \text{with} \quad s = \tilde{P}^\dagger \tilde{s},$$

using the same Galerkin-Krylov method and $\mathbb{P}x = Mx$ are equivalent.

Generalised eigenproblem $Ax = \lambda Mx$

Use $\mathbb{P}x = Mx$ Matrix `sherman5.mtx` with a pos. def. tridiagonal M
Rayleigh quotient shift; preconditioned FOM as inner solver

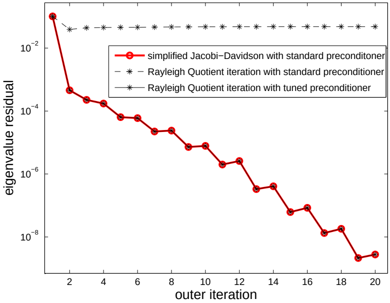

Figure: Rayleigh quotient iteration and Jacobi-Davidson method - standard and tuned preconditioner

Another motivation for $\mathbb{P}x = Ax$

More detailed GMRES theory for $(A - \sigma I)y = x$

$$\|x - (A - \sigma I)y_k\| \leq \tilde{\kappa}(W) \frac{|\lambda_2 - \lambda_1|}{\lambda_1} \min_{p \in \mathcal{P}_{k-1}} \max_{j=2,\ldots,n} |p(\lambda_j)| \|\mathcal{Q}x\| \leq \tau$$

where λ_j are eigenvalues of $A - \sigma I$.

Number of inner iterations

$$k \geq C_1 + C_2 \log \frac{\|\mathcal{Q}x\|}{\tau},$$

where $\mathcal{Q}$ projects onto the space *not* spanned by the eigenvector.

Another motivation for $\mathbb{P}x = Ax$

Good news!

$$k^{(i)} \geq C_1 + C_2 \log \frac{C_3\|r^{(i)}\|}{\tau^{(i)}},$$

where $\tau^{(i)} = C\|r^{(i)}\|$. Iteration number approximately constant!

Another motivation for $\mathbb{P}x = Ax$

Good news!

$$k^{(i)} \geq C_1 + C_2 \log \frac{C_3 \|r^{(i)}\|}{\tau^{(i)}},$$

where $\tau^{(i)} = C\|r^{(i)}\|$. Iteration number approximately constant!

Bad news :-(

For a standard preconditioner P

$$(A - \sigma I)P^{-1}\tilde{y}^{(i)} = x^{(i)} \qquad P^{-1}\tilde{y}^{(i)} = y^{(i)}$$

$$k^{(i)} \geq C_1' + C_2' \log \frac{\|\tilde{\mathcal{Q}}x^{(i)}\|}{\tau^{(i)}} = C_1' + C_2' \log \frac{C}{\tau^{(i)}},$$

where $\tau^{(i)} = C\|r^{(i)}\|$. Iteration number increases!

Another motivation for $\mathbb{P}x = Ax$

How to overcome this problem

Use tuned preconditioner:

$$\mathbb{P}_i x^{(i)} = Ax^{(i)}, \quad \mathbb{P}_i := P + (A - P)x^{(i)}{x^{(i)}}^H$$

Why does that work?

Assume we have found eigenvector x_1

$$Ax_1 = \mathbb{P}x_1 = \lambda_1 x_1 \quad \Rightarrow \quad (A - \sigma I)\mathbb{P}^{-1}x_1 = \frac{\lambda_1 - \sigma}{\lambda_1}x_1$$

and convergence of Krylov method applied to $(A - \sigma I)\mathbb{P}^{-1}\tilde{y} = x_1$ in one iteration. For general $x^{(i)}$

$$k^{(i)} \geq C_1' + C_2' \log \frac{C_3\|r^{(i)}\|}{\tau^{(i)}}, \quad \text{where} \quad \tau^{(i)} = C\|r^{(i)}\|.$$

Convection-Diffusion operator

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 $\tau^{(i)} = 0.01\|r^{(i)}\|$,
- standard and tuned preconditioner (incomplete LU).

Convection-Diffusion operator

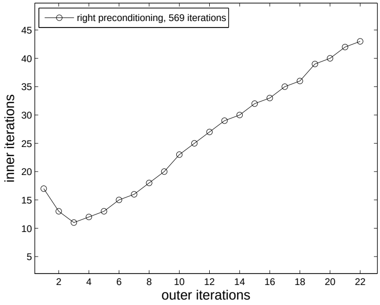

Figure: Inner iterations vs outer iterations

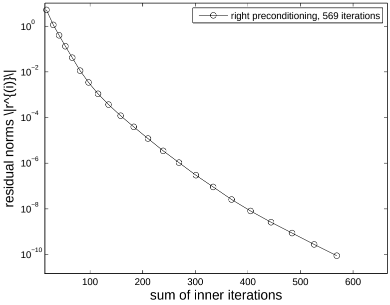

Figure: Eigenvalue residual norms vs total number of inner iterations

Convection-Diffusion operator

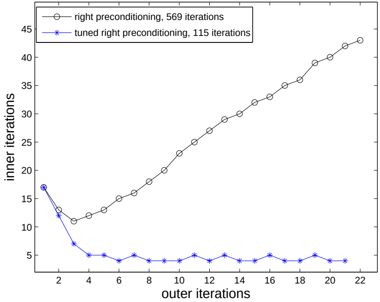

Figure: Inner iterations vs outer iterations

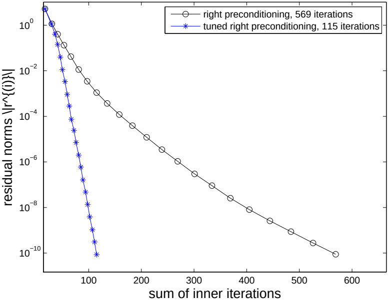

Figure: Eigenvalue residual norms vs total number of inner iterations

Extensions

Possible Extensions (ongoing work)

1. subspace iteration
2. Shift-invert Arnoldi iteration using a tuned preconditioner

$$\mathbb{P}_i Q^{(i)} = AQ^{(i)}; \quad \text{given by} \quad \mathbb{P}_i = P + (A - P)Q^{(i)}{Q^{(i)}}^H$$

is equivalent to the Jacobi-Davidson method with a standard preconditioner

Numerical Example

`sherman5.mtx` matrix from the Matrix Market library (3312×3312).

- smallest eigenvalue: $\lambda_1 \approx 4.69 \times 10^{-2}$,
- Preconditioned GMRES as inner solver (fixed tolerance and relaxation strategy),
- standard and tuned preconditioner (incomplete LU).

No tuning and standard preconditioner

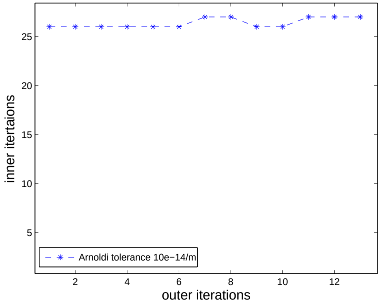

Figure: Inner iterations vs outer iterations

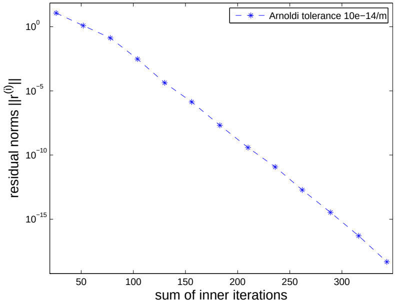

Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning

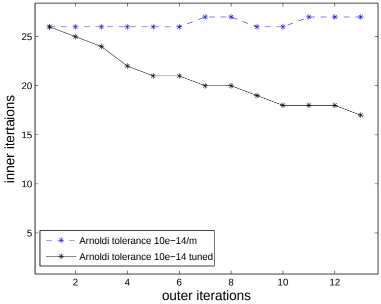

Figure: Inner iterations vs outer iterations

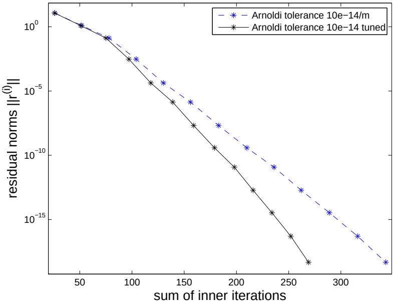

Figure: Eigenvalue residual norms vs total number of inner iterations

Conclusions

- For eigencomputations it is advantageous to consider modified preconditioners (works for any preconditioner)
- Analysis provides further understanding of preconditioned Jacobi-Davidson method
- Numerical results on eigenvalue problems obtained from Mixed FEM Navier-Stokes with DD preconditioner show the same gains.

- M. A. Freitag and A. Spence, *Convergence rates for inexact inverse iteration with application to preconditioned iterative solves*, BIT, 47 (2007), pp. 27–44.
- ——, *Convergence theory for inexact inverse iteration applied to the generalised nonsymmetric eigenproblem*, Electron. Trans. Numer. Anal., 28 (2007), pp. 40–64.
- ——, *Rayleigh quotient iteration and simplified Jacobi-Davidson method with preconditioned iterative solves*, Linear Algebra Appl., 428 (2008), pp. 2049–2060.
- M. Robbé, M. Sadkane, and A. Spence, *Inexact inverse subspace iteration with preconditioning applied to non-Hermitian eigenvalue problems*, 2007.
  To appear in SIAM J. Matrix Anal. Appl.
- F. Xue and H. C. Elman, *Convergence analysis of iterative solvers in inexact Rayleigh quotient iteration*, Preprint UMCP-CSD:CS-TR-4902, University of Maryland, Department of Computer Science and Institute for Advanced Computer Studies, 2008.