Preconditioned inexact inverse iteration and inexact shift-invert Arnoldi method

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SAMBa Student-Led Symposium
Preparation for ITT2
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Outline

1. Introduction

2. Inexact inverse iteration

3. Inexact Shift-invert Arnoldi method

4. Conclusions

Motivation

Alastairs lecture:

$$(I - \sigma_s K_\sigma)\Phi = \lambda \nu \sigma_f K_\sigma \Phi,$$

- Eigenvalue problem arising from reactor criticality computation
- Theory on the derivation in the thesis by Fynn Scheben
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- In this talk: $B = I$ (but all results extend to $B \neq I$)

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  - Power method
  - Simultaneous iteration
  - Arnoldi method
  - Jacobi-Davidson method
- repeated application of the matrix A to a vector
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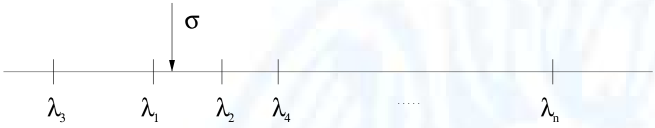
Shift-invert strategy

- Wish to find a few eigenvalues close to a shift σ



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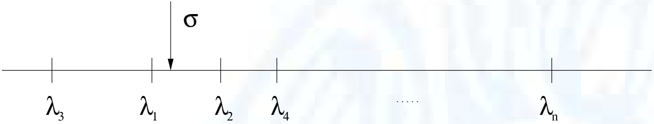

- Problem becomes

$$(A - \sigma I)^{-1} x = \frac{1}{\lambda - \sigma} x$$

- each step of the iterative method involves repeated application of $\mathcal{A} = (A - \sigma I)^{-1}$ to a vector
- Inner iterative solve:

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

  using Krylov method for linear systems. (CG, MINRES, GMRES, ...)
- leading to inner-outer iterative method.

Shift-invert strategy

This talk:

Convergence of outer iteration

Inner iteration and preconditioning

Inverse iteration and Arnoldi method

Outline

Classical methods for finding one eigenvalue

Inverse iteration/Rayleigh quotient iteration

INPUT: Matrix A shift $\sigma \approx \lambda$, initial vector x_0 with $\|x_0\| = 1$.
OUTPUT: Approximate eigenpair (λ, x)
for $i = 1$ to $\dots$ **do**
  Choose shift σ.
  Solve for $\hat{x}$
$$(A - \sigma I)\hat{x} = x$$
  Rescale $x = \dfrac{\hat{x}}{\|\hat{x}\|}$,
  Update $\lambda = \rho(x) = x^H A x$,
  Test for convergence (using eigenvalue residual ($r = (A - \lambda I)x$).
end for

Inexact Inverse iteration/Inexact Rayleigh quotient iteration

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for $i = 1$ to $\ldots$ **do**
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  Run k steps of a Krylov subspace method to obtain $\hat{x}$ such that

$$0 \leq \|(A - \sigma I)\hat{x} - x\| \leq \xi,$$

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Classical methods for finding one eigenvalue

Convergence rates of exact methods

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- Rayleigh quotient iteration (RQI): cubic convergence for normal A (otherwise quadratic)

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Convergence rate analysis of inexact methods

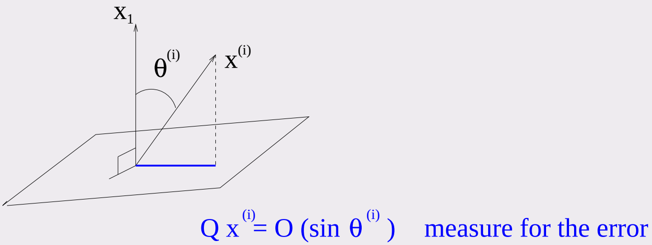
Main requirement: decreasing accuracy of the inner solves:

$$\xi^{(i+1)} \leq \xi^{(i)}$$

The convergence speed of the exact methods can be re-established.
[Lai/Lin/Lin '97, Golub/Ye '00, Simoncini/Elden '02, F./Spence '07, Elman/Xue '09, ...]

Error indicator

Error indicator (Orthogonal decomposition, symmetric A)



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

Generalisations to nonsymmetric A exist.

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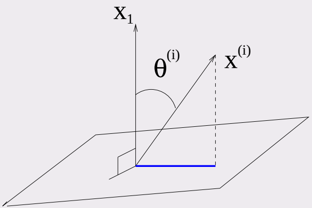

Q x$^{(i)}$ = O (sin θ$^{(i)}$)   measure for the error

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Eigenvalue residual

$$C_1 |\sin\theta^{(i)}| \leq \|r^{(i)}\| \leq C_2 |\sin\theta^{(i)}|$$

Convergence rates of inexact inverse iteration - independent of the inner solver

Error in θ (eigenvector)

$$\tan\theta^{(i+1)} \leq \frac{|\lambda_1 - \sigma^{(i)}|}{|\lambda_2 - \sigma^{(i)}|} T^{(i)}$$

- Exact solves: $T^{(i)} = \tan\theta^{(i)}$
- Inexact solves $T^{(i)} = \dfrac{|\sin\theta^{(i)}| + \|(I - x_1 x_1^*) s^{(i)}\|}{|\cos\theta^{(i)} - \|x_1^* s^{(i)}\|}$, $\quad \|s^{(i)}\| \leq \xi^{(i)}$

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Choice of τ

- Choice 1: $\xi^{(i)} = C\|r^{(i)}\| = \mathcal{O}(\sin\theta^{(i)}) \Rightarrow T^{(i)} = \mathcal{O}(\tan\theta^{(i)})$
- Choice 2: $\xi^{(i)} = \text{constant} \Rightarrow T^{(i)} = \mathcal{O}(1)$

Classical methods for finding one eigenvalue

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Convergence rates

If the solve tolerance is decreased, i.e.

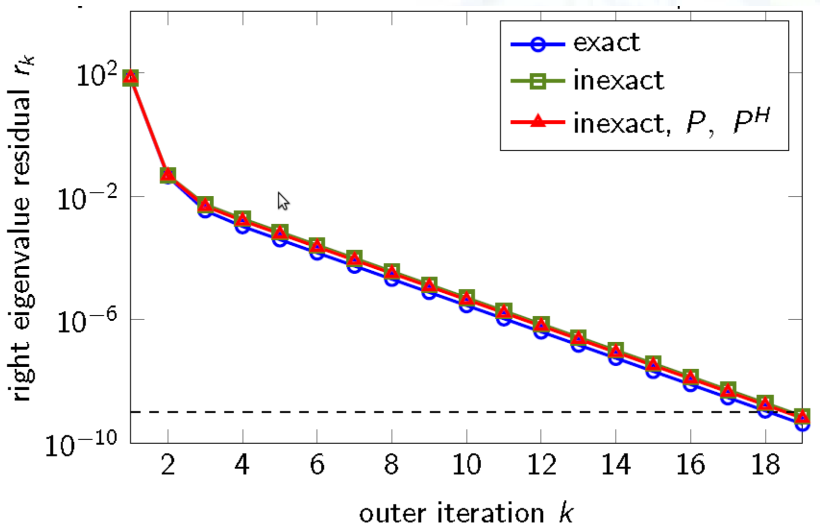
$$\xi^{(i)} = C\|r^{(i)}\|$$

then convergence rate is linear (same convergence rate as for exact solves).

Example: matrix `sherman5`, $n = 3312$, fixed shift $\sigma = 0$.

- exact solution (Matlab backslash)
- inexact solution (full GMRES) with decreasing tolerance
- termination when $\|r^{(i)}\| \leq 10^{-9}$, where
- preconditioned GMRES with incomplete LU preconditioners P

Example: matrix `sherman5`, $n = 3312$, fixed shift $\sigma = 0$.



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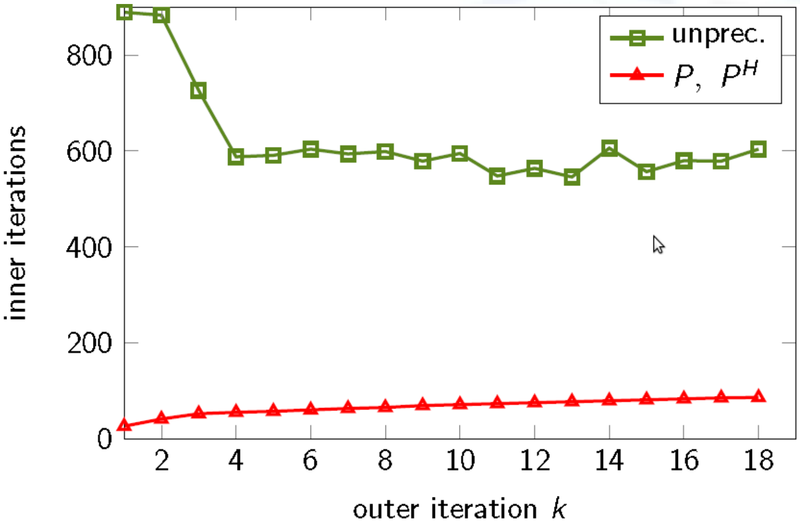

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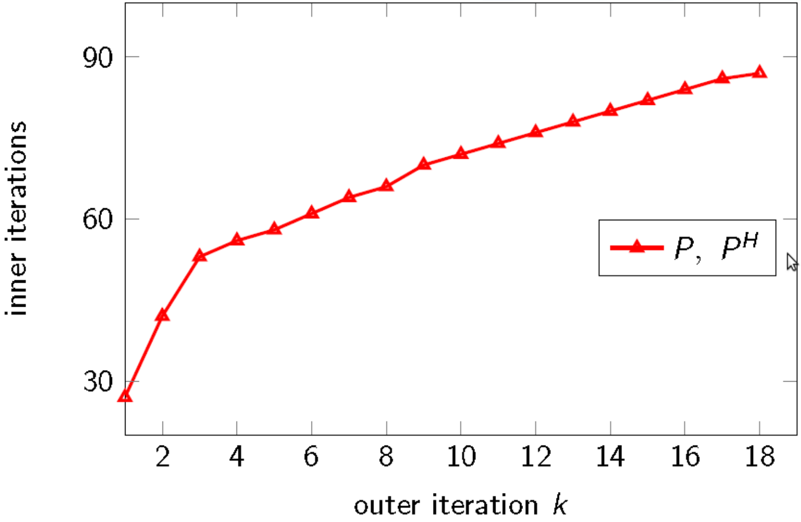

Inexact methods - observation

Observation in the *unpreconditioned* case

increasing accuracy $\Rightarrow$ number of inner iterations remains $\approx$ constant
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- right hand side x is an approximate eigenvector in inexact RQI
- beneficial for Krylov subspace methods! [F./Spence '07-09]

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Basic idea - key observation

Solving $Bx = b$ with a Krylov method, where b is an eigenvector of B:

$$\begin{aligned} \Rightarrow \mathcal{K}_1(B,b) &= \text{span}\{b\} \\ \mathcal{K}_2(B,b) &= \text{span}\{b, Bb\} = \text{span}\{b, \alpha b\} = \text{span}\{b\} \end{aligned}$$

Krylov method converges in one step!

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- Solution of $(A - \sigma I)\hat{x} = x$ with a (left) preconditioned Krylov subspace method:

$$P^{-1}(A - \sigma I)\hat{x} = P^{-1}x$$

but $P^{-1}x$ is a poor eigenvector approximation of $P^{-1}(A - \sigma I)$!.

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Question

Can we reduce the number of inner steps, e.g. to an $\approx$ constant level?

Tuned preconditioners

We need a preconditioner $\mathbb{P}$ such that $\mathbb{P}^{-1}x$ is an approximate eigenvector of $\mathbb{P}^{-1}(A - \sigma I)$:

$$\mathbb{P}^{-1}(A - \sigma I)\mathbb{P}^{-1}x = (\lambda - \sigma)\mathbb{P}^{-1}x$$

Has to satisfy $\mathbb{P}x = x$ (or $\mathbb{P}x = Ax$)

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The tuned preconditioner for one-sided RQI [F./Spence '09]

For $P \approx A$, the **tuned preconditioner** $\mathbb{P}$ is defined by

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

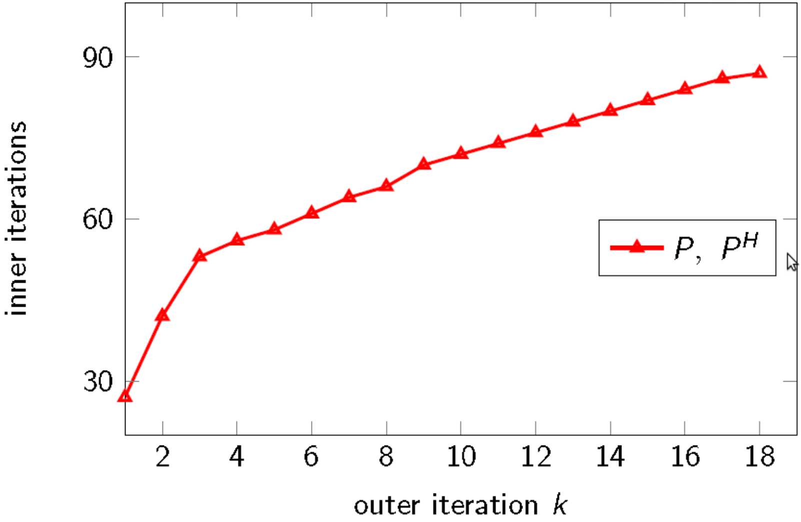
and we obtain

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

Minor modification and minor extra computational cost.

Inexact two-sided methods - dilemma!

Example: matrix `sherman5`, $n = 3312$, fixed shift $\sigma = 0$.



Inexact two-sided methods - dilemma resolved!

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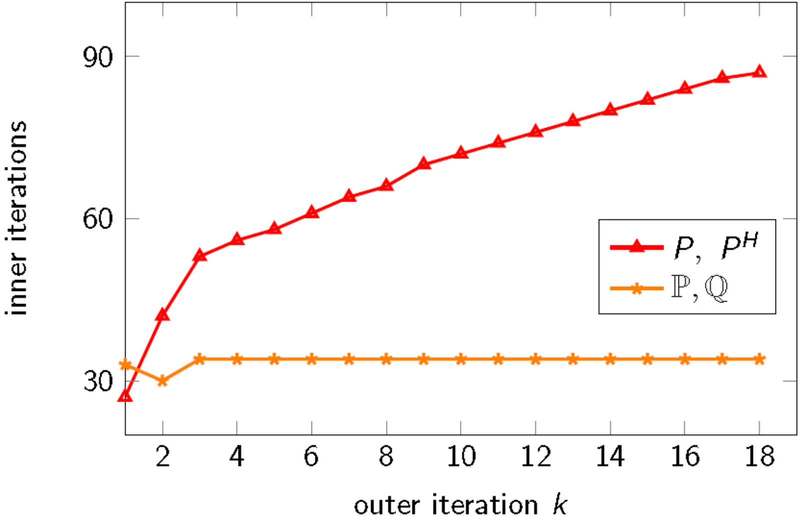

The inner iteration for $(A - \sigma I)y = x$

Standard GMRES theory for $y_0 = 0$ and A diagonalisable

$$\|x - (A - \sigma I)y_k\| \leq \kappa(W) \min_{p \in \mathcal{P}_k} \max_{j=1,\dots,n} |p(\lambda_j)| \|x\|$$

where λ_j are eigenvalues of $A - \sigma I$ and $(A - \sigma I) = W \Lambda W^{-1}$.

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Number of inner iterations

$$k \ge C_1 + C_2 \log \frac{\|x\|}{\xi}$$

for $\|x - (A - \sigma I)y_k\| \le \xi$.

The inner iteration for $(A - \sigma I)y = x$

More detailed GMRES theory for $y_0 = 0$

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

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

Number of inner iterations

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

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

The inner iteration for $(A - \sigma I)y = x$

Good news!

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

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

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Bad news :-(

For a standard preconditioner P

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

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

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

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

Convection-Diffusion operator

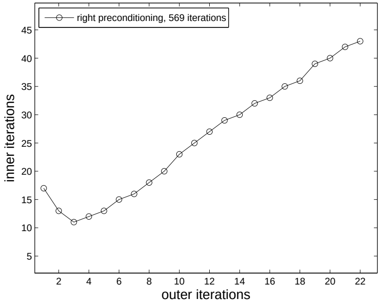

Figure: Inner iterations vs outer iterations

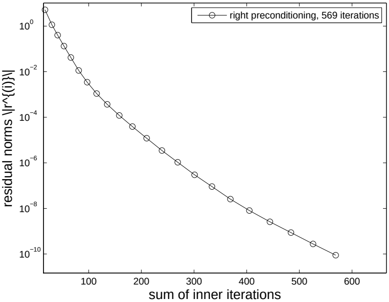

Figure: Eigenvalue residual norms vs total number of inner iterations

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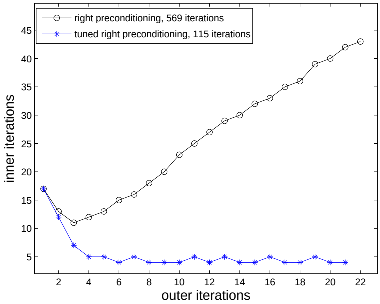

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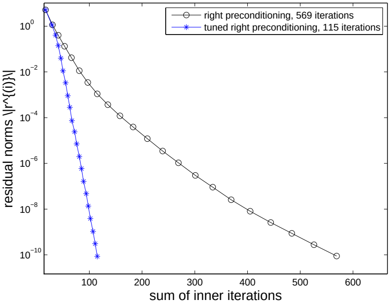

Figure: Eigenvalue residual norms vs total number of inner iterations

Outline

The algorithm

Arnoldi's method

- Arnoldi method constructs an orthogonal basis of k-dimensional Krylov subspace

$$\mathcal{K}_k(\mathcal{A}, q^{(1)}) = \mathrm{span}\{q^{(1)}, \mathcal{A}q^{(1)}, \mathcal{A}^2 q^{(1)}, \ldots, \mathcal{A}^{k-1} q^{(1)}\},$$

$$\mathcal{A}Q_k = Q_k H_k + q_{k+1} h_{k+1,k} e_k^H = Q_{k+1} \begin{bmatrix} H_k \\ h_{k+1,k} e_k^H \end{bmatrix}$$

$$Q_k^H Q_k = I.$$

The algorithm

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- Eigenvalues of H_k are eigenvalue approximations of (outlying) eigenvalues of $\mathcal{A}$

$$\|r_k\| = \|\mathcal{A}x - \theta x\| = \|(\mathcal{A}Q_k - Q_k H_k)u\| = |h_{k+1,k}||e_k^H u|,$$

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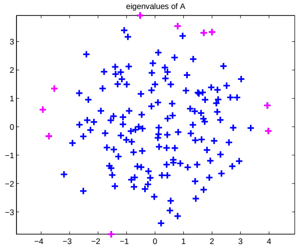
- at each step, application of $\mathcal{A}$ to q_k: $\mathcal{A}q_k = \tilde{q}_{k+1}$

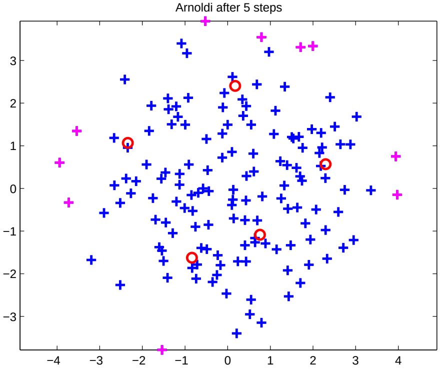
Example

random complex matrix of dimension $n = 144$ generated in MATLAB:

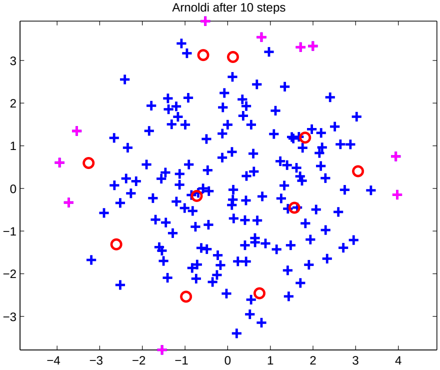
```
G=numgrid('N',14);B=delsq(G);A=sprandn(B)+i*sprandn(B)
```



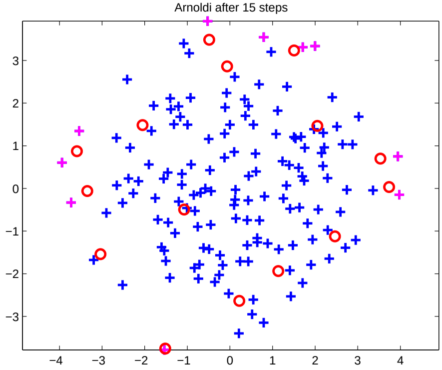
after 5 Arnoldi steps



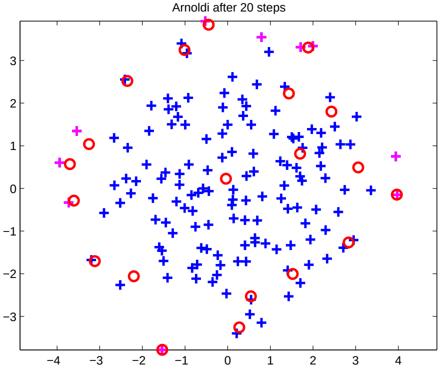
after 10 Arnoldi steps



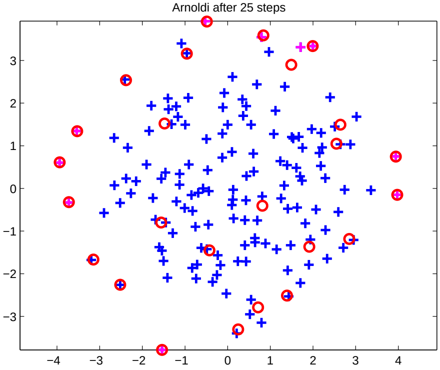
after 15 Arnoldi steps



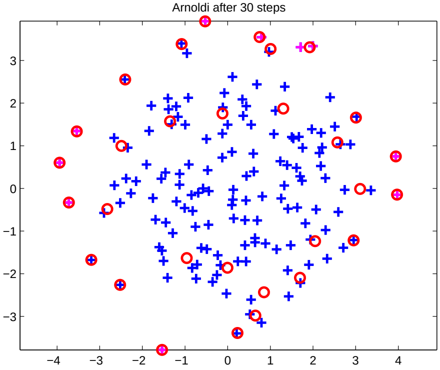
after 20 Arnoldi steps



after 25 Arnoldi steps



after 30 Arnoldi steps



The algorithm: take $\sigma = 0$

Shift-Invert Arnoldi's method $\mathcal{A} := A^{-1}$

- Arnoldi method constructs an orthogonal basis of k-dimensional Krylov subspace

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$$Q_k^H Q_k = I.$$

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- at each step, application of A^{-1} to q_k: $A^{-1}q_k = \tilde{q}_{k+1}$

Inexact solves

Inexact solves (Simoncini 2005), Bouras and Frayssé (2000)

- Wish to solve

$$\|q_k - A\tilde{q}_{k+1}\| = \|\tilde{d}_k\| \leq \tau_k$$

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$$\|q_k - A\tilde{q}_{k+1}\| = \|\tilde{d}_k\| \leq \tau_k$$

- leads to inexact Arnoldi relation

$$A^{-1}Q_k = Q_{k+1}\left[\begin{array}{c} H_k \\ h_{k+1,k}e_k^H \end{array}\right] + D_k = Q_{k+1}\left[\begin{array}{c} H_k \\ h_{k+1,k}e_k^H \end{array}\right] + [d_1|\ldots|d_k]$$

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$$\|r_k\| = \|(A^{-1}Q_k - Q_kH_k)u\| = |h_{k+1,k}||e_k^H u| + D_k u,$$

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- Linear combination of the columns of D_k

$$D_k u = \sum_{l=1}^{k} d_l u_l, \quad \text{if} \quad u_l \quad \text{small, then} \quad \|d_l\| \quad \text{allowed to be large!}$$

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$$\|d_l u_l\| \leq \frac{1}{k}\varepsilon \Rightarrow \|D_k u\| < \varepsilon$$

and

$$|u_l| \leq C(l,k)\|r_{l-1}\| \qquad \star$$

leads to

$$\|q_k - A\tilde{q}_{k+1}\| = \|\tilde{d}_k\|$$

$$\|\tilde{d}_k\| = C\frac{1}{\|r_{k-1}\|} \qquad \diamond$$

Solve tolerance can be relaxed.

The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

Preconditioning

GMRES convergence bound

$$\|q_k - AP^{-1}\tilde{q}^l_{k+1}\| = \kappa \min_{p\in\Pi_l} \max_{i=1,\ldots,n} |p(\mu_i)| \|q_k\|$$

depending on

The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

Preconditioning

GMRES convergence bound

$$\|q_k - AP^{-1}\tilde{q}_{k+1}^{l}\| = \kappa \min_{p\in\Pi_l} \max_{i=1,\dots,n} |p(\mu_i)|\|q_k\|$$

depending on

- the eigenvalue clustering of AP^{-1}
- the condition number
- the right hand side (initial guess)

The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

Preconditioning

- Introduce preconditioner P and solve

$$AP^{-1}\tilde{q}_{k+1} = q_k, \quad P^{-1}\tilde{q}_{k+1} = q_{k+1}$$

using GMRES

The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

Preconditioning

- Introduce preconditioner P and solve

$$AP^{-1}\tilde{q}_{k+1} = q_k, \quad P^{-1}\tilde{q}_{k+1} = q_{k+1}$$

  using GMRES

Tuned Preconditioner

using a tuned preconditioner for Arnoldi's method

$$\mathbb{P}_k Q_k = AQ_k; \quad \text{given by} \quad \mathbb{P}_k = P + (A - P)Q_k Q_k^H$$

The inner iteration for $A\tilde{q} = q$

Theorem (Properties of the tuned preconditioner)

Let P with $P = A + E$ be a preconditioner for A and assume k steps of Arnoldi's method have been carried out; then k eigenvalues of $A\mathbb{P}_k^{-1}$ are equal to one:

$$[A\mathbb{P}_k^{-1}]AQ_k = AQ_k$$

and $n - k$ eigenvalues are close to the corresponding eigenvalues of AP^{-1}.

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Implementation

- Sherman-Morrison-Woodbury.
- Only minor extra costs (one back substitution per outer iteration)

Numerical Example

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

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

No tuning and standard preconditioner

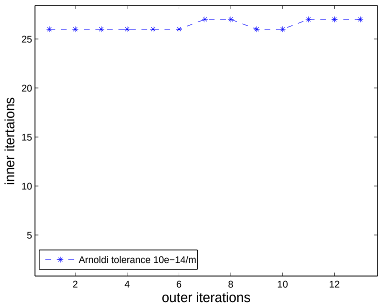

Figure: Inner iterations vs outer iterations

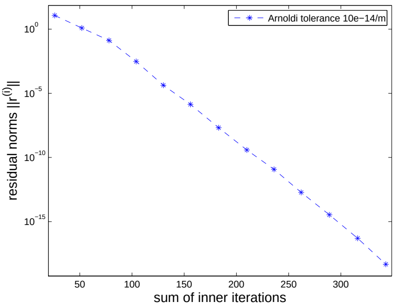

Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning the preconditioner

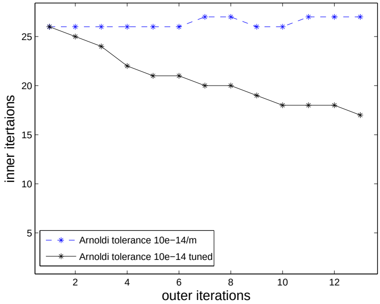

Figure: Inner iterations vs outer iterations

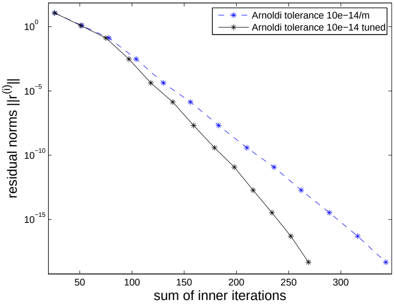

Figure: Eigenvalue residual norms vs total number of inner iterations

Relaxation

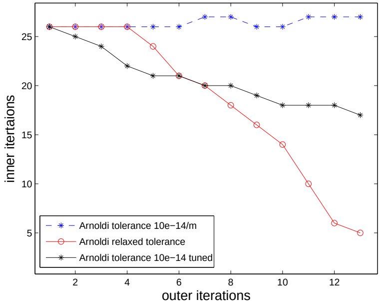

Figure: Inner iterations vs outer iterations

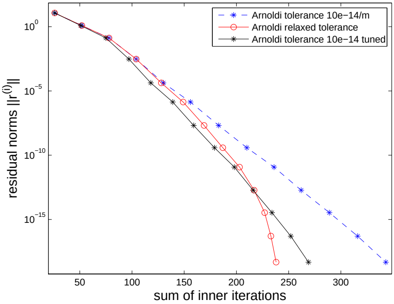

Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning and relaxation strategy

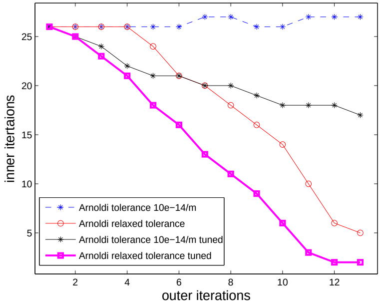

Figure: Inner iterations vs outer iterations

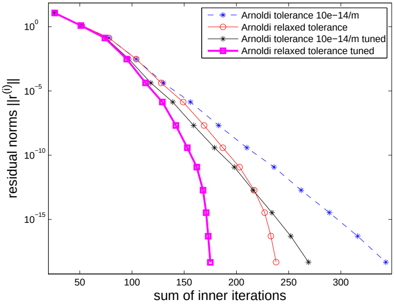

Figure: Eigenvalue residual norms vs total number of inner iterations

Ritz values of exact and inexact Arnoldi

Exact eigenvalues	Ritz values (exact Arnoldi)	Ritz values (inexact Arnoldi, tuning)
+4.69249563e-02	+4.69249563e-02	+4.69249563e-02
+1.25445378e-01	+1.25445378e-01	+1.25445378e-01
+4.02658363e-01	+4.02658347e-01	+4.02658244e-01
+5.79574381e-01	+5.79625498e-01	+5.79817301e-01
+6.18836405e-01	+6.18798666e-01	+6.18650849e-01

Table: Ritz values of exact Arnoldi's method and inexact Arnoldi's method with the tuning strategy compared to exact eigenvalues closest to zero after 14 shift-invert Arnoldi steps.

Outline

Conclusions

- For eigenvalue computations it is advantageous to consider small rank changes to the standard preconditioners
- Works for any preconditioner
- Works for SI versions of Power method, Simultaneous iteration, Arnoldi method

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