Inexact preconditioned shift-and-invert Arnoldi’s method and implicit restarts for eigencomputations

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joint work with Alastair Spence (Bath)
Problem and iterative methods

Find a small number of eigenvalues close to a shift $\sigma$ and corresponding eigenvectors of:

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

- $A$ is large, sparse, nonsymmetric $\Rightarrow$ iterative solves (e.g. Arnoldi method)
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- Problem becomes

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

- each step of the iterative method involves repeated application of $(A - \sigma I)^{-1}$ to a vector
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$$\quad (A - \sigma I)^{-1}x = \frac{1}{\lambda - \sigma}x$$

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

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

using Krylov or Galerkin-Krylov method for linear systems.

- leading to inner-outer iterative method.
The algorithm

**Arnoldi’s method**

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

$$\mathcal{K}_k(A, q_1) = \text{span}\{q_1, Aq_1, A^2q_1, \ldots, A^{k-1}q_1\},$$

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

$$Q_k^H Q_k = I.$$ 

- Eigenvalues of the upper Hessenberg matrix $H_k$ are eigenvalue approximations of ("outlying") eigenvalues of $A$

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

- at each step: application of $A$ to $q_k$:

$$Aq_k = \tilde{q}_{k+1}$$
Enhancements: Shift-Invert Arnoldi and IRA

Shift-Invert Arnoldi’s method $A := A^{-1}$ ($\sigma = 0$)

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

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Implicitly Restarted Arnoldi

- perform $m = k + p$ Arnoldi iterations
- IRA: restart from step $k$: $A Q_k = Q_k H_k + q_{k+1} h_{k+1,k} e_k^H \rightarrow 0$
This talk

Extend the results by Simoncini (2005) for Arnoldi to IRA

Extend the idea of tuning (previous talk) to Arnoldi and IRA
Inexact solves (Simoncini 2005), Bouras and Frayssé (2000)

- Wish to solve

\[ \| q_k - A \tilde{q}_{k+1} \| = \| \tilde{d}_k \| \leq \tau_k \]
Inexact solves (Simoncini 2005), Bouras and Frayssé (2000)

- Wish to solve

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

- after \( m \) steps leads to inexact Arnoldi relation

\[
A^{-1} Q_m = Q_{m+1} \begin{bmatrix} H_m \\ h_{m+1, m} e_k^H \end{bmatrix} + D_m = Q_{m+1} \begin{bmatrix} H_m \\ h_{m+1, m} e_m^H \end{bmatrix} + [d_1 | \ldots | d_m]
\]
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- \( u \) eigenvector of \( H_m \):

\[
\|r_m\| = \|(A^{-1}Q_m - Q_m H_m)u\| = |h_{m+1,m}| \|e_m^H u\| + D_m u,
\]

\[
D_m u = \sum_{k=1}^{m} d_k u_k, \quad \text{if } |u_k| \text{ small, then } \|d_k\| \text{ allowed to be large!}
\]
Inexact solves (Simoncini 2005), Bouras and Frayssé (2000)

- Wish to solve
  \[ \| q_k - A \tilde{q}_{k+1} \| = \| \tilde{d}_k \| \leq \tau_k \]
- after \( m \) steps leads to inexact Arnoldi relation
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  A^{-1} Q_m = Q_{m+1} \left[ \begin{array}{c} H_m \\ h_{m+1,m} e_k^H \end{array} \right] + D_m = Q_{m+1} \left[ \begin{array}{c} H_m \\ h_{m+1,m} e_m^H \end{array} \right] + [d_1 | \ldots | d_m]
  \]
- \( u \) eigenvector of \( H_m \):
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  \| r_m \| = \| (A^{-1} Q_m - Q_m H_m) u \| = |h_{m+1,m}| |e_m^H u| + D_m u,
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  D_m u = \sum_{k=1}^{m} d_k u_k, \quad \text{if} \quad |u_k| \text{ small, then} \quad \|d_k\| \text{ allowed to be large!}
  \]
- Simoncini (2005) has shown
  \[
  |u_k| \leq C(k, m)|r_{k-1}|
  \]
  which leads to
  \[
  \| \tilde{d}_k \| = C(k, m) \frac{1}{|r_{k-1}|} \varepsilon
  \]
  for \( \|D_m u\| < \varepsilon \).
Numerical Examples

\texttt{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).
Fixed tolerance

Figure: Inner iterations vs outer iterations

Figure: Eigenvalue residual norms vs total number of inner iterations
Relaxation (Simoncini 2005)

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Relaxation strategy for invariant subspaces (F./Spence 2008)

- \( m = k + p \) steps of the Arnoldi factorisation

\[
AQ_{k+p} = Q_{k+p}H_{k+p} + q_{k+p+1}h_{k+p+1,k+p}e^H_{k+p}
\]

- let \( H_m \) have Schur decomposition

\[
H_m = H_{k+p} = \begin{bmatrix} U & W_2 \end{bmatrix} \begin{bmatrix} \Theta & \ast \\ 0 & T_{22} \end{bmatrix}^H \begin{bmatrix} U & W_2 \end{bmatrix}
\]
Relaxation strategy for invariant subspaces (F./Spence 2008)

- \( m = k + p \) steps of the Arnoldi factorisation

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- let \( H_k \) be decomposed as \( \Theta_k = U_k^H H_k U_k \)

- let \( R_k = q_{k+1} h_{k+1,k} e_k^H U_k \) be the residual after \( k \) Arnoldi steps.
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- $m = k + p$ steps of the Arnoldi factorisation

$$AQ_{k+p} = Q_{k+p}H_{k+p} + q_{k+p+1}h_{k+p+1,k+p}e_{k+p}^H$$

- let $H_m$ have Schur decomposition

$$H_m = H_{k+p} = \begin{bmatrix} U & W_2 \end{bmatrix} \begin{bmatrix} \Theta & 0 \\ 0 & T_{22} \end{bmatrix}^* \begin{bmatrix} U & W_2 \end{bmatrix}^H$$

- let $H_k$ be decomposed as $\Theta_k = U_k^HH_kU_k$

- let $R_k = q_{k+1}h_{k+1,k}e_k^H U_k$ be the residual after $k$ Arnoldi steps.

- Then $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$ with $U^HU = I$, such that

$$\|U_2\| \leq \frac{\|R_k\|}{\text{sep}(T_{22}, \Theta_k)}$$

where $\text{sep}(T_{22}, \Theta_k) := \min_{\|V\|_1 = 1} \|T_{22}V - V\Theta_k\|$. 
Relaxation strategy for IRA (F./Spence 2008)

### Theorem

For any given $\varepsilon \in \mathbb{R}$ with $\varepsilon > 0$ assume that

\[
\|d_l\| \leq \begin{cases} 
\frac{\varepsilon}{2(m-k)} \frac{\text{sep}(T_{22}, \Theta_k)}{\|R_k\|} & \text{if } l > k, \\
\frac{\varepsilon}{2k} & \text{otherwise.}
\end{cases}
\]

Then

\[
\|AQ_mU - Q_mU\Theta - R_m\| \leq \varepsilon.
\]
Relaxation strategy for IRA (F./Spence 2008)

**Theorem**

*For any given $\varepsilon \in \mathbb{R}$ with $\varepsilon > 0$ assume that*

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*Then*

$$\|AQ_mU - Q_mU\Theta - R_m\| \leq \varepsilon.$$ 

*In practice: perform $m = k + p$ initial steps and then relax the tolerance from the first restart.*
Numerical Example

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

- $k = 8$ eigenvalues closest to zero
- IRA with exact shifts $p = 4$
- Preconditioned GMRES as inner solver (fixed tolerance and relaxation strategy),
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Fixed tolerance

**Figure:** Inner iterations vs outer iterations

**Figure:** Eigenvalue residual norms vs total number of inner iterations
Relaxation

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Tuning the preconditioner \( AP^{-1} \tilde{q}_{k+1} = q_k \)

- 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:

\[
\|d_l\| = \kappa \min_{p \in \Pi_l} \max_{i=1, \ldots, n} |p(\mu_i)| \|d_0\|
\]
Tuning the preconditioner $AP^{-1}q_{k+1} = q_k$

- Introduce preconditioner $P$ and solve

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

using GMRES:

$$\|d_l\| = \kappa \min_{p \in \Pi_l} \max_{i=1,\ldots,n} |p(\mu_i)| \|d_0\|$$

- use a tuned preconditioner for Arnoldi’s method

$$P_kQ_k = AQ_k; \quad \text{given by} \quad P_k = P + (A - P)Q_kQ_k^H$$
The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

**Theorem (Properties of the tuned preconditioner $P_k Q_k = AQ_k$)**

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 $AP_k^{-1}$ are equal to one:

$$[AP_k^{-1}]AQ_k = AQ_k$$

and $n - k$ eigenvalues equivalent to eigenvalues of $L \in \mathbb{C}^{n-k \times n-k}$ with

$$\|L - I\| \leq C\|E\|.$$
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**Theorem (Properties of the tuned preconditioner $P_k Q_k = AQ_k$)**

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 $A P_k^{-1}$ are equal to one:

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**Implementation**

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

Why does tuning help?

- Arnoldi decomposition

\[ A^{-1}Q_k = Q_k H_k + q_{k+1} h_{k+1,k} e_k^H \]
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\[ A^{-1}Q_k = Q_kH_k + q_{k+1}h_{k+1,k}e_k^H \]

- let \( A^{-1} \) be transformed into upper Hessenberg form

\[
\begin{bmatrix}
Q_k & Q_k^\perp
\end{bmatrix}^H A^{-1} \begin{bmatrix}
Q_k & Q_k^\perp
\end{bmatrix} = \begin{bmatrix}
H_k & T_{12} \\
h_{k+1,k}e_1e_k^H & T_{22}
\end{bmatrix},
\]

where \( \begin{bmatrix}
Q_k & Q_k^\perp
\end{bmatrix} \) is unitary and \( H_k \in \mathbb{C}^{k,k} \) and \( T_{22} \in \mathbb{C}^{n-k,n-k} \) are upper Hessenberg.
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If \( h_{k+1, k} \neq 0 \) then

\[
\begin{bmatrix}
Q_k & Q_k^\perp
\end{bmatrix}^H A P_k^{-1} \begin{bmatrix}
Q_k & Q_k^\perp
\end{bmatrix} = 
\begin{bmatrix}
I + \star & Q_k^H A P_k^{-1} Q_k^\perp \\
\star & T_{22}^{-1} (Q_k^H P Q_k^\perp)^{-1} + \star
\end{bmatrix}
\]
Tuning

Why does tuning help?

- Assume we have found an approximate invariant subspace, that is

\[ A^{-1}Q_k = Q_kH_k + q_{k+1}h_{k+1,k}e_k^H \approx 0 \]

- let \( A^{-1} \) have the upper Hessenberg form

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If \( h_{k+1,k} = 0 \) then

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\]
Another advantage of tuning

- System to be solved at each step of Arnoldi’s method is

\[ A \mathbb{P}^{-1}_k \tilde{\mathbf{q}}_{k+1} = \mathbf{q}_k, \quad \mathbb{P}^{-1}_k \tilde{\mathbf{q}}_{k+1} = \mathbf{q}_{k+1} \]
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- Assuming invariant subspace found then \((A^{-1}Q_k = Q_kH_k)\):

\[ A\mathbb{P}_k^{-1}q_k = q_k \]
Tuning

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- Assuming invariant subspace found then \((A^{-1}Q_k = Q_kH_k)\):

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

- the right hand side of the system matrix is an eigenvector of the system matrix!

- Krylov methods converge in one iteration
Numerical Example (Arnoldi)

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Conclusions

- For eigencomputations it is advantageous to consider small rank changes to the standard preconditioners (works for any preconditioner)
- Extension of the relaxation strategy to IRA
- Best results are obtained when relaxation and tuning are combined
- Link to Jacobi-Davidson method?