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Eigenvalues and eigenvectors II

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$$\mathbf{Ax} = \mathbf{b}$$

$$\mathbf{Ax} = \lambda \mathbf{x}$$

Subspace methods

Iterate until sufficiently accurate:

- **Expansion.** Expand the search subspace \mathcal{V}_k .
Restart if $\dim(\mathcal{V}_k)$ is too large.
- **Extraction.** Extract an appropriate approximate solution from the search subspace.

Example. Krylov subspace methods
as GMRES, CG, Arnoldi, Lanczos: expansion by $\mathbf{t}_k = \mathbf{A}\mathbf{v}_k$

Goal.

Expansion. $\angle(\mathbf{x}, \mathcal{V}_{k+1}) \ll \angle(\mathbf{x}, \mathcal{V}_k)$

Extraction. Find $\mathbf{u} = \mathbf{V}_k \mathbf{y}_k$ s.t. $\angle(\mathbf{x}, \mathbf{u}) \approx \angle(\mathbf{x}, \mathcal{V}_{k+1})$

$$\mathbf{Ax} = \mathbf{b}$$

$$\mathbf{Ax} = \lambda \mathbf{x}$$

Subspace methods

Iterate until sufficiently accurate:

- **Expansion.** Expand the search subspace \mathcal{V}_k .
Restart if $\dim(\mathcal{V}_k)$ is too large.
- **Extraction.** Extract an appropriate approximate solution (ϑ, \mathbf{u}) from the search subspace.

This lecture, for $\mathbf{Ax} = \lambda \mathbf{x}$ with \mathbf{A} $n \times n$, focusses on:

- Expansion
- Restart
- Deflation

Notation.

\mathbf{u} is a approximation of \mathbf{x} (in direction) with
 ϑ the approximate eigenvalue, $\|\mathbf{x}\|_2 = \|\mathbf{u}\|_2 = 1$,
 $\mathbf{r} \equiv \mathbf{A}\mathbf{u} - \vartheta\mathbf{u}$ is the residual,

Program Lecture 13

- Expansion
 - Krylov subspace approach
 - Lanczos, Arnoldi, Shift and Invert Arnoldi**
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 - Accelerated **R**ayleigh **Q**uotient **I**teration
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Krylov subspace expansion

The columns of $\mathbf{V}_k = [\mathbf{v}_1, \dots, \mathbf{v}_k]$ form a (orthonormal) Krylov basis: then $\mathbf{t} = \mathbf{A}\mathbf{v}_k$ is an expansion vector.

Examples. For $\mathbf{A}\mathbf{x} = \mathbf{b}$

- GMRES (minimal residual extraction),
- CG for $\mathbf{A}\mathbf{x} = \mathbf{b}$ if $\mathbf{A}^* = \mathbf{A}$ (Galerkin extraction).

For $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$

- **Arnoldi** ((harmonic) Ritz extraction).
- **Lanczos** in case \mathbf{A} is Hermitian.

Lanczos

$$\mathbf{A} = \mathbf{A}^* \quad \Rightarrow \quad \mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\underline{T}_k,$$

$\mathbf{V}_k = [\mathbf{v}_1, \dots, \mathbf{v}_k]$ orthonormal, \underline{T}_k is $(k+1) \times k$ tridiagonal.

If **only** eigenvalues of \mathbf{A} are to be computed (no eigenvectors), then there is no need to store the “old” \mathbf{v}_j . Moreover, eigenvalues of symmetric tridiagonal matrices as T_k can fairly efficiently be computed (QR-alg., Sylvester’s law, Sturm sequences, Divide and Conquer). This makes Lanczos very suitable for searching very high dimensional Krylov subspaces (low costs in flops and in storage) and finding many eigenvalues.

Eigenvectors can also be computed with one (or a few) steps of Shift and Invert with a detected eigenvalue as shift.

Lanczos in floating point arithmetic

Sensitive to errors

Lanczos is very unstable

The Lanczos vectors \mathbf{v}_j lose orthogonality upon convergence:

Theorem. If $\sin \angle(\mathbf{x}, \mathbf{u}_k)$ is of order machine precision (**mp**), then $\angle(\mathbf{v}_k, \text{span}(\mathbf{v}_1, \dots, \mathbf{v}_{k-1}))$ is of order **mp**.

Effect: This leads to **ghost eigenvalues** (eigenvalues of T_k that result from floating point errors).

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Surprise. Ghost eigenvalues converge to eigenvalues of **A**. Due to rounding errors Lanczos produces clusters of approximate eigenvalues around true eigenvalues.

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Surprise. Ghost eigenvalues converge to eigenvalues of \mathbf{A} . Due to rounding errors Lanczos produces clusters of approximate eigenvalues around true eigenvalues.

Detecting ghost eigenvalues. Let T'_k be T_k from which the first row and first column have been removed. If ϑ is an eigenvalue of both T_k and T'_k , then ϑ is a ghost eigenvalue.

Lanczos in floating point arithmetic

Strategies to deal with the sensitivity to errors

1) Detect ghost eigenvalues.

For the other strategies the \mathbf{v}_j have to be stored.

2) **Full reorthogonalisation.**

(Like Arnoldi, but use T_k for computing eigenvalues)
(expensive expans., expensive stor., cheap extrac.)

3) **Selective reorthogonalisation:**

Orthogonalise \mathbf{v}_k and \mathbf{v}_{k+1} against all $\mathbf{v}_1, \dots, \mathbf{v}_{k-1}$
iff the loss of orthogonality is of order $\sqrt{\mathbf{u}}$
with \mathbf{u} machine precision.

There are cheap recurrences to estimate

$\mathbf{E}_k \equiv I_k - \mathbf{V}_k^* \mathbf{V}_k$, i.e., the loss of orthogonality.

(cheaper expans., expensive stor., cheap extrac.)

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- **Shift and Invert Arnoldi** ((harmonic) Ritz extraction):
$$\mathbf{t} = (\mathbf{A} - \tau\mathbf{I})^{-1}\mathbf{v}_k$$
 to generate a basis
for the search subspace $\mathcal{K}_k((\mathbf{A} - \tau\mathbf{I})^{-1}, \mathbf{v}_1)$.

Shift and Invert Lanczos in case \mathbf{A} is Hermitian.

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Recall that SI expansion amplifies components of eigenvectors with eigenvalue close to the target τ .

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Convergence without subspace acceleration

Shift & Invert $\mathbf{u}_{k+1} = (\mathbf{A} - \tau\mathbf{I})^{-1}\mathbf{u}_k.$ (s&i)

Then $\tan \angle(\mathbf{x}, \mathbf{u}_k) \sim \left(\frac{\lambda - \tau}{\lambda_j - \tau} \right)^k,$

where $\lambda = \lambda_{j_0}$, $\mathbf{x} = \mathbf{x}_{j_0}$, and $|\lambda_{j_0} - \tau| < |\lambda_j - \tau|$ all $j \neq j_0$.

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Rayleigh Quotient Iteration

$$\mathbf{u}_{k+1} = (\mathbf{A} - \rho_k \mathbf{I})^{-1} \mathbf{u}_k, \quad \text{where } \rho_k \equiv \rho(\mathbf{u}_k).$$

$$\mathbf{A}^* = \mathbf{A}, \quad \gamma \equiv \min_{\lambda_j \neq \lambda} |\lambda - \lambda_j|,$$

$$\alpha_k \equiv \frac{|\rho_k - \lambda|}{\gamma - |\rho_k - \lambda|}, \quad \zeta_k \equiv \tan \angle(\mathbf{u}_k, \mathbf{x}).$$

Then, $\zeta_{k+1} \leq \alpha_k \zeta_k, \quad \alpha_{k+1} \leq (\alpha_k \zeta_k)^2.$

\Rightarrow asymptotic cubic convergence (as soon as $\alpha_{k_0} \zeta_{k_0} < 1$).

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$\mathbf{A}^* \neq \mathbf{A} \quad \Rightarrow \quad$ asymptotic quadratic convergence.

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Rayleigh Quotient Iteration

$$\mathbf{u}_{k+1} = (\mathbf{A} - \rho_k \mathbf{I})^{-1} \mathbf{u}_k, \text{ where } \rho_k \equiv \rho(\mathbf{u}_k).$$

$$\mathbf{A}^* \neq \mathbf{A}$$

With $\mathbf{u}_{k+1} = (\mathbf{A} - \rho_k \mathbf{I})^{-1} \mathbf{u}_k$ and $\mathbf{w}_{k+1}^* = \mathbf{w}_k^* (\mathbf{A} - \rho_k \mathbf{I})^{-1},$

where $\rho_k \equiv \frac{\mathbf{w}_k^* \mathbf{A} \mathbf{u}_k}{\mathbf{w}_k^* \mathbf{u}_k} \Rightarrow$ asymptotic cubic convergence.

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Accelerated RQI.

Expand the search subspace $\mathcal{V} = \text{span}(\mathbf{V})$ with

$$\mathbf{t} = (\mathbf{A} - \rho \mathbf{I})^{-1} \mathbf{u}, \quad (\text{rqi})$$

where $\rho = \mathbf{u}^* \mathbf{A} \mathbf{u}$ and \mathbf{u} approximate eigenvector in \mathcal{V} .

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- + Fast convergence (RQI)
- Search subspace is not a Krylov subspace.

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Rational Krylov Sequence method allows efficient computations.

[Ruhe 82]

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Rational Krylov Sequence method allows efficient computations.

[Ruhe 82]

— **Computational costs**

S& I: Solving $(\mathbf{A} - \tau \mathbf{I}) \mathbf{u}_k = \mathbf{u}_{k+1}$ at **one** LU-dec. in total.

RQI: Solving $(\mathbf{A} - \rho_k \mathbf{I}) \mathbf{u}_k = \mathbf{u}_{k+1}$ at one LU-dec. **each step**.

May not be feasible if n large.

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Optimal expansion

$$\mathbf{Ax} = \mathbf{b}.$$

If $\mathbf{x}_k = \mathbf{V}_k y$ is an approximate solution, then the solution \mathbf{t} of $\mathbf{At} = \mathbf{r}_k \equiv \mathbf{b} - \mathbf{Ax}_k$ is the correction of \mathbf{x}_k .

Expansion: solve (approximately) $\mathbf{At} = \mathbf{r}_k$ for \mathbf{t}

↪ flexible version of GCR

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Expansion: solve (approximately) $\mathbf{At} = \mathbf{r}_k$ for \mathbf{t}

↪ flexible version of GCR

$$\mathbf{Ax} = \lambda \mathbf{x}.$$

If $(\vartheta \equiv \rho(\mathbf{u}), \mathbf{u})$ is an approximate eigenpair, $\mathbf{r} \equiv \mathbf{Au} - \vartheta \mathbf{u}$, then the solution $\mathbf{t} \perp \mathbf{u}$ of

$$(\mathbf{I} - \mathbf{u}\mathbf{u}^*)(\mathbf{A} - \vartheta \mathbf{I})(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{t} = -\mathbf{r}$$

is the (first order wrt $\|\mathbf{r}\|_2$) correction of \mathbf{u} .

↪ **Jacobi-Davidson**

[Sleijpen vd Vorst 95]

(Approximately) solving for $\mathbf{t} \perp \mathbf{u}$

$$(\mathbf{I} - \mathbf{u}\mathbf{u}^*)(\mathbf{A} - \vartheta\mathbf{I})(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{t} = -\mathbf{r} \quad (\text{jd})$$

If solved exactly \Rightarrow asymptotic quadratic convergence

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The **Jacobi-Davidson correction equation** (jd) can be viewed as a Newton correction equation for the non-linear problem

$$F(\lambda, \mathbf{x}) \equiv (1 - \|\mathbf{x}\|_2^2, \mathbf{A}\mathbf{x} - \lambda\mathbf{x}) = (0, \mathbf{0}) :$$

(jd) can be related to the Jacobian of $F : \mathbb{C}^{n+1} \rightarrow \mathbb{C}^{n+1}$.

(Approximately) solving for $\mathbf{t} \perp \mathbf{u}$

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Note. If $\vartheta \approx \lambda$,

then the system $(\mathbf{A} - \vartheta\mathbf{I})\mathbf{t} = \mathbf{u}$ is ill conditioned.

Whereas, if λ is simple and $(\vartheta, \mathbf{u}) \approx (\lambda, \mathbf{x})$, then the system (jd) as a system in the space \mathbf{u}^\perp is well-conditioned.

Krylov subspace solvers with initial guess $\mathbf{x}_0 = \mathbf{0}$ are suitable for solving in \mathbf{u}^\perp .

Better conditioning \rightsquigarrow

- faster convergence of the linear solver (deflation of small eigenvalue),
- more stability.

(Approximately) solving for $\mathbf{t} \perp \mathbf{u}$

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There are block-versions to deal with the non-simple eigenvalue case (but the simple eigenvalue version often works well also in the non-simple case).

Block versions require to know the multiplicity in advance.

Block versions are attractive for computational reasons (exploit parallelism).

(Approximately) solving for $\mathbf{t} \perp \mathbf{u}$

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If solved exactly \Rightarrow asymptotic quadratic convergence

Solve approximately with preconditioned iterative linear solver as GMRES (or MINRES of $\mathbf{A}^* = \mathbf{A}$).

Often a fixed modest number of steps already lead to fast convergence.

Issue. How many steps are optimal?

Many steps in the inner loop (to solve (jd)) \rightsquigarrow high quality search subspace of low dimension.

Optimal strategy is available in case $\mathbf{A} = \mathbf{A}^*$.

Effective strategy (optimal?) is available for the general case.

(Approximately) solving for $\mathbf{t} \perp \mathbf{u}$

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If solved exactly \Rightarrow asymptotic quadratic convergence

Approximate solves. $\mathbf{M} \approx \mathbf{A} - \vartheta\mathbf{I}$

$\mathbf{t} \perp \mathbf{u}$ such that $(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{M}(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{t} = -\mathbf{r}$

$$\Leftrightarrow \mathbf{M}\mathbf{t} = -\mathbf{r} + \beta\mathbf{u} \quad \text{with } \beta \text{ st } \mathbf{t} \perp \mathbf{u}$$

$$\Leftrightarrow \mathbf{t} = -\mathbf{M}^{-1}\mathbf{r} + \beta\mathbf{M}^{-1}\mathbf{u} \perp \mathbf{u} \quad \Rightarrow \quad \beta = \frac{\mathbf{u}^*\mathbf{M}^{-1}\mathbf{r}}{\mathbf{u}^*\mathbf{M}^{-1}\mathbf{u}}$$

$$\Leftrightarrow \mathbf{t} = -\left(\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right)\mathbf{M}^{-1}\mathbf{r}, \quad \text{where } \mathbf{w} \equiv \mathbf{M}^{-1}\mathbf{u}.$$

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Expansion by $\mathbf{t} = -\mathbf{M}^{-1}\mathbf{r}$ (d) **Davidson** '75

Expansion by $\mathbf{t} = -\left(\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right)\mathbf{M}^{-1}\mathbf{r}$ (o) **Olsen** '93

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Interpretation. If $\mathbf{M} = \mathbf{A} - \vartheta\mathbf{I}$, then $\mathbf{u} = \mathbf{M}^{-1}\mathbf{r}$. Hence, effective expansion with $\mathbf{w} = \mathbf{M}^{-1}\mathbf{u}$: RQI expansion.

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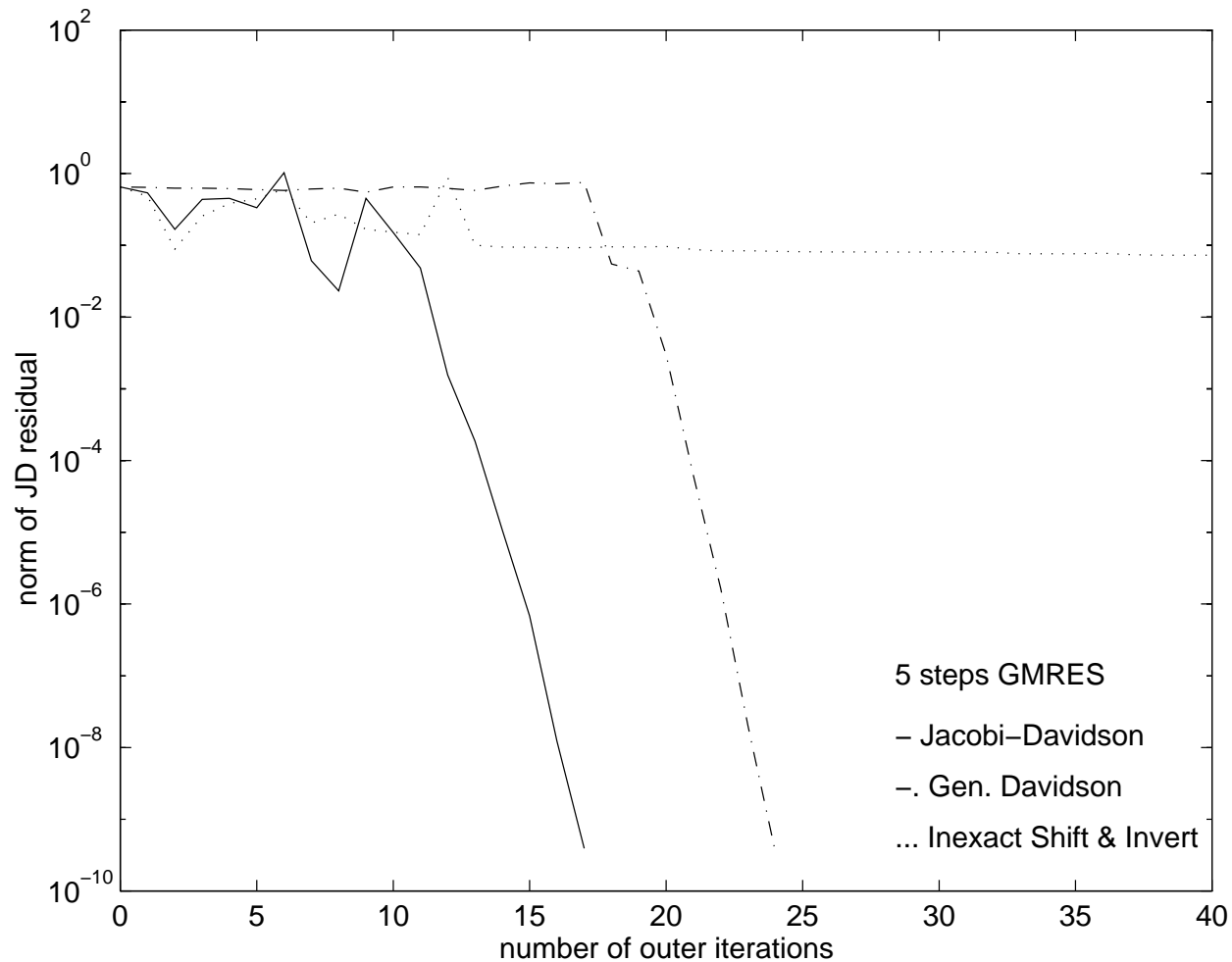
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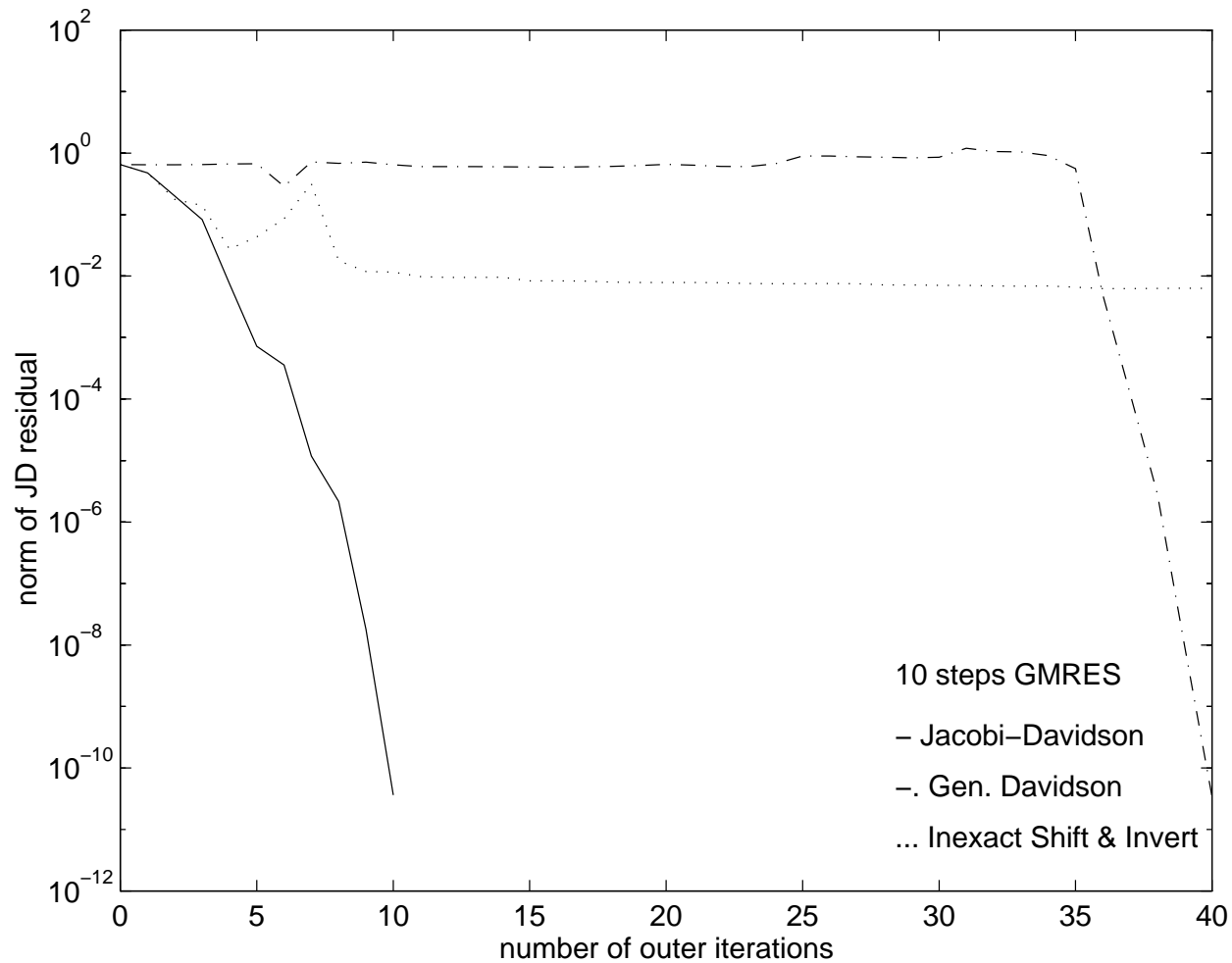
$$\Leftrightarrow \mathbf{t} = -\left(\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right)\mathbf{M}^{-1}\mathbf{r}, \quad \text{where } \mathbf{w} \equiv \mathbf{M}^{-1}\mathbf{u}.$$

Interpretation. If $\mathbf{M} = \mathbf{A} - \vartheta\mathbf{I}$, then $\mathbf{u} = \mathbf{M}^{-1}\mathbf{r}$. Hence, effective expansion with $\mathbf{w} = \mathbf{M}^{-1}\mathbf{u}$: RQI expansion.

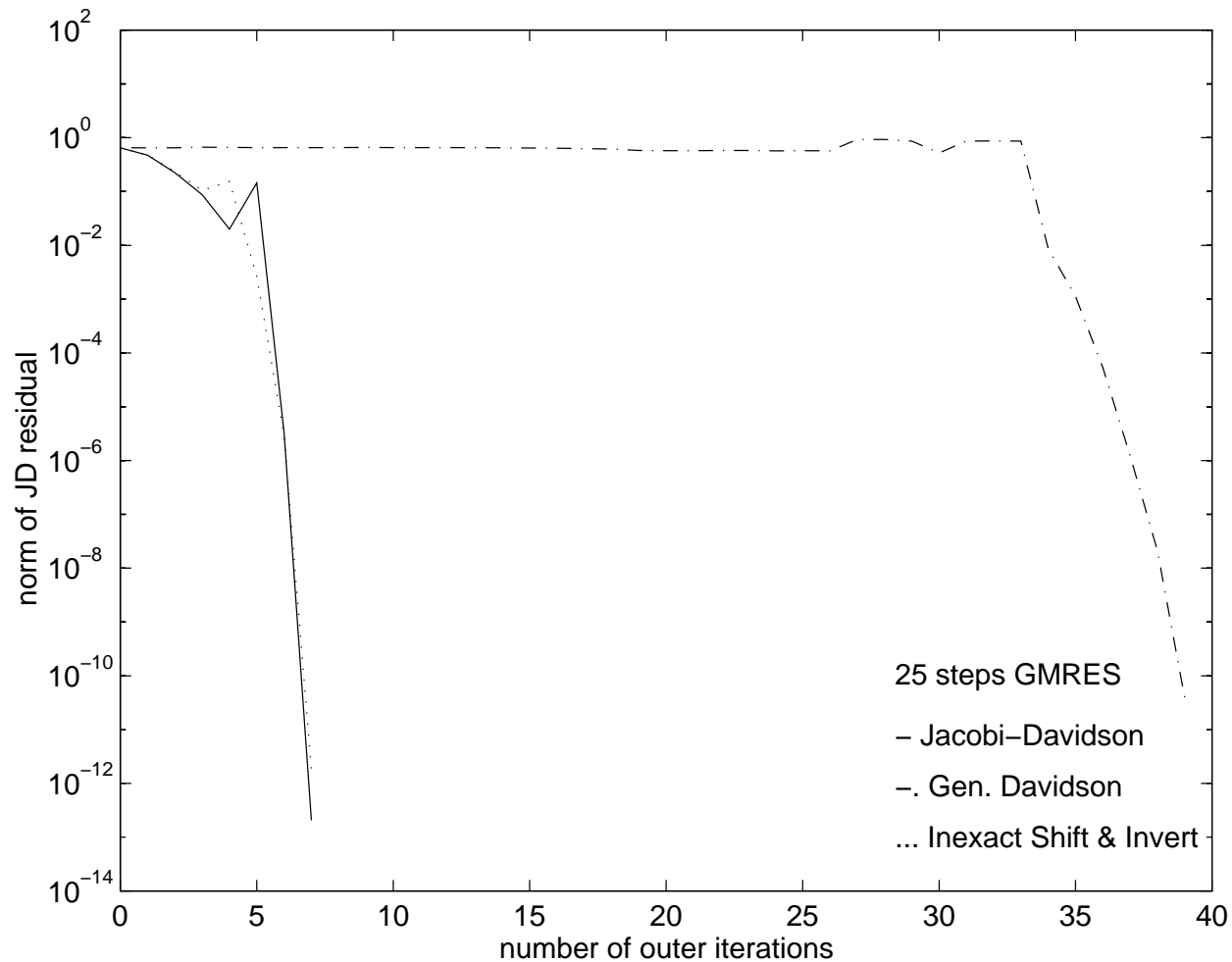
+ expansion equation (jd) better conditioned than (rqi).



A is SHERMAN4 finding the eigenvalue closests to $\tau = 0.5$
 (which is the fifth smallest eigenvalue),
M is ILU(2) of **A** - τ **I**



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(Approximately) solving for $\mathbf{t} \perp \mathbf{u}$

$$(\mathbf{I} - \mathbf{u}\mathbf{u}^*)(\mathbf{A} - \vartheta\mathbf{I})(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{t} = -\mathbf{r} \quad (\text{jd})$$

If solved exactly \Rightarrow asymptotic quadratic convergence

Approximate solves. $\mathbf{M} \approx \mathbf{A} - \vartheta\mathbf{I}$

$\mathbf{t} \perp \mathbf{u}$ such that $(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{M}(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{t} = -\mathbf{r}$

$$\Leftrightarrow \mathbf{t} = -\left(\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right)\mathbf{M}^{-1}\mathbf{r}, \quad \text{where } \mathbf{w} \equiv \mathbf{M}^{-1}\mathbf{u}.$$

Precondition (jd) by $\left(\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right)\mathbf{M}^{-1}$, where $\mathbf{w} \equiv \mathbf{M}^{-1}\mathbf{u}$

Preconditioned Krylov requires mult. by

$$\left(\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right)\mathbf{M}^{-1}(\mathbf{A} - \vartheta\mathbf{I})$$

with righthand side vector $\left(\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right)\mathbf{M}^{-1}\mathbf{r}$.

(Approximately) solving for $\mathbf{t} \perp \mathbf{u}$

$$(\mathbf{I} - \mathbf{u}\mathbf{u}^*)(\mathbf{A} - \vartheta\mathbf{I})(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{t} = -\mathbf{r} \quad (\text{jd})$$

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Additional costs for solving (jd).

(additional to RQI for solving $(\mathbf{A} - \vartheta\mathbf{I})\mathbf{t} = \mathbf{u}$)

Per step mult. by $\mathbf{I} - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}$: 1 AXPY, 1 DOT per step.

Per Krylov run for solving (jd): 1 solve of $\mathbf{M}\mathbf{w} = \mathbf{u}$.

Jacobi–Davidson

- Subspace method
 - + Accelerated convergence
 - + Steering possibilities
 - + variety of selection methods
 - More costly steps
- Expansion vectors from JD equation
 - + Locally optimal expansion (with exact solves)
 - + Asymptotic quadratic convergence possible (with exact solves)
 - + Well-conditioned (when λ is simple)
 - + Fast convergence with moderate accurate solves
 - + Preconditioners can be exploited
 - Additional costs per step

Program Lecture 13

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- Restart
 - LOGG, Implicitly Restarted Arnoldi Method**
- Deflation

For ease of discussion . . .

Recall that harmonic Ritz vectors are better suited for selecting approximate eigenpairs than Ritz vectors. In our discussion below, we refer to Ritz pairs, but the discussion can be extended to harmonic Ritz pairs.

For stability we need a well-conditioned bases of the search subspace. To ease discussion, we assume the basis $\mathbf{v}_1, \dots, \mathbf{v}_k$ to be orthonormal and the expansion vector \mathbf{t} is to be orthonormalised against $\mathbf{v}_1, \dots, \mathbf{v}_k$ to obtain the next basis vector \mathbf{v}_{k+1} . However, it may be more efficient to have orthonormality with respect to other non-standard inner product (as the \mathbf{A} -, or \mathbf{M} -inner product, . . .) or to have bi-orthogonality.

The most promising Ritz vectors

If $\mathbf{V}_k = [\mathbf{v}_1, \dots, \mathbf{v}_k]$ spans the search subspace \mathcal{V}_k , then we can compute k Ritz pairs $(\vartheta_1, \mathbf{u}_1), \dots, (\vartheta_k, \mathbf{u}_k)$, i.e., $\mathbf{u}_j \in \mathcal{V}_k$ and $\vartheta_j \in \mathbb{C}$ such that

$$\mathbf{A}\mathbf{u}_j - \vartheta_j \mathbf{u}_j \perp \mathbf{V}_k \quad (j = 1, \dots, k)$$

or, equivalently, with $H_k \equiv \mathbf{V}_k^* \mathbf{A} \mathbf{V}_k$,

$$\mathbf{u}_j = \mathbf{V}_k \mathbf{y}_j \quad \text{such that} \quad H_k \mathbf{y}_j = \vartheta_j \mathbf{y}_j \quad (j = 1, \dots, k).$$

The ℓ most **promising Ritz vectors** $\mathbf{u}_1, \dots, \mathbf{u}_\ell$ are the ones with Ritz value that ‘best’ have the property that we want our wanted eigenvalue of \mathbf{A} to have.

Examples. • $\operatorname{Re}(\vartheta_j) \geq \operatorname{Re}(\vartheta_{j+1}) \quad (j = 1, \dots, k-1)$

if the eigenvalue of \mathbf{A} with largest real part is wanted.

• $|\vartheta_j - \tau| \leq |\vartheta_{j+1} - \tau| \quad (j = 1, \dots, k-1)$

if the eigenvalue of \mathbf{A} closest to some target $\tau \in \mathbb{C}$ is wanted.

The most promising Ritz vectors

If $\mathbf{V}_k = [\mathbf{v}_1, \dots, \mathbf{v}_k]$ spans the search subspace \mathcal{V}_k , then we can compute k Ritz pairs $(\vartheta_1, \mathbf{u}_1), \dots, (\vartheta_k, \mathbf{u}_k)$.

For stability, we rather compute the **Schur decomposition**

$$H_k = USU^*$$

of H_k rather than the eigenvector decomposition: here U is $k \times k$ unitary and S is $k \times k$ upper triangular.

The Ritz values are the diagonal entries of S : $\vartheta_j = S_{jj}$.
If $Sz_j = \vartheta_j z_j$ then $y_j = Uz_j$.

Theorem. The first ℓ columns of U form an orthonormal basis of the space spanned by the eigenvectors y_1, \dots, y_ℓ of H_k with eigenvalues the top ℓ diagonal entries $S_{11}, \dots, S_{\ell\ell}$ of S .

The most promising Ritz vectors

If $\mathbf{V}_k = [\mathbf{v}_1, \dots, \mathbf{v}_k]$ spans the search subspace \mathcal{V}_k , then we can compute k Ritz pairs $(\vartheta_1, \mathbf{u}_1), \dots, (\vartheta_k, \mathbf{u}_k)$.

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A Schur decomposition can be re-ordered (using unitary transforms, Givens rotations) such that the most promising Ritz values are the top diagonal entries of 'new' S :

Theorem. There is a Schur decomposition of H_k such that the diagonal elements of S appear in prescribed order.

Assumption. $\mathbf{u}_1, \dots, \mathbf{u}_\ell$ are the most promising Ritz vectors and $\text{span}(\mathbf{u}_1, \dots, \mathbf{u}_\ell) = \text{span}(\mathbf{V}_k U(:, 1:\ell))$.

Restart

$\dim(\mathcal{V}) = k$ is too high, $k = k_{\max} \Rightarrow$ restart to limit

- high memory demands (to store $\mathbf{V}_{k+1} = [\mathbf{v}_1, \dots, \mathbf{v}_k, \mathbf{v}_{k+1}]$),
- high computational costs (to orthonormalise \mathbf{t} against \mathbf{V}_k).

Simple restart. Take $\tilde{\mathcal{V}} = \text{span}(\mathbf{u}_1)$, i.e., $\tilde{\mathbf{V}}_1 = [\mathbf{u}_1]$.

Thick resart. Take $\tilde{\mathcal{V}} = \text{span}(\mathbf{u}_1, \dots, \mathbf{u}_\ell)$ with $\ell = k_{\min}$,
i.e., $\tilde{\mathbf{V}}_\ell = \mathbf{V}_k U(:, 1:\ell)$.

Why thick restart? i.e., why $\ell = k_{\min} > 1$?

- to (partially) maintain super linear convergence
- to maintain a space that provides a good initial guess when the search to a next eigenpair is started.

Explanation. The second Ritz pair is likely to converge to the second eigenpair (recall the convergence proof of the power method). The main component of the error in \mathbf{u}_1 is probably in the direction of \mathbf{u}_2 , etc.

Restart

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Example. For the case where $\mathbf{A}^* = \mathbf{A}$.

Locally Optimal CG takes $k_{\max} = 3$ and $k_{\min} = 2$ and restarts with the two dimensional space spanned by the best Ritz vector and the best Ritz vector from the preceding step.

LOCG expands with a Davidson step, solve \mathbf{t} from $\mathbf{M}\mathbf{t} = \mathbf{r}$.

Restarting Arnoldi

Arnoldi's method requires a start with an Arnoldi relation.

If, with $\eta \equiv h_{k+1,k}$,

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1} \underline{H}_k = \mathbf{V}_k H_k + \eta \mathbf{v}_{k+1} e_k^*,$$

then, with $\tilde{U} \equiv U(:, 1:\ell)$, $\tilde{S} \equiv S(1:\ell, 1:\ell)$, and $q^* \equiv e_k^* \tilde{U}$,

$$\mathbf{A}\mathbf{V}_k \tilde{U} = \mathbf{V}_k \tilde{U} \tilde{S} + \eta \mathbf{v}_{k+1} q^*. \quad (*)$$

The ℓ -vector q will not be a multiple of e_ℓ and (*) is **not** an Arnoldi relation (no Hessenberg matrix).

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The ℓ -vector q will not be a multiple of e_ℓ and (*) is **not** an Arnoldi relation (no Hessenberg matrix).

Th. [Arnoldi–Schur restart]. There is a unitary matrix Q (product of Householder reflections) such that

$$\widetilde{H}_\ell \equiv \begin{bmatrix} Q & 0 \\ 0^* & 1 \end{bmatrix}^* \begin{bmatrix} \tilde{S} \\ \eta q^* \end{bmatrix} Q \quad \text{is } (\ell + 1) \times \ell \text{ upper Hessenberg.}$$

Note. Except for vector updates for $\tilde{\mathbf{V}}_{\ell+1} \equiv [\mathbf{V}_k(\tilde{U}Q), \mathbf{v}_{k+1}]$, this allows a restart at the cost of only low dim. operations.

Implicitly Restarted Arnoldi Method

More elegant and more efficient and stable implementation to compute $U(:, 1:\ell)Q$ by Sorenson is based on idea QR-algorithm for eigenvalue computation of dense systems.

Implicitly Restarted Arnoldi Method

Select $\mu_{\ell+1}, \dots, \mu_{k-1}, \mu_k$ in \mathbb{C} . Let p be the polynomial

$$p(\zeta) \equiv (\zeta - \mu_k) \cdot \dots \cdot (\zeta - \mu_{\ell+1}) \quad (\zeta \in \mathbb{C}).$$

Let $\tilde{\mathbf{v}}_1 \equiv p(\mathbf{A})\mathbf{v}_1$. Consider the Arnoldi relation

$$\mathbf{A} \tilde{\mathbf{V}}_\ell = \tilde{\mathbf{V}}_{\ell+1} \tilde{H}_\ell \quad \text{with} \quad \tilde{\mathbf{V}}_\ell e_1 = \tilde{\mathbf{v}}_1.$$

Theorem. This Arnoldi relation can be obtained by applying $k - \ell$ steps of the shifted QR-algorithm to H_k with **shifts** μ_j finding $H_k U = U \tilde{H}_k$ and then use the first ℓ columns of U to form $\tilde{\mathbf{V}}_\ell \equiv \mathbf{V}_k U(:, 1:\ell)$.

IRAM selects $\mu_j = \vartheta_j$ (the less 'best' Ritz values). This gives the desired Arnoldi relation: the columns of $\tilde{\mathbf{V}}_\ell$ form an orthonormal basis of the space spanned by $\mathbf{u}_1, \dots, \mathbf{u}_\ell$. The eigenvalues of \tilde{H}_ℓ are precisely $\vartheta_1, \dots, \vartheta_\ell$.

Implicitly Restarted Arnoldi Method

`eigs.m` in **Matlab** is IRAM (with deflation)

`eigs.m` is based on ARPACK, a collection of FORTRAN routines that implements IRAM

Lehoucq, Sorensen and Yang 1998

Program Lecture 13

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Towards the next eigenpair

Suppose an eigenpair (λ, \mathbf{x}) has been detected in search subspace \mathcal{V} , i.e., $\mathbf{x} \in \mathcal{V}$ up to the required accuracy.

How to continue the search for the next eigenpair?

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How to continue the search for the next eigenpair?

1) **Deflate the search subspace:**

- Deflate \mathbf{x} from the search subspace \mathcal{V} ,
that is, remove \mathbf{x} -components from \mathcal{V} :
normalize \mathbf{x} , $\tilde{\mathcal{V}} \equiv (\mathbf{I} - \mathbf{x}\mathbf{x}^*)\mathcal{V}$.
- Continue the search, with initial search subspace $\tilde{\mathcal{V}}$.
- Select Ritz pairs for the next eigenpair.

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- Select Ritz pairs for the next eigenpair.

Very **unstable**: (λ, \mathbf{x}) might/will be recomputed in $\tilde{\mathcal{V}}_j$, where $\tilde{\mathcal{V}}_0 \equiv \tilde{\mathcal{V}}$. (It may even prevent the process from finding a next eigenpair.)

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- Continue the search, with initial search subspace $\tilde{\mathcal{V}}$.
- Select Ritz pairs for the next eigenpair.

2) **Deflate the matrix** as well: As 1), but continue the search with the **deflated matrix**:

$$(\mathbf{I} - \mathbf{x}\mathbf{x}^*)\mathbf{A}(\mathbf{I} - \mathbf{x}\mathbf{x}^*)$$

rather than with \mathbf{A} .

Eigenvectors or Schur vectors

Assume the wanted $\lambda_1, \dots, \lambda_\ell, \lambda_{\ell+1}, \dots$ are simple.

Eigenvectors. Let $(\lambda_i, \mathbf{x}_i, \mathbf{y}_i)$ be an eigen triple:

$$\mathbf{A}\mathbf{x}_i = \lambda_i\mathbf{x}_i \quad \text{and} \quad \mathbf{y}_i^*\mathbf{A} = \lambda_i\mathbf{y}_i^*.$$

Scale such that $\|\mathbf{x}_i\|_2 = 1$, $\mathbf{y}_i^*\mathbf{x}_i = 1$. Note $\mathbf{y}_j^*\mathbf{x}_i = 0$ ($i \neq j$):

$$\mathbf{A}\mathbf{X}_\ell = \mathbf{X}_\ell\Lambda_\ell, \quad \mathbf{Y}_\ell^*\mathbf{A} = \Lambda_\ell\mathbf{Y}_\ell^*, \quad \text{and} \quad \mathbf{Y}_\ell^*\mathbf{X}_\ell = I_\ell.$$

Use $\mathbf{I} - \mathbf{X}_\ell\mathbf{Y}_\ell^*$ for deflation.

Note that $(\lambda_{\ell+1}, \mathbf{x}_{\ell+1}, \mathbf{y}_{\ell+1})$ is an eigen triple of the **deflated matrix**

$$(\mathbf{I} - \mathbf{X}_\ell\mathbf{Y}_\ell^*)\mathbf{A}(\mathbf{I} - \mathbf{X}_\ell\mathbf{Y}_\ell^*)$$

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Disadvantage.

- $\mathbf{X}_\ell, \mathbf{Y}_\ell$ may be ill-conditioned
- each step requires two search subspaces:
 - \mathcal{V} for forming \mathbf{x}_i
 - \mathcal{W} for forming \mathbf{y}_i .

Stopping criterion checks for convergence of both \mathbf{x}_i and \mathbf{y}_i .

Advantage.

- Information on the conditioning of the eigenvalues is available.

Eigenvectors or Schur vectors

$$\mathbf{A}\mathbf{Q}_\ell = \mathbf{Q}_\ell S_\ell$$

Is a **partial Schur decomposition** if \mathbf{Q}_ℓ is $n \times \ell$ orthonormal and S_ℓ is $\ell \times \ell$ upper triangular. Assume $\text{diag}(S_\ell) = \Lambda_\ell$.

Theorem. If $S_\ell X_\ell = X_\ell \Lambda_\ell$ then $\mathbf{X}_\ell = \mathbf{Q}_\ell X_\ell$.

Use $\mathbf{I} - \mathbf{Q}_\ell \mathbf{Q}_\ell^*$ for deflation.

Note that \mathbf{q}_1 is an eigenvector of \mathbf{A} with eigenvalue λ_1 , and $\mathbf{q}_{\ell+1}$ is an eigenvector with eigenvalue $\lambda_{\ell+1}$ of the **deflated matrix**

$$(\mathbf{I} - \mathbf{Q}_\ell \mathbf{Q}_\ell^*) \mathbf{A} (\mathbf{I} - \mathbf{Q}_\ell \mathbf{Q}_\ell^*).$$

Eigenvectors or Schur vectors

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Theorem. If $\mathbf{S}_\ell \mathbf{X}_\ell = \mathbf{X}_\ell \Lambda_\ell$ then $\mathbf{X}_\ell = \mathbf{Q}_\ell \mathbf{X}_\ell$.

Advantage.

- \mathbf{Q}_ℓ is well-conditioned.
- per step only one search subspace \mathcal{V} is needed.

Disadvantage. Generally $\text{span}(\mathbf{Q}_\ell) \neq \text{span}(\mathbf{Y}_\ell)$.

- Only “weak” information on the left eigenvector available (i.p. “weak” information on conditioning eigenvalues):
 \mathbf{x}_i may be in \mathbf{V} (sufficiently accurate), while \mathbf{y}_i is not in \mathbf{V} .

Deflation with Schur vectors

The approach based on Schur vectors (for deflation and computing Schur vectors) is the most popular one.

In JD, this leads to the following JD correction equation:

$$(\mathbf{I} - [\mathbf{Q}_\ell, \mathbf{u}][\mathbf{Q}_\ell, \mathbf{u}]^*)(\mathbf{A} - \nu\mathbf{I})(\mathbf{I} - [\mathbf{Q}_\ell, \mathbf{u}][\mathbf{Q}_\ell, \mathbf{u}]^*)\mathbf{t} = -\mathbf{r}$$

for determining the expansion for the search space for searching for $\mathbf{q}_{\ell+1}$: $\mathbf{u} \approx \mathbf{q}_{\ell+1}$.

Recall that enhancing the conditioning is one of the benefits of including a projection in the 'Shift and Invert' equation. Including \mathbf{Q}_ℓ in the projections amplifies this effect. Note that the solution \mathbf{t} is orthogonal to \mathbf{Q}_ℓ and the search subspace gets automatically expanded with vectors $\perp \mathbf{Q}_\ell$.

Deflation with Schur vectors

The approach based on Schur vectors (for deflation and computing Schur vectors) is the most popular one.

IRA uses the deflated matrix

$$(\mathbf{I} - \mathbf{Q}_\ell \mathbf{Q}_\ell^*) \mathbf{A} (\mathbf{I} - \mathbf{Q}_\ell \mathbf{Q}_\ell^*)$$

in an implicit way:

It keeps the columns of \mathbf{Q}_ℓ in the search subspace (\mathcal{V} is not deflated), putting these columns as first vectors in the orthonormal matrix for the search subspace: $\tilde{\mathbf{V}}_{k+j} = [\mathbf{Q}_\ell, \tilde{\mathbf{V}}]$.

Since $\mathbf{v}_{k+j} \perp \mathbf{Q}_\ell$ and $\mathbf{A}\mathbf{v}_{k+j}$ is orthogonalized also against \mathbf{Q}_ℓ to obtain \mathbf{v}_{k+j+1} , the same vector \mathbf{v}_{k+j+1} would have been obtained by expansion using the deflated matrix.

For extraction, IRA uses $H \equiv \tilde{\mathbf{V}}^* \mathbf{A} \tilde{\mathbf{V}}$. This interaction matrix equals the interaction matrix for the deflated matrix.

Deflating Arnoldi's relation

We want to retain an Arnoldi relation at deflation.

Theorem. If $\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\underline{H}_k$, then the following properties are equivalent

- One of the Ritz vectors \mathbf{u}_j is an eigenvector.
- A subdiagonal element, say $h_{\ell+1,\ell}$, of \underline{H}_k is 0.
- $\text{span}(\mathbf{V}_\ell)$ is \mathbf{A} -invariant (whence, spanned by eigenvectors).

Idea 1. Replace small subdiagonal elements of \underline{H}_k , say $|h_{\ell+1,\ell}| \leq \epsilon$, by 0.

Idea 2. Keep \mathbf{V}_ℓ in the Arnoldi basis for orthogonalisation, use $\mathbf{V}(:, [\ell + 1 : k])$ for selection (restart).

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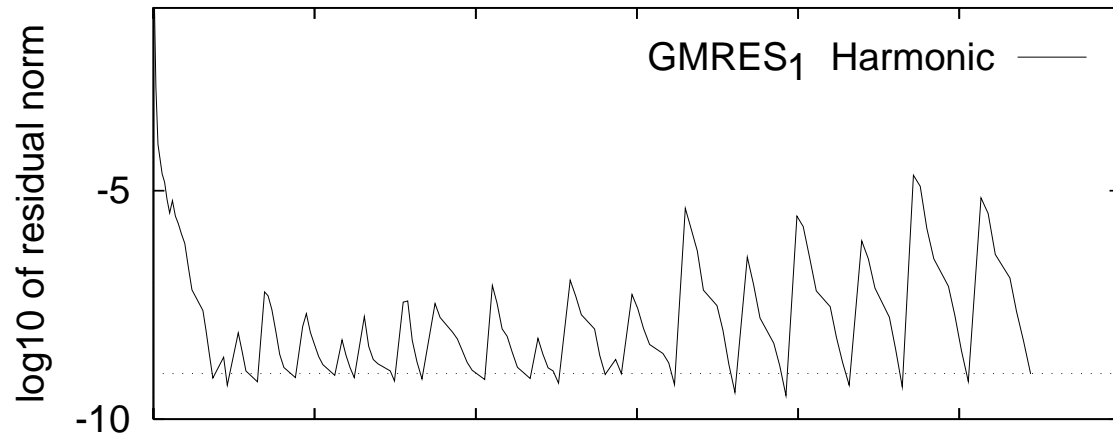
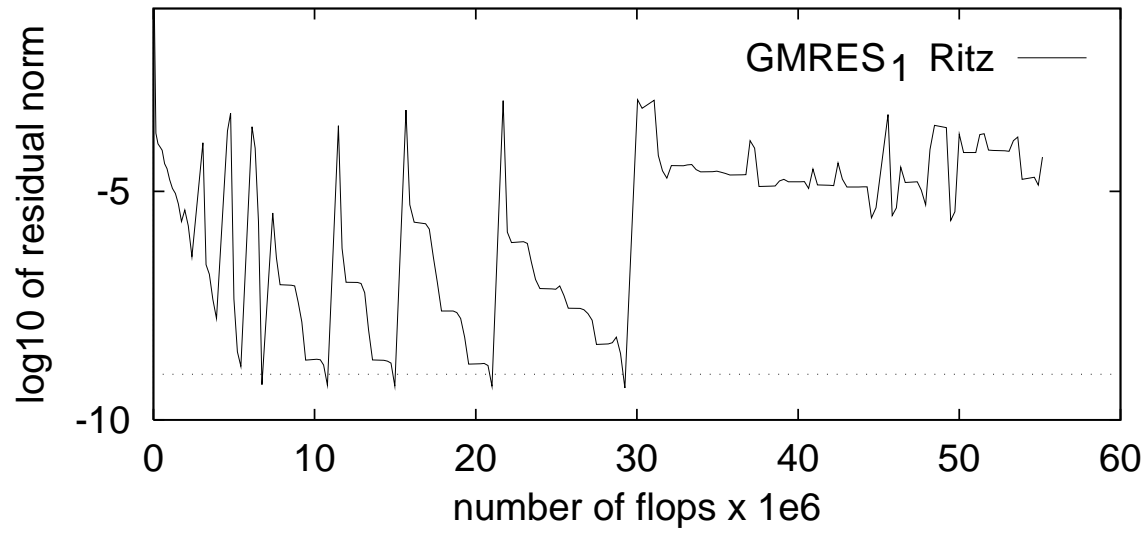
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Idea 2. Keep \mathbf{V}_ℓ in the Arnoldi basis for orthogonalisation, use $\mathbf{V}(:, [\ell + 1 : k])$ for selection (restart).

Note. Idea 1 is unstable and needs stabilisation.

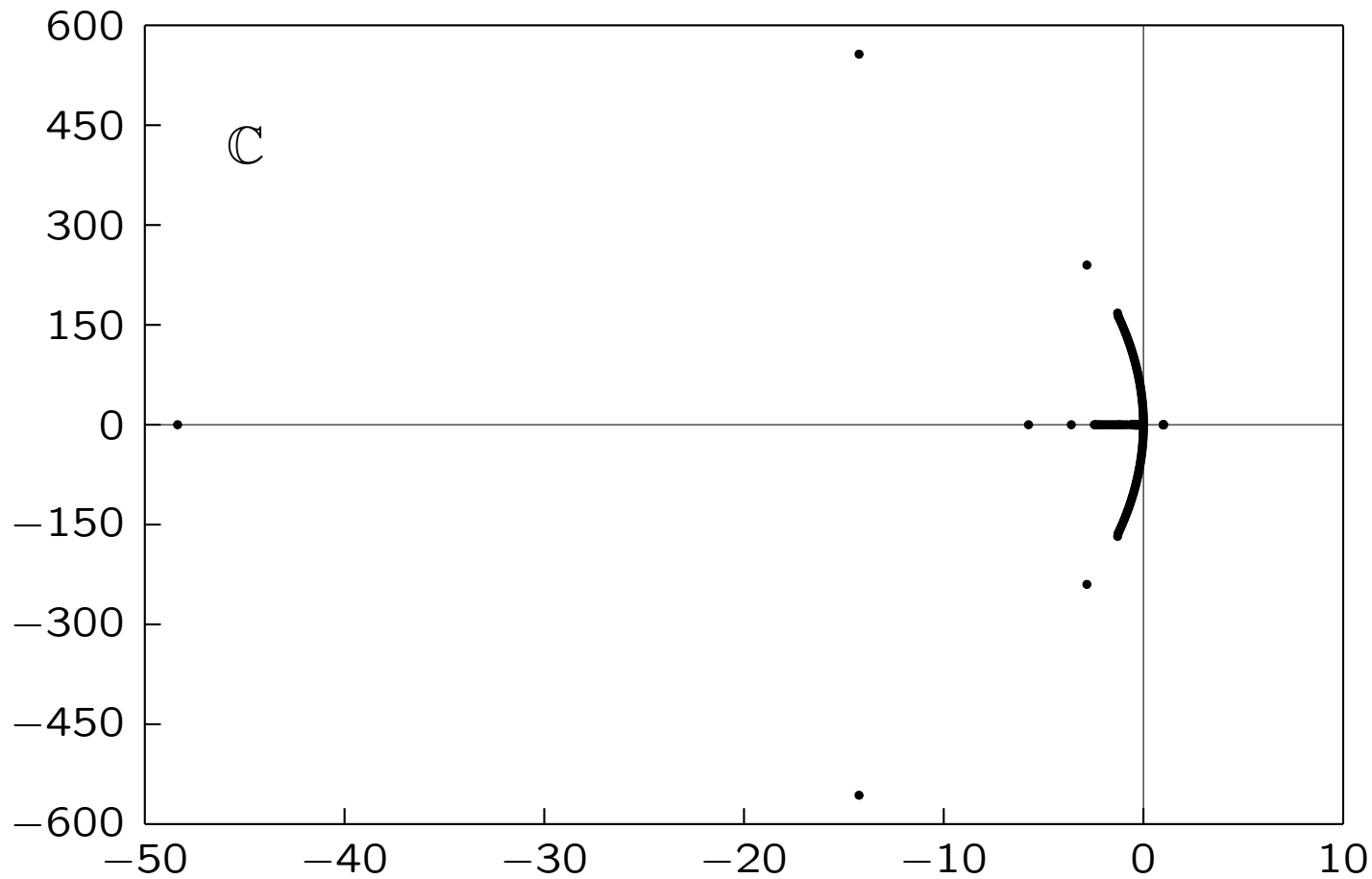
The next transparencies illustrate Jacobi-Davidson with thick restart and deflation

1. **Start:** Choose an initial \mathbf{z} .
 - Set $\Lambda = []$, $\mathbf{U} = []$, $\mathbf{V} = []$.
2. **Repeat:**
 - a. $\mathbf{V} \leftarrow \text{ModGS}([\mathbf{V} | \mathbf{z}])$, $\mathbf{W} \leftarrow \mathbf{A}\mathbf{V}$
 - b. Compute $H \leftarrow \mathbf{V}^*\mathbf{W}$.
 - c. Compute $H = QRQ^*$
with $Q^*Q = I$, R upper Δ ,
 $|R_{11} - \tau| \leq |R_{22} - \tau| \leq \dots$
 - d. $\vartheta \leftarrow R_{11}$, $y \leftarrow Qe_1$, $\mathbf{u} \leftarrow \mathbf{V}y$,
 $\mathbf{r} \leftarrow \text{ModGS}_{\mathbf{U}}(\mathbf{A}\mathbf{u} - \vartheta\mathbf{u})$.
 - e. **If** $\|\mathbf{r}\| \leq \text{tol}$
 - $\Lambda \leftarrow [\Lambda | \vartheta]$, $\mathbf{U} \leftarrow [\mathbf{U} | \mathbf{u}]$.
 - $J = [e_2 | \dots | e_{\dim(\mathbf{V})}]$,
 $\mathbf{V} \leftarrow \mathbf{V}(QJ)$, $Q \leftarrow I$, $R \leftarrow J^*RJ$.
 - **Goto** 2.d.
 - f. Solve (app.) $\mathbf{z} \perp \tilde{\mathbf{U}} \equiv [\mathbf{U} | \mathbf{u}]$
 $(\mathbf{I} - \tilde{\mathbf{U}}\tilde{\mathbf{U}}^*)(\mathbf{A} - \vartheta\mathbf{I})(\mathbf{I} - \tilde{\mathbf{U}}\tilde{\mathbf{U}}^*)\mathbf{z} = -\mathbf{r}$.



$\max(\dim(\text{span}(\mathbf{V}))) = 15$, after restart $\dim(\mathbf{V}) = 10$

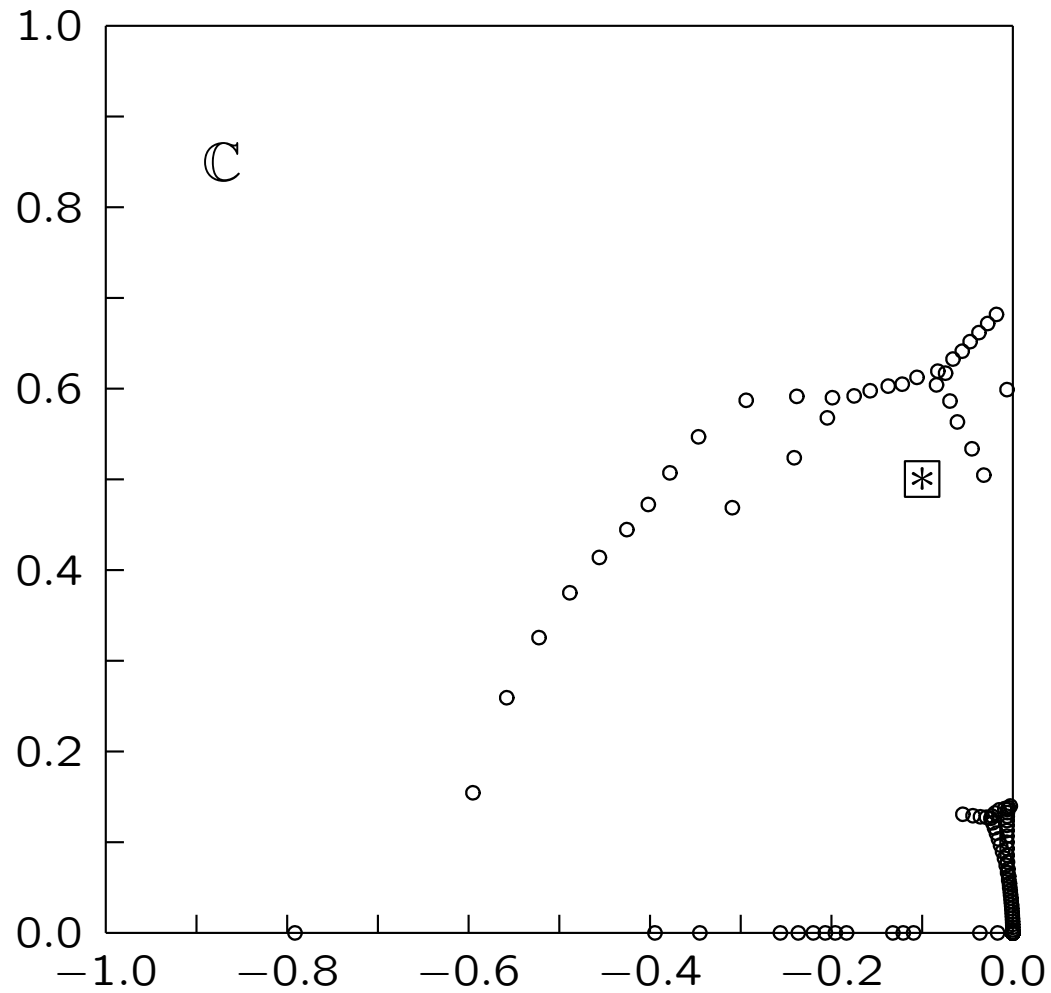
Spectrum MHD test problem



Entire spectrum MHD test problem ($n = 416$).

Correct eigenvalues (.) are shown.

Alfvén spectrum



MHD test problem ($n = 416$).

Correct eigenvalues (\circ), target (\boxtimes).