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Eigenvalues and eigenvectors II

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

Program Lecture 13

- Expansion
  - Krylov subspace approach
    Lanczos, **Arnoldi**, **Shift and Invert** Arnoldi
  - Convergence
  - Accelerated **R**ayleigh **Q**uotient **I**teration
    Rational **K**rylov **S**equence method
  - Optimal expansion
    Jacobi-Davidson
- Restart
  LOCG, **I**mplicitly **R**estarted **A**rnoldi **M**ethod
- Deflation

Lanczos

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

$\mathbf{V}_k = [\mathbf{v}_1, \ldots, \mathbf{v}_k]$ 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 **Unstability is stable**

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

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

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

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 $\mathbf{v}_1,\ldots,\mathbf{v}_{k-1}$ 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 ortogonality.
(cheaper expans., expensive stor., cheap extrac.)

Krylov subspace expansion

The columns of $\mathbf{V}_k = [\mathbf{v}_1,\ldots,\mathbf{v}_k]$ 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.
- **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 $\mathcal{K}_k((\mathbf{A}-\tau\mathbf{I})^{-1}, \mathbf{v}_1)$.

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

Convergence without subspace accelaration

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 $j \neq j_0$.

Rayleigh Quotient Iteration

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

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

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

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

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

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

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

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

\+ Fast convergence (RQI)

\− Search subspace is not a Krylov subspace.

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.

Optimal expansion

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

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

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

$\rightsquigarrow$ flexible version of GCR

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

If $(\vartheta \equiv \rho(\mathbf{u}), \mathbf{u})$ is an approximate eigenpair, $\mathbf{r} \equiv \mathbf{A}\mathbf{u} - \vartheta\mathbf{u}$, 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 $\mathbf{u}$.

$\rightsquigarrow$ **Jacobi-Davidson** [Sleijpen vd Vorst 95]

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

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

If solved exactly $\Rightarrow$ asymptotic quadratic convergence

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 $\mathbf{t} \perp \mathbf{u}$

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

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 $\mathbf{t} \perp \mathbf{u}$

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

If solved exactly $\Rightarrow$ asymptotic quadratic convergence

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

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

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

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

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

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

If solved exactly $\Rightarrow$ asymptotic quadratic convergence

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

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

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 $\mathbf{M}\mathbf{w} = \mathbf{u}$.

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

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

If solved exactly $\Rightarrow$ asymptotic quadratic convergence

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

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 then (rqi).

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

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 $\mathbf{v}_1, \ldots, \mathbf{v}_k$ to be orthonormal and the expansion vector $\mathbf{t}$ is to be orthonormalised against $\mathbf{v}_1, \ldots, \mathbf{v}_k$ 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 $\mathbf{V}_k = [\mathbf{v}_1, \ldots, \mathbf{v}_k]$ spans the search subspace $\mathcal{V}_k$,
then we can compute k Ritz pairs $(\vartheta_1, \mathbf{u}_1), \ldots, (\vartheta_k, \mathbf{u}_k)$.

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.

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

The most promising Ritz vectors

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

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

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

$$\mathbf{u}_j = \mathbf{V}_k y_j \quad \text{such that} \quad H_k y_k = \vartheta_j y_k \qquad (j = 1, \ldots, k).$$

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

Examples. • $\operatorname{Re}(\vartheta_j) \geq \operatorname{Re}(\vartheta_{j+1}) \quad (j = 1, \ldots, k-1)$
if the eigenvalue of $\mathbf{A}$ with largest real part is wanted.

• $|\vartheta_j - \tau| \leq |\vartheta_{j+1} - \tau| \quad (j = 1, \ldots, k-1)$
if the eigenvalue of $\mathbf{A}$ closest to some target $\tau \in \mathbb{C}$ is wanted.

Restart

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

• high memory demands (to store $\mathbf{V}_{k+1} = [\mathbf{v}_1, \ldots, \mathbf{v}_k, \mathbf{v}_{k+1}]$),

• high computational costs (to orthonormalise $\mathbf{t}$ against $\mathbf{V}_k$).

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

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

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

• to (partially) maintain super linear convergence

• to maintain a space that provids 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

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

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

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

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

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 $\mathbf{Mt} = \mathbf{r}$.

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 $q^* \equiv e_k^* \tilde{U}$,

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

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

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

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

Implicitly Restarted Arnoldi Method

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

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

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

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

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 $H_k U = U \widetilde{H}_k$ and then use the first ℓ columns of U to form $\widetilde{\mathbf{V}}_\ell \equiv \mathbf{V}_k U(:, 1\!:\!\ell)$.

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

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

Towards the next eigenpair

Suppose an eigenpair $(\lambda, \mathbf{x})$ 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?

1) **Deflate the search subspace**:
   - Deflate $\mathbf{x}$ form the search subspace $\mathcal{V}$,
     that is, remove $\mathbf{x}$-components from $\mathcal{V}$:
     normalize $\mathbf{x}$, $\widetilde{\mathcal{V}} \equiv (\mathbf{I} - \mathbf{x}\mathbf{x}^*)\mathcal{V}$.
   - Continue the search, with initial search subspace $\widetilde{\mathcal{V}}$.
   - 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 $\lambda_1, \ldots, \lambda_\ell, \lambda_{\ell+1}, \ldots$ are simple.

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

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

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

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

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

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

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

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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**

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

Eigenvectors or Schur vectors

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

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

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

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

Advantage.
– $\mathbf{Q}_\ell$ is well-conditioned.
– per step only one search subspace $\mathcal{V}$ is needed.

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

De 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 $\mathbf{Q}_\ell$ in the search subspace ($\mathcal{V}$ is not deflated), putting these columns as first vectors in the orthonormal matrix for the search subspace: $\mathbf{V}_{k+j} = [\mathbf{Q}_\ell, \widetilde{\mathbf{V}}]$.
Since $\mathbf{v}_{k+j} \perp \mathbf{Q}_\ell$ and $\mathbf{A}\mathbf{v}_{k+j}$ is orthogonalized also against $\mathbf{Q}_\ell$ 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 $H \equiv \widetilde{\mathbf{V}}^* \mathbf{A} \widetilde{\mathbf{V}}$. This interaction matrix equals the interaction matrix for the deflated matrix.

Deflation with Schur vectors

De 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:

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

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