

## Solution of eigenvalue problems

- Introduction – motivation
- Projection methods for eigenvalue problems
- Subspace iteration, The symmetric Lanczos algorithm
- Nonsymmetric Lanczos procedure;
- Implicit restarts
- Harmonic Ritz values, Jacobi-Davidson's method

## Background. Origins of Eigenvalue Problems

- Structural Engineering [ $Ku = \lambda Mu$ ] (Goal: frequency response)
  - Electronic structure calculations [Schrödinger equation..]
  - Stability analysis [e.g., electrical networks, mechanical system,..]
  - Bifurcation analysis [e.g., in fluid flow]
- Large eigenvalue problems in quantum chemistry use up biggest portion of the time in supercomputer centers

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## Background. New applications in data analytics

- Machine learning problems often require a (partial) *Singular Value Decomposition* -
- Somewhat different issues in this case:
- Very large matrices, update the SVD
  - Compute dominant singular values/vectors
  - Many problems of approximating a matrix (or a **tensor**) by one of lower rank (Dimension reduction, ...)
- But: Methods for computing SVD often based on those for standard eigenvalue problems

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## Background. The Problem (s)

- Standard eigenvalue problem:

$$Ax = \lambda x$$

Often:  $A$  is symmetric real (or Hermitian complex)

- Generalized problem  $Ax = \lambda Bx$  Often:  $B$  is symmetric positive definite,  $A$  is symmetric or nonsymmetric

- Quadratic problems:  $(A + \lambda B + \lambda^2 C)u = 0$

- Nonlinear eigenvalue problems (NEVP)

$$\left[ A_0 + \lambda B_0 + \sum_{i=1}^n f_i(\lambda) A_i \right] u = 0$$

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➤ General form of NEVP  $A(\lambda)x = 0$

➤ Nonlinear **eigenvector** problems:

$$[A + \lambda B + F(u_1, u_2, \dots, u_k)]u = 0$$

### What to compute:

- A few  $\lambda_i$  's with smallest or largest real parts;
- All  $\lambda_i$ 's in a certain region of  $\mathbb{C}$ ;
- A few of the dominant eigenvalues;
- All  $\lambda_i$ 's (rare).

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### Large eigenvalue problems in applications

➤ Some applications require the computation of a large number of eigenvalues and vectors of very large matrices.

➤ Density Functional Theory in electronic structure calculations: 'ground states'

➤ *Excited states* involve transitions and invariably lead to much more complex computations. → Large matrices, \*many\* eigen-pairs to compute

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### Background: The main tools

#### Projection process:

(a) Build a 'good' subspace  $K = \text{span}(V)$ ;

(b) get approximate eigenpairs by a Rayleigh-Ritz process:

$\tilde{\lambda}, \tilde{u} \in K$  satisfy:  $(A - \tilde{\lambda}I)\tilde{u} \perp K \rightarrow$

$$V^H(A - \tilde{\lambda}I)Vy = 0$$

- $\tilde{\lambda}$  = Ritz value,  $\tilde{u} = Vy$  = Ritz vector
- Two common choices for  $K$ :
  - 1) Power subspace  $K = \text{span}\{A^k X_0\}$ ; or  $\text{span}\{P_k(A)X_0\}$ ;
  - 2) Krylov subspace  $K = \text{span}\{v, Av, \dots, A^{k-1}v\}$

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### Background. The main tools (cont)

#### Shift-and-invert:

➤ If we want eigenvalues near  $\sigma$ , replace  $A$  by  $(A - \sigma I)^{-1}$ .

**Example:** power method:  $v_j = Av_{j-1}$ /scaling replaced by

$$v_j = \frac{(A - \sigma I)^{-1}v_{j-1}}{\text{scaling}}$$

- Works well for computing a few eigenvalues near  $\sigma$ /
- Used in commercial package NASTRAN (for decades!)
- Requires factoring  $(A - \sigma I)$  (or  $(A - \sigma B)$  in generalized case.) But convergence will be much faster.
- A solve each time - Factorization done once (ideally).

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## Background. The main tools (cont)

### Deflation:

- Once eigenvectors converge remove them from the picture (e.g., with power method, second largest becomes largest eigenvalue after deflation).

### Restarting Strategies :

- Restart projection process by using information gathered in previous steps
- 
- ALL available methods use some combination of these ingredients. [e.g. ARPACK: Arnoldi/Lanczos + 'implicit restarts' + shift-and-invert (option).]

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## Current state-of-the art in eigensolvers

- Eigenvalues at one end of the spectrum:
  - Subspace iteration + filtering [e.g. FEAST, Chev,...]
  - Lanczos+variants (no restart, thick restart, implicit restart, Davidson,..), e.g., ARPACK code, PRIMME.
  - Block Algorithms [Block Lanczos, TraceMin, LOBPCG, SlepSc,...]
  - + Many others - more or less related to above
- 'Interior' eigenvalue problems (middle of spectrum):
  - Combine shift-and-invert + Lanczos/block Lanczos. Used in, e.g., NASTRAN
  - Rational filtering [FEAST, Sakurai et al,... ]

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## Projection Methods for Eigenvalue Problems

### General formulation:

Projection method onto  $K$  orthogonal to  $L$

- Given: Two subspaces  $K$  and  $L$  of same dimension.
- Find:  $\tilde{\lambda}, \tilde{u}$  such that

$$\tilde{\lambda} \in \mathbb{C}, \tilde{u} \in K; (\tilde{\lambda}I - A)\tilde{u} \perp L$$

### Two types of methods:

Orthogonal projection methods: situation when  $L = K$ .

Oblique projection methods: When  $L \neq K$ .

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## Rayleigh-Ritz projection

**Given:** a subspace  $X$  known to contain good approximations to eigenvectors of  $A$ .

**Question:** How to extract good approximations to eigenvalues/eigenvectors from this subspace?

**Answer:** Rayleigh Ritz process.

Let  $Q = [q_1, \dots, q_m]$  an orthonormal basis of  $X$ . Then write an approximation in the form  $\tilde{u} = Qy$  and obtain  $y$  by writing

$$Q^H(A - \tilde{\lambda}I)\tilde{u} = 0$$

- $Q^H A Q y = \tilde{\lambda} y$

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### Procedure:

1. Obtain an orthonormal basis of  $X$
2. Compute  $C = Q^H A Q$  (an  $m \times m$  matrix)
3. Obtain Schur factorization of  $C$ ,  $C = Y R Y^H$
4. Compute  $\tilde{U} = Q Y$

**Property:** if  $X$  is (exactly) invariant, then procedure will yield exact eigenvalues and eigenvectors.

**Proof:** Since  $X$  is invariant,  $(A - \tilde{\lambda} I)u = Qz$  for a certain  $z$ .  $Q^H Q z = 0$  implies  $z = 0$  and therefore  $(A - \tilde{\lambda} I)u = 0$ .

➤ Can use this procedure in conjunction with the subspace obtained from subspace iteration algorithm

### Subspace Iteration

➤ Original idea: projection technique onto a subspace if the form  $Y = A^k X$

➤ In practice: Replace  $A^k$  by suitable polynomial [Chebyshev]

Advantages:

- Easy to implement (in symmetric case);
- Easy to analyze;

Disadvantage: Slow.

➤ Often used with polynomial acceleration:  $A^k X$  replaced by  $C_k(A)X$ . Typically  $C_k =$  Chebyshev polynomial.

### Algorithm: Subspace Iteration with Projection

1. **Start:** Choose an initial system of vectors  $X = [x_0, \dots, x_m]$  and an initial polynomial  $C_k$ .
2. **Iterate:** Until convergence do:
  - (a) Compute  $\hat{Z} = C_k(A)X_{old}$ .
  - (b) Orthonormalize  $\hat{Z}$  into  $Z$ .
  - (c) Compute  $B = Z^H A Z$  and use the QR algorithm to compute the Schur vectors  $Y = [y_1, \dots, y_m]$  of  $B$ .
  - (d) Compute  $X_{new} = ZY$ .
  - (e) Test for convergence. If satisfied stop. Else select a new polynomial  $C'_{k'}$  and continue.

**THEOREM:** Let  $S_0 = \text{span}\{x_1, x_2, \dots, x_m\}$  and assume that  $S_0$  is such that the vectors  $\{P x_i\}_{i=1, \dots, m}$  are linearly independent where  $P$  is the spectral projector associated with  $\lambda_1, \dots, \lambda_m$ . Let  $\mathcal{P}_k$  the orthogonal projector onto the subspace  $S_k = \text{span}\{X_k\}$ . Then for each eigenvector  $u_i$  of  $A$ ,  $i = 1, \dots, m$ , there exists a unique vector  $s_i$  in the subspace  $S_0$  such that  $P s_i = u_i$ . Moreover, the following inequality is satisfied

$$\|(I - \mathcal{P}_k)u_i\|_2 \leq \|u_i - s_i\|_2 \left( \left| \frac{\lambda_{m+1}}{\lambda_i} \right| + \epsilon_k \right)^k, \quad (1)$$

where  $\epsilon_k$  tends to zero as  $k$  tends to infinity.

## Krylov subspace methods

Principle: Projection methods on Krylov subspaces, i.e., on

$$K_m(A, v_1) = \text{span}\{v_1, Av_1, \dots, A^{m-1}v_1\}$$

- probably the most important class of projection methods [for linear systems and for eigenvalue problems]
- many variants exist depending on the subspace  $L$ .

Properties of  $K_m$ . Let  $\mu = \text{deg. of minimal polynomial of } v$ . Then,

- $K_m = \{p(A)v \mid p = \text{polynomial of degree } \leq m - 1\}$
- $K_m = K_\mu$  for all  $m \geq \mu$ . Moreover,  $K_\mu$  is invariant under  $A$ .
- $\dim(K_m) = m$  iff  $\mu \geq m$ .

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## Arnoldi's Algorithm

- Goal: to compute an orthogonal basis of  $K_m$ .
- Input: Initial vector  $v_1$ , with  $\|v_1\|_2 = 1$  and  $m$ .

**ALGORITHM : 1.** *Arnoldi's procedure*

```

For  $j = 1, \dots, m$  do
  Compute  $w := Av_j$ 
  For  $i = 1, \dots, j$ , do  $\begin{cases} h_{i,j} := (w, v_i) \\ w := w - h_{i,j}v_i \end{cases}$ 
   $h_{j+1,j} = \|w\|_2; v_{j+1} = w/h_{j+1,j}$ 
End

```

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## Result of Arnoldi's algorithm

Let

$$\bar{H}_m = \begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ & x & x & x & x \\ & & x & x & x \\ & & & x & x \\ & & & & x \end{bmatrix}; \quad H_m = \bar{H}_m(1:m, 1:m)$$

1.  $V_m = [v_1, v_2, \dots, v_m]$  orthonormal basis of  $K_m$ .
2.  $AV_m = V_{m+1}\bar{H}_m = V_m H_m + h_{m+1,m}v_{m+1}e_m^T$
3.  $V_m^T AV_m = H_m \equiv \bar{H}_m - \text{last row.}$

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## Application to eigenvalue problems

- Write approximate eigenvector as  $\tilde{u} = V_m y$  + Galerkin condition

$$(A - \tilde{\lambda}I)V_m y \perp \mathcal{K}_m \rightarrow V_m^H (A - \tilde{\lambda}I)V_m y = 0$$

- Approximate eigenvalues are eigenvalues of  $H_m$

$$H_m y_j = \tilde{\lambda}_j y_j$$

Associated approximate eigenvectors are

$$\tilde{u}_j = V_m y_j$$

Typically a few of the outermost eigenvalues will converge first.

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## Restarted Arnoldi

In practice: Memory requirement of algorithm implies restarting is necessary

- Restarted Arnoldi for computing rightmost eigenpair:

### ALGORITHM : 2. Restarted Arnoldi

1. **Start:** Choose an initial vector  $v_1$  and a dimension  $m$ .
2. **Iterate:** Perform  $m$  steps of Arnoldi's algorithm.
3. **Restart:** Compute the approximate eigenvector  $u_1^{(m)}$
4. associated with the rightmost eigenvalue  $\lambda_1^{(m)}$ .
5. If satisfied stop, else set  $v_1 \equiv u_1^{(m)}$  and goto 2.

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## Example:

Small Markov Chain matrix [ Mark(10) , dimension = 55]. Restarted Arnoldi procedure for computing the eigenvector associated with the eigenvalue with algebraically largest real part. We use  $m = 10$ .

$m$	$\Re(\lambda)$	$\Im(\lambda)$	Res. Norm
10	0.9987435899D+00	0.0	0.246D-01
20	0.9999523324D+00	0.0	0.144D-02
30	0.1000000368D+01	0.0	0.221D-04
40	0.1000000025D+01	0.0	0.508D-06
50	0.9999999996D+00	0.0	0.138D-07

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## Restarted Arnoldi (cont.)

- Can be generalized to more than \*one\* eigenvector :

$$v_1^{(new)} = \sum_{i=1}^p \rho_i u_i^{(m)}$$

- However: often does not work well – (hard to find good coefficients  $\rho_i$ 's)
- Alternative : compute eigenvectors (actually Schur vectors) one at a time.
- Implicit deflation.

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## Deflation

- Very useful in practice.
- Different forms: locking (subspace iteration), selective orthogonalization (Lanczos), Schur deflation, ...

**A little background** Consider Schur canonical form

$$A = URU^H$$

where  $U$  is a (complex) upper triangular matrix.

- Vector columns  $u_1, \dots, u_n$  called **Schur vectors**.
- Note: Schur vectors are not unique. In particular, they depend on the order of the eigenvalues

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**Wiedlandt Deflation:** Assume we have computed a right eigenpair  $\lambda_1, u_1$ . Wielandt deflation considers eigenvalues of

$$A_1 = A - \sigma u_1 v^H$$

Note:

$$\Lambda(A_1) = \{\lambda_1 - \sigma, \lambda_2, \dots, \lambda_n\}$$

Wielandt deflation preserves  $u_1$  as an eigenvector as well all the left eigenvectors not associated with  $\lambda_1$ .

- An interesting choice for  $v$  is to take simply  $v = u_1$ . In this case Wielandt deflation preserves Schur vectors as well.
- Can apply above procedure successively.

**ALGORITHM : 3. Explicit Deflation**

1.  $A_0 = A$
2. For  $j = 0 \dots \mu - 1$  Do:
3.   Compute a dominant eigenvector of  $A_j$
4.   Define  $A_{j+1} = A_j - \sigma_j u_j u_j^H$
5. End

- Computed  $u_1, u_2, \dots$  form a set of Schur vectors for  $A$ .
- Alternative: implicit deflation (within a procedure such as Arnoldi).

**Deflated Arnoldi**

- When first eigenvector converges, put it in 1st column of  $V_m = [v_1, v_2, \dots, v_m]$ . Arnoldi will now start at column 2, orthogonalizing still against  $v_1, \dots, v_j$  at step  $j$ .
- Accumulate each new converged eigenvector in columns 2, 3, ... ['locked' set of eigenvectors.]

Thus, for  $k = 2$ :

$$V_m = \begin{bmatrix} \underbrace{v_1, v_2}_{\text{Locked}}, \overbrace{v_3, \dots, v_m}^{\text{active}} \end{bmatrix}$$

$$H_m = \begin{pmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ \hline & & * & * & * & * \\ & & * & * & * & * \\ & & & * & * & * \\ & & & & * & * \end{pmatrix}$$

- Similar techniques in Subspace iteration [G. Stewart's SRRIT]

**Example:** Matrix Mark(10) – small Markov chain matrix ( $N = 55$ ).

- First eigenpair by iterative Arnoldi with  $m = 10$ .

$m$	$\Re(\lambda)$	$\Im(\lambda)$	Res. Norm
10	0.9987435899D+00	0.0	0.246D-01
20	0.9999523324D+00	0.0	0.144D-02
30	0.1000000368D+01	0.0	0.221D-04
40	0.1000000025D+01	0.0	0.508D-06
50	0.9999999996D+00	0.0	0.138D-07

- Computing the next 2 eigenvalues of Mark(10).

Eig.	Mat-Vec's	$\Re(\lambda)$	$\Im(\lambda)$	Res. Norm
2	60	0.9370509474	0.0	0.870D-03
	69	0.9371549617	0.0	0.175D-04
	78	0.9371501442	0.0	0.313D-06
	87	0.9371501564	0.0	0.490D-08
3	96	0.8112247133	0.0	0.210D-02
	104	0.8097553450	0.0	0.538D-03
	112	0.8096419483	0.0	0.874D-04
	⋮	⋮	⋮	⋮
	⋮	⋮	⋮	⋮
	152	0.8095717167	0.0	0.444D-07

### Hermitian case: The Lanczos Algorithm

- The Hessenberg matrix becomes tridiagonal :

$$A = A^H \quad \text{and} \quad V_m^H A V_m = H_m \quad \rightarrow \quad H_m = H_m^H$$

- We can write

$$H_m = \begin{bmatrix} \alpha_1 & \beta_2 & & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & & \beta_m & \alpha_m \end{bmatrix} \quad (2)$$

- Consequence: three term recurrence

$$\beta_{j+1} v_{j+1} = A v_j - \alpha_j v_j - \beta_j v_{j-1}$$

### ALGORITHM : 4. Lanczos

1. Choose  $v_1$  of norm unity. Set  $\beta_1 \equiv 0, v_0 \equiv 0$
2. For  $j = 1, 2, \dots, m$  Do:
3.  $w_j := A v_j - \beta_j v_{j-1}$
4.  $\alpha_j := (w_j, v_j)$
5.  $w_j := w_j - \alpha_j v_j$
6.  $\beta_{j+1} := \|w_j\|_2$ . If  $\beta_{j+1} = 0$  then Stop
7.  $v_{j+1} := w_j / \beta_{j+1}$
8. EndDo

Hermitian matrix + Arnoldi  $\rightarrow$  Hermitian Lanczos

- In theory  $v_i$ 's defined by 3-term recurrence are orthogonal.
- However: in practice severe loss of orthogonality;

### Lanczos with reorthogonalization

Observation [Paige, 1981]: Loss of orthogonality starts suddenly, when the first eigenpair converges. It indicates loss of linear independence of the  $v_i$ 's. When orthogonality is lost, then several copies of the same eigenvalue start appearing.

- Full reorthogonalization – reorthogonalize  $v_{j+1}$  against all previous  $v_i$ 's every time.
- Partial reorthogonalization – reorthogonalize  $v_{j+1}$  against all previous  $v_i$ 's only when needed [Parlett & Simon]
- Selective reorthogonalization – reorthogonalize  $v_{j+1}$  against computed eigenvectors [Parlett & Scott]
- No reorthogonalization – Do not reorthogonalize - but take measures to deal with 'spurious' eigenvalues. [Cullum & Willoughby]



## Partial reorthogonalization

- Partial reorthogonalization: reorthogonalize only when deemed necessary.
- Main question is **when?**
- Uses an inexpensive recurrence relation
- Work done in the 80's [Parlett, Simon, and co-workers] + more recent work [Larsen, '98]
- Package: PROPACK [Larsen] V 1: 2001, most recent: V 2.1 (Apr. 05)
- Often, need for reorthogonalization not too strong

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## The Lanczos Algorithm in the Hermitian Case

Assume eigenvalues sorted increasingly

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$$

- Orthogonal projection method onto  $K_m$ ;
- To derive error bounds, use the Courant characterization

$$\tilde{\lambda}_1 = \min_{u \in K, u \neq 0} \frac{(Au, u)}{(u, u)} = \frac{(A\tilde{u}_1, \tilde{u}_1)}{(\tilde{u}_1, \tilde{u}_1)}$$

$$\tilde{\lambda}_j = \min_{\substack{u \in K, u \neq 0 \\ u \perp \tilde{u}_1, \dots, \tilde{u}_{j-1}}} \frac{(Au, u)}{(u, u)} = \frac{(A\tilde{u}_j, \tilde{u}_j)}{(\tilde{u}_j, \tilde{u}_j)}$$

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- Bounds for  $\lambda_1$  easy to find – similar to linear systems.
- Ritz values approximate eigenvalues of  $A$  inside out:



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## A-priori error bounds

Theorem [Kaniel, 1966]:

$$0 \leq \lambda_1^{(m)} - \lambda_1 \leq (\lambda_N - \lambda_1) \left[ \frac{\tan \angle(v_1, u_1)}{T_{m-1}(1 + 2\gamma_1)} \right]^2$$

where  $\gamma_1 = \frac{\lambda_2 - \lambda_1}{\lambda_N - \lambda_2}$ ; and  $\angle(v_1, u_1)$  = angle between  $v_1$  and  $u_1$ .

+ results for other eigenvalues. [Kaniel, Paige, YS]

Theorem

$$0 \leq \lambda_i^{(m)} - \lambda_i \leq (\lambda_N - \lambda_i) \left[ \kappa_i^{(m)} \frac{\tan \angle(v_i, u_i)}{T_{m-i}(1 + 2\gamma_i)} \right]^2$$

where  $\gamma_i = \frac{\lambda_{i+1} - \lambda_i}{\lambda_N - \lambda_{i+1}}$ ,  $\kappa_i^{(m)} = \prod_{j < i} \frac{\lambda_j^{(m)} - \lambda_N}{\lambda_j^{(m)} - \lambda_i}$

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## The Lanczos biorthogonalization ( $A^H \neq A$ )

### ALGORITHM : 5. Lanczos bi-orthogonalization

1. Choose two vectors  $v_1, w_1$  such that  $(v_1, w_1) = 1$ .
2. Set  $\beta_1 = \delta_1 \equiv 0, w_0 = v_0 \equiv 0$
3. For  $j = 1, 2, \dots, m$  Do:
4.  $\alpha_j = (Av_j, w_j)$
5.  $\hat{v}_{j+1} = Av_j - \alpha_j v_j - \beta_j v_{j-1}$
6.  $\hat{w}_{j+1} = A^T w_j - \alpha_j w_j - \delta_j w_{j-1}$
7.  $\delta_{j+1} = |(\hat{v}_{j+1}, \hat{w}_{j+1})|^{1/2}$ . If  $\delta_{j+1} = 0$  Stop
8.  $\beta_{j+1} = (\hat{v}_{j+1}, \hat{w}_{j+1}) / \delta_{j+1}$
9.  $w_{j+1} = \hat{w}_{j+1} / \beta_{j+1}$
10.  $v_{j+1} = \hat{v}_{j+1} / \delta_{j+1}$
11. EndDo

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- Builds a pair of biorthogonal bases for the two subspaces

$$\mathcal{K}_m(A, v_1) \quad \text{and} \quad \mathcal{K}_m(A^H, w_1)$$

- Many choices for  $\delta_{j+1}, \beta_{j+1}$  in lines 7 and 8. Only constraint:

$$\delta_{j+1} \beta_{j+1} = (\hat{v}_{j+1}, \hat{w}_{j+1})$$

Let

$$T_m = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \delta_2 & \alpha_2 & \beta_3 & & \\ & \cdot & \cdot & \cdot & \\ & & \delta_{m-1} & \alpha_{m-1} & \beta_m \\ & & & \delta_m & \alpha_m \end{bmatrix} \cdot$$

- $v_i \in \mathcal{K}_m(A, v_1)$  and  $w_j \in \mathcal{K}_m(A^T, w_1)$ .

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If the algorithm does not break down before step  $m$ , then the vectors  $v_i, i = 1, \dots, m$ , and  $w_j, j = 1, \dots, m$ , are biorthogonal, i.e.,

$$(v_j, w_i) = \delta_{ij} \quad 1 \leq i, j \leq m.$$

Moreover,  $\{v_i\}_{i=1,2,\dots,m}$  is a basis of  $\mathcal{K}_m(A, v_1)$  and  $\{w_i\}_{i=1,2,\dots,m}$  is a basis of  $\mathcal{K}_m(A^H, w_1)$  and

$$\begin{aligned} AV_m &= V_m T_m + \delta_{m+1} v_{m+1} e_m^H, \\ A^H W_m &= W_m T_m^H + \bar{\beta}_{m+1} w_{m+1} e_m^H, \\ W_m^H AV_m &= T_m \quad \cdot \end{aligned}$$

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- If  $\theta_j, y_j, z_j$  are, respectively an eigenvalue of  $T_m$ , with associated right and left eigenvectors  $y_j$  and  $z_j$  respectively, then corresponding approximations for  $A$  are

Ritz value	Right Ritz vector	Left Ritz vector
$\theta_j$	$V_m y_j$	$W_m z_j$

[Note: terminology is abused slightly - Ritz values and vectors normally refer to Hermitian cases.]

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## Advantages and disadvantages

### Advantages:

- Nice three-term recurrence – requires little storage in theory.
- Computes left and a right eigenvectors at the same time

### Disadvantages:

- Algorithm can break down or nearly break down.
- Convergence not too well understood. Erratic behavior
- Not easy to take advantage of the tridiagonal form of  $T_m$ .

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## Look-ahead Lanczos

Algorithm breaks down when:

$$(\hat{v}_{j+1}, \hat{w}_{j+1}) = 0$$

Three distinct situations.

- 'lucky breakdown' when either  $\hat{v}_{j+1}$  or  $\hat{w}_{j+1}$  is zero. In this case, eigenvalues of  $T_m$  are eigenvalues of  $A$ .
- $(\hat{v}_{j+1}, \hat{w}_{j+1}) = 0$  but of  $\hat{v}_{j+1} \neq 0$ ,  $\hat{w}_{j+1} \neq 0 \rightarrow$  **serious breakdown**. Often possible to bypass the step (+ a few more) and continue the algorithm. If this is not possible then we get an ...
- ... Incurable break-down. [very rare]

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**Look-ahead Lanczos algorithms** deal with the second case.

See Parlett 80, Freund and Nachtigal '90.... Main idea: when break-down occurs, skip the computation of  $v_{j+1}, w_{j+1}$  and define  $v_{j+2}, w_{j+2}$  from  $v_j, w_j$ . For example by orthogonalizing  $A^2 v_j$  ... Can define  $v_{j+1}$  somewhat arbitrarily as  $v_{j+1} = A v_j$ . Similarly for  $w_{j+1}$ .

- Drawbacks: (1) projected problem no longer tridiagonal (2) difficult to know what constitutes near-breakdown.

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