Hessenberg Eigenvalue – Eigenvector Relations and their Application to the Error Analysis of Finite Precision Krylov Subspace Methods

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Talk at the Gesellschaft für Angewandte Mathematik und Mechanik Workshop

Numerical Linear Algebra with special emphasis on Multilevel and Krylov Subspace Methods

September 13–14, 2002

University of Bielefeld, Germany
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The Menagerie of Krylov Methods

- **Lanczos** based methods (short–term methods)
- **Arnoldi** based methods (long–term methods)

**eigensolvers:** $Av = v\lambda$
**linear system solvers:** $Ax = b$
  - (quasi-) orthogonal residual approaches: (Q)OR
  - (quasi-) minimal residual approaches: (Q)MR

Extensions:
- **Lanczos** based methods:
  - look-ahead
  - product-type (LTPMs)
  - applied to normal equations (CGN)
- **Arnoldi** based methods:
  - restart (thin/thick, explicit/implicit)
  - truncation (standard/optimal)
A Unified Matrix Description of Krylov Methods

Krylov methods as projection onto 'simpler' matrices:
- \( Q^H Q = I, \ Q^H AQ = H \) Hessenberg (Arnoldi),
- \( \tilde{Q}^H Q = I, \ \tilde{Q}^H AQ = T \) tridiagonal (Lanczos)

Introduce computed (condensed) matrix \( C = T, H \)

\[
Q^{-1}AQ = C \quad \Rightarrow \quad AQ = QC
\]

Iteration implied by unreduced Hessenberg structure:

\[
AQ_k = Q_{k+1}C_k, \quad Q_k = [q_1, \ldots, q_k], \quad C_k \in \mathbb{K}^{(k+1)\times k}
\]

Stewart: 'Krylov Decomposition'

Iteration spans Krylov subspace \((q = q_1)\):

\[
\text{span}\{Q_k\} = \mathcal{K}_k = \text{span}\{q, Aq, \ldots, A^{k-1}q\}
\]
Perturbed Krylov Decompositions

A Krylov decomposition analogue holds true in finite precision:

\[
AQ_k = Q_{k+1}C_k - F_k = Q_kC_k + q_{k+1}c_{k+1, k}e_k^T - F_k \\
= Q_kC_k + M_k - F_k
\]

We have to investigate the impacts of the method on
- the structure of the basis \( Q_k \) (local orthogonality/duality)
- the structure of the computed \( C_k, C_k \)
- the size/structure of the error term \(-F_k\)

Convergence theory:
- is usually based on inductively proven properties: orthogonality, bi-orthogonality, \( A \)-conjugacy, . . .

What can be said about these properties?

'Standard' error analysis:
- splits into forward and backward error analysis.

Does this type of analysis apply to Krylov methods?
All methods fit **pictorially** into:

\[
A \quad Q_k \quad - \quad Q_k \quad = \quad 0 \quad - \quad F_k
\]

This is a perturbed Krylov decomposition, as **subspace equation**.
Examination of the methods can be grouped according to
- methods directly based on the Krylov decomposition
- methods based on a split Krylov decomposition
- LTPMs

The matrix $C_k$ plays a crucial role:
- $C_k$ is Hessenberg or even tridiagonal (basics),
- $C_k$ may be blocked or banded (block Krylov methods),
- $C_k$ may have humps, spikes, ... (more sophisticated)

The error analysis and convergence theory splits further up:
- knowledge on Hessenberg (tridiagonal) matrices
- knowledge on orthogonality, duality, conjugacy, ...

We start with results on Hessenberg matrices.
An Excursion on Matrix Structure

Eigendecomposition of $A$:

$$AV = VJ_{\lambda}$$

Left eigenmatrices:

$$\tilde{V} \equiv V^{-H} \Rightarrow \tilde{V}^H A = J_{\lambda} \tilde{V}^H$$

$$\check{V} \equiv V^{-T} \Rightarrow \check{V}^T A = J_{\lambda} \check{V}^T$$

The adjoint of $\lambda I - A$ fulfills

$$\text{adj} (\lambda I - A)(\lambda I - A) = \text{det}(\lambda I - A)I \equiv \chi_A(\lambda)I.$$}

Suppose that $\lambda$ is not contained in the spectrum of $A$. 
We form the resolvent $R(\lambda) = (\lambda I - A)^{-1}$ of $\lambda$ and obtain

$$\text{adj} (\lambda I - A) = \chi_A(\lambda) R(\lambda) = \chi_A(\lambda) V J_{\lambda - \lambda_i}^{-1} V^H.$$

One shifted and inverted Jordan block:

$$J_{\lambda - \lambda_i}^{-1} = S_i E_i S_i \equiv S_i \left( \begin{array}{cccc}
(\lambda - \lambda_i)^{-1} & (\lambda - \lambda_i)^{-2} & \ldots & (\lambda - \lambda_i)^{-k} \\
(\lambda - \lambda_i)^{-1} & \ldots & \vdots \\
& \ldots & \vdots \\
& & (\lambda - \lambda_i)^{-1}
\end{array} \right) S_i,$$

Observation: Terms with negative exponent cancel with factors in the characteristic polynomial $\chi_A(\lambda)$.

The resulting expression is a source of eigenvalue – eigenvector relations.
We express the adjugate with the aid of compound matrices,

\[ \text{adj } A \equiv SC_{n-1}(A^T)S. \]

Then we have equality

\[ P \equiv C_{n-1}(\lambda I - A^T) = (SVS)G(S\hat{V}^HS) \equiv (SVS)\chi_A(\lambda)E(S\hat{V}^HS). \]

The compound matrix \( P \) is composed of polynomials in \( \lambda \):

\[ p_{ij} = p_{ij}(\lambda; A) \equiv \det L_{ji}, \quad \text{where} \quad L \equiv \lambda I - A. \]

\( G \) is composed of rational functions in \( \lambda \):

\[ G = \chi_A(\lambda) \cdot (\oplus_i E_i). \]

Since many terms cancel, the elements of \( G \) are polynomials.

We divide by maximal factor \( (\lambda - \lambda_i)^\ell \) and compute the limes \( \lambda \to \lambda_i \).
Observation: Only few elements of $\lim \mathcal{G}$ are non-zero. Choice of eigenvectors based on non-zero positions $i, j$:

We consider here only the special case of non-derogatory eigenvalues.

We arrive at equations involving the elements of $P$, $\lim \mathcal{G}$ and products of components of left and right eigenvectors.
Theorem: Let $A \in \mathbb{K}^{n \times n}$. Let $\lambda_l = \lambda_{l+1} = \ldots = \lambda_{l+k}$ be a geometrically simple eigenvalue of $A$. Let $k + 1$ be the algebraic multiplicity of $\lambda$. Let $\tilde{v}_{l+k}^H$ and $v_l$ be the corresponding left and right eigenvectors with appropriate normalization.

Then

$$v_{jl} \tilde{v}_{i,l+k} = (-1)^{(j+i+k)} \frac{p_{ji}(\lambda_l; A)}{\prod_{\lambda_s \neq \lambda_l} (\lambda_l - \lambda_s)}$$

holds true.

The sign matrices bear the blame for the minus one, $P$ for the numerator and $\lim G$ for the denominator.

This setting matches every eigenvalue of non-derogatory $A$. 
Unreduced Hessenberg matrices are non-derogatory matrices. This is easily seen by a simple rank argument. In the following let $H = H_m$ be unreduced Hessenberg of size $m \times m$,

$$\text{rank}(H - \theta I) \geq m - 1.$$ 

Many polynomials can be evaluated in case of Hessenberg matrices:

**Theorem:** The polynomial $p_{ji}$, $i \leq j$ has degree $(i - 1) + (m - j)$ and can be evaluated as follows:

$$p_{ji}(\theta; H) = \begin{vmatrix} \theta I - H_{1:i-1} & \ast \\ 0 & \theta I - H_{j+1:m} \end{vmatrix} = (-1)^{i+j} \chi_{H_{1:i-1}}(\theta) \prod \text{diag}(H_{i:j}, -1) \chi_{H_{j+1:m}}(\theta).$$
Denote by $\mathcal{H}(m)$ the set of unreduced Hessenberg matrices of size $m \times m$. The general result on eigenvalue – eigenvector relations can be simplified to read:

**Theorem:** Let $H \in \mathcal{H}(m)$. Let $i \leq j$. Let $\theta$ be an eigenvalue of $H$ with multiplicity $k + 1$. Let $s$ be the unique left eigenvector and $\tilde{s}^H$ be the unique right eigenvector to eigenvalue $\theta$.

Then

$$(-1)^k \tilde{s}(i)s(j) = \left[ \frac{\chi_{H_{1:i-1}H_{j+1:m}}(\theta)}{\chi_{H_{1:m}}} \right]^{j-1} \prod_{l=i}^{j-1} h_{l+1,l}$$

holds true.

**Remark:** We ignored the implicit scaling in the eigenvectors imposed by the choice of eigenvector-matrices, i.e. by $\tilde{S}^T S = I$. 
Error Analysis Revisited

For simplicity we assume that the perturbed Krylov decomposition

\[ M_k = AQ_k - Q_k C_k + F_k \]

is diagonalisable, i.e. that \( A \) and \( C_k \) are diagonalisable. Let \( y_j \equiv Q_k s_j \).

**Theorem:** The recurrence of the basis vectors in eigenparts is given by

\[
\hat{v}_i^H q_{k+1} = \left( \lambda_i - \theta_j \right) \hat{v}_i^H y_j + \hat{v}_i^H F_k s_j \cdot c_{k+1,k} s_{kj} \quad \forall \ i, j (, k).
\]

This *local error amplification formula* consists of four ingredients:

- the left eigenpart of \( q_{k+1} \): \( \hat{v}_i^H q_{k+1} \),
- a measure of convergence: \( (\lambda_i - \theta_j) \hat{v}_i^H y_j \),
- an error term: \( \hat{v}_i^H F_k s_j \),
- an amplification factor: \( c_{k+1,k} s_{kj} \).
The formula depends on the Ritz pair of the actual step. Using the eigenvector basis we can get rid of the Ritz vector:

\[ I = SS^{-1} = S\tilde{S}^T \quad \Rightarrow \quad e_l = S\tilde{S}^T e_l \equiv \sum_{j=1}^{k} \tilde{s}_{lj}s_{j}. \]

**Theorem**: The recurrence between vectors \( q_l \) and \( q_{k+1} \) is given by

\[
\begin{bmatrix}
\sum_{j=1}^{k} \frac{c_{k+1,k}\tilde{s}_{lj}s_{kj}}{\lambda_i - \theta_j}
\end{bmatrix} \hat{v}_i^H q_{k+1} = \hat{v}_i^H q_l + \hat{v}_i^H F_k \begin{bmatrix}
\sum_{j=1}^{k} \left( \frac{\tilde{s}_{lj}}{\lambda_i - \theta_j} \right) s_j
\end{bmatrix}.
\]

For \( l = 1 \) we obtain a formula that reveals how the errors affect the recurrence from the beginning:

\[
\begin{bmatrix}
\sum_{j=1}^{k} \frac{c_{k+1,k}\tilde{s}_{1j}s_{kj}}{\lambda_i - \theta_j}
\end{bmatrix} \hat{v}_i^H q_{k+1} = \hat{v}_i^H q_1 + \hat{v}_i^H F_k \begin{bmatrix}
\sum_{j=1}^{k} \left( \frac{\tilde{s}_{1j}}{\lambda_i - \theta_j} \right) s_j
\end{bmatrix}.
\]
**Interpretation:** The size of the deviation depends on the size of the first component of the left eigenvector $\hat{s}_j$ of $C_k$ and the shape and size of the right eigenvector $s_j$.

Next step: Application of the eigenvector – eigenvalue relation (1), (set $k = 1, i = 1, m = k, j = k$):

$$(-1)^k \hat{s}(i)s(j) = \left[ \frac{\chi C_{1:i-1}\chi C_{j+1:m}}{\chi C_{(k+1):1:m}(\theta)} \right] \prod_{l=i}^{j-1} c_{l+1, l}.$$ 

**Theorem:** The recurrence between basis vectors $q_1$ and $q_{k+1}$ can be described by

$$\sum_{j=1}^{k} \frac{\prod_{p=1}^{k} c_{p+1, p}}{\prod_{s \neq j} (\theta_s - \theta_j) (\lambda_i - \theta_j)} \hat{v}_i^H q_{k+1} = \hat{v}_i^H q_1 + \hat{v}_i^H F_k \left[ \sum_{j=1}^{k} \left( \frac{\hat{s}_{1j}}{\lambda_i - \theta_j} \right) s_j \right].$$
A result from polynomial interpolation theory (Lagrange):

\[
\sum_{j=1}^{k} \frac{1}{\prod_{l \neq j} (\theta_j - \theta_l) (\lambda_i - \theta_j)} = \frac{1}{\chi C_k(\lambda_i)} \sum_{j=1}^{k} \frac{\prod_{l \neq j} (\lambda_i - \theta_l)}{\prod_{l \neq j} (\theta_j - \theta_l)} = \frac{1}{\chi C_k(\lambda_i)}
\]

The following theorem holds true:

**Theorem:** The recurrence between basis vectors \( q_1 \) and \( q_{k+1} \) can be described by

\[
\hat{v}_i^H q_{k+1} = \frac{\chi C_k(\lambda_i)}{\prod_{p=1}^{k} c_{p+1,p}} \left( \hat{v}_i^H q_1 + \hat{v}_i^H F_k \left[ \sum_{j=1}^{k} \left( \frac{\tilde{s}_{1j}}{\lambda_i - \theta_j} \right) s_j \right] \right)
\]
Similarly we can get rid of the eigenvectors $s_j$ in the error term:

$$e^T_l \left[ \sum_{j=1}^{k} \left( \frac{\tilde{s}_{1j}}{\lambda_i - \theta_j} \right) s_j \right] = \sum_{j=1}^{k} \left( \frac{\tilde{s}_{1j} s_{lj}}{\lambda_i - \theta_j} \right) = \frac{\prod_{p=1}^{l} c_{p+1,p} \chi_{C_{l+1:1}}(\lambda_i)}{\chi_{C_{k}}(\lambda_i)}$$

This results in the following theorem:

**Theorem:** The recurrence between basis vectors $q_1$ and $q_{k+1}$ can be described by

$$\hat{v}_i^H q_{k+1} = \frac{\chi_{C_{k}}(\lambda_i)}{\prod_{p=1}^{k} c_{p+1,p}} \left( \hat{v}_i^H q_1 + \hat{v}_i^H \sum_{l=1}^{k} \frac{\prod_{p=1}^{l} c_{p+1,p} \chi_{C_{l+1:1}}(\lambda_i)}{\chi_{C_{k}}(\lambda_i)} f_l \right)$$

$$= \frac{\chi_{C_{k}}(\lambda_i)}{\prod_{p=1}^{k} c_{p+1,p}} \hat{v}_i^H q_1 + \sum_{l=1}^{k} \left( \frac{\chi_{C_{l+1:1}}(\lambda_i)}{\prod_{p=l+1}^{k} c_{p+1,p}} \hat{v}_i^H f_l \right).$$
Multiplication by the right eigenvectors $v_i$ and summation gives the familiar result:

**Theorem**: The recurrence of the basis vectors of a finite precision Krylov method can be described by

$$q_{k+1} = \frac{\chi_{C_k}(A)}{\prod_{p=1}^{k} c_{p+1,p}} q_1 + \sum_{l=1}^{k} \left( \frac{\chi_{C_{l+1:k}}(A)}{\prod_{p=l+1}^{k} c_{p+1,p}} f_l \right).$$

This result holds true even for non-diagonalisable matrices $A, C_k$.

The method can be interpreted as an *additive mixture* of several instances of the same method with several starting vectors.

A *severe deviation* occurs when one of the characteristic polynomials $\chi_{C_{l+1:k}}(A)$ becomes large compared to $\chi_{C_k}(A)$. 
Open Questions

- Can Krylov methods be forward or backward stable?
- If so, which can?
- Are there any sets of matrices $A$ for which Krylov methods are stable?
- Does the stability depend on the starting vector?
- Are there any a priori results on
  - the behaviour to be expected and
  - the rate of convergence?
$A \in \mathbb{R}^{100 \times 100}$ normal, eigenvalues equidistant in $[0, 1]$.  

Behaviour of **CGS-Arnoldi, MGS-Arnoldi, DO-Arnoldi**, convergence to eigenvalue of largest modulus.
\( A \in \mathbb{R}^{100 \times 100} \) non-normal, eigenvalues equidistant in \([0, 1]\).

$A = A^T \in \mathbb{R}^{100 \times 100}$, random entries in $[0, 1]$. Perron root well separated.

Behaviour of symmetric Lanczos, convergence to eigenvalue of largest modulus.
$A = A^T \in \mathbb{R}^{100 \times 100}$, random entries in $[0, 1]$. Perron root well separated.

Behaviour of symmetric Lanczos, convergence to eigenvalue of largest and second largest modulus.