Hessenberg eigenvalue – eigenvector relations and their application to the error analysis of finite precision Krylov subspace methods

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The Menagerie of Krylov Methods

o Lanczos based methods (short–term methods)
o Arnoldi based methods (long–term methods)

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

Extensions:
o Lanczos based methods:
- o look-ahead
- o product-type (LTPMs)
- o applied to normal equations (CGN)

o Arnoldi based methods:
- o restart (thin/thick, explicit/implicit)
- o truncation (standard/optimal)

A Unified Matrix Description of Krylov Methods

Krylov methods as projection onto 'simpler' matrices:

- o $Q^H Q = I$, $Q^H A Q = H$ Hessenberg (Arnoldi),
- o $\hat{Q}^H Q = I$, $\hat{Q}^H A Q = T$ tridiagonal (Lanczos)

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

$$Q^{-1} A Q = C \quad \Rightarrow \quad AQ = QC$$

Iteration implied by unreduced Hessenberg structure:

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

Stewart: 'Krylov Decomposition'

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

$$\mathrm{span}\{Q_k\} = \mathcal{K}_k = \mathrm{span}\{q, Aq, \ldots, A^{k-1} q\}$$

Perturbed Krylov Decompositions

A Krylov decomposition analogue holds true in finite precision:

$$\begin{aligned} AQ_k = Q_{k+1}\underline{C}_k - F_k &= Q_k C_k + q_{k+1} c_{k+1,k} e_k^T - F_k \\ &= Q_k C_k + M_k - F_k \end{aligned}$$

We have to investigate the impacts of the method on
- o the structure of the basis Q_k (local orthogonality/duality)
- o the structure of the computed C_k, $\underline{C}_k$
- o the size/structure of the error term $-F_k$

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

What can be said about these properties?

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

Does this analysis apply to Krylov methods?

All methods fit pictorially into:

$$A Q_k - Q_k C_k = 0 - F_k.$$

This is a perturbed Krylov decomposition, as subspace equation.

Examination of the methods has to be done according to

- o methods directly based on the Krylov decomposition
- o methods based on a split Krylov decomposition
- o LTPMs

The matrix C_k plays a crucial role:

- o C_k is Hessenberg or even tridiagonal (basics),
- o C_k may be blocked or banded (block Krylov methods),
- o C_k may have humps, spikes, ... (more sophisticated)

The error analysis and convergence theory splits further up:

- o knowledge on Hessenberg (tridiagonal) matrices
- o knowledge on orthogonality, duality, conjugacy, ...

We start with results on Hessenberg matrices.

A Short Excursion on Matrix Structure

J_Λ	Jordan matrix of A
V	right eigenvector-matrix, $AV = VJ_\Lambda$
$\widehat{V} \equiv V^{-H}$	left eigenvector-matrix, $\widehat{V}^H A = J_\Lambda \widehat{V}^H$
$\check{V} \equiv V^{-T}$	alternate eigenvector-matrix, $\check{V}^T A = J_\Lambda \check{V}^T$
$\chi_A(\lambda) \equiv \det(\lambda I - A)$	characteristic polynomial of A
$R(\lambda) \equiv (\lambda I - A)^{-1}$	resolvent
$\mathcal{C}_k(A)$	kth compound matrix of A
$\operatorname{adj}(A)$	classical adjoint, adjugate of A
A_{ij}	A with row i and column j deleted
S, S_i	sign matrices

The adjoint of $\lambda I - A$ fulfils

$$\operatorname{adj}(\lambda I - A)(\lambda I - A) = \det(\lambda I - A) I.$$

Suppose that λ is not contained in the spectrum of A.

We form the resolvent of λ and obtain

$$\begin{aligned} \operatorname{adj}(\lambda I - A) &= \det(\lambda I - A)\, R(\lambda) \\ &= V \left(\chi_A(\lambda)\, J^{-1}_{\lambda - \Lambda}\right) \widehat{V}^H. \end{aligned}$$

The shifted and inverted Jordan matrix looks like

$$J^{-1}_{\lambda-\lambda_i} = S_i E_i S_i \equiv S_i \begin{pmatrix} (\lambda-\lambda_i)^{-1} & (\lambda-\lambda_i)^{-2} & \dots & (\lambda-\lambda_i)^{-k} \\ & (\lambda-\lambda_i)^{-1} & & \\ & & \ddots & \vdots \\ & & & \\ & & & (\lambda-\lambda_i)^{-1} \end{pmatrix} S_i,$$

The multiplication with the characteristic polynomial allows to cancel the terms with negative exponent.

The resulting expression is a source of eigenvalue – eigenvector relations.

We express the adjugate with the aid of compound matrices,

$$\operatorname{adj} A \equiv S\mathcal{C}_{n-1}(A^T)S.$$

Then we have equality

$$\begin{aligned} P \equiv \mathcal{C}_{n-1}(\lambda I - A^T) &= (SVS)\, G\, (S\widehat{V}^H S) \\ &\equiv (SVS)\, \chi_A(\lambda)\, E\, (S\widehat{V}^H S). \end{aligned}$$

The elements of the compound matrix P are *polynomials* in λ of the form

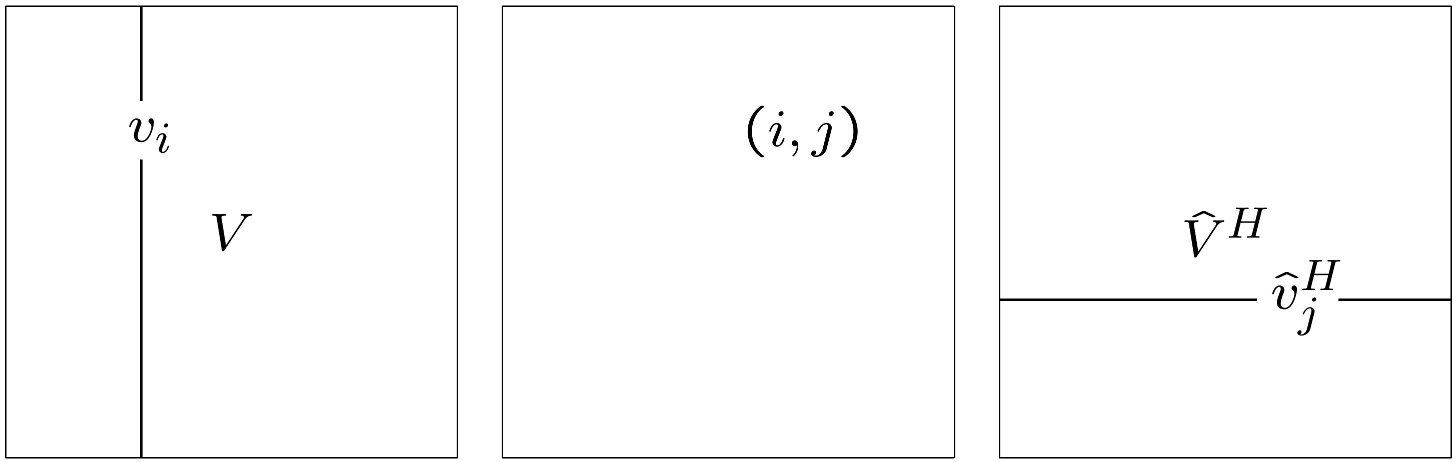
$$p_{ij} = p_{ij}(\lambda; A) \equiv \det L_{ji}, \qquad \text{where} \qquad L \equiv \lambda I - A.$$

The elements of G are obviously given by *rational functions* in λ, since

$$G = \chi_A(\lambda) \cdot (\oplus_i E_i)\,.$$

Many terms cancel, the elements of G are *polynomials*. We divide by the maximal factor and compute the limes $\lambda \to \lambda_i$.

The choice of eigenvectors is based on the non-zero positions i, j in the matrix (the sign matrices are left out):



Amongst others, the well-known result on eigenvalue – eigenvector relations by Thompson and McEnteggert is included. This is one of the basic results used in Paige's analysis of the finite precision symmetric Lanczos method.

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

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 λ. Let $\hat{v}_l^H$ and v_{l+k} be the corresponding left and right eigenvectors with appropriate normalization.

Then

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

holds true.

The minus one stems from the sign matrices, the polynomial from the definition of the adjoint as matrix of cofactors and the denominator by division with the maximal factor.

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 $m \times m$,

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

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:

$$\begin{aligned} p_{ji}(\theta; H) &= \begin{vmatrix} \theta I - H_{1:i-1} & & \star \\ & R_{i+1:j-1} & \\ 0 & & \theta I - H_{j+1:m} \end{vmatrix} \\ &= (-1)^{i+j} \chi_{H_{1:i-1}}(\theta) \prod \mathrm{diag}(H_{i:j}, -1) \chi_{H_{j+1:m}}(\theta). \end{aligned}$$

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 θ be an eigenvalue of H with multiplicity $k+1$. Let s be the unique left eigenvector and $\widehat{s}^H$ be the unique right eigenvector to eigenvalue θ.

Then

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

holds true.

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

Among these relations of special interest is the case of index pairs (i, m), $(1, m)$ and $(1, m)$, $(1, j)$:

$$
\begin{aligned}
(-1)^k \, \breve{s}(i) s(m) &= \left[\frac{\chi_{H_{1:i-1}}}{\chi^{(k+1)}_{H_{1:m}}}(\theta) \right] \prod_{l=i}^{m-1} h_{l+1,l}, \\
(-1)^k \, \breve{s}(1) s(m) &= \left[\frac{1}{\chi^{(k+1)}_{H_{1:m}}}(\theta) \right] \prod_{l=1}^{m-1} h_{l+1,l}, \\
(-1)^k \, \breve{s}(1) \, s(j) &= \left[\frac{\chi_{H_{j+1:m}}}{\chi^{(k+1)}_{H_{1:m}}}(\theta) \right] \prod_{l=1}^{j-1} h_{l+1,l}.
\end{aligned}
$$

These relations are used to derive relations between eigenvalues and *one* eigenvector.

They are also of interest for the understanding of the convergence of Krylov methods, at least in context of Krylov eigensolvers.

Theorem: Let $H \in \mathcal{H}(m)$. Let θ be an eigenvalue of H. Then $\hat{s} = \overline{\check{s}}$ defined by non-zero $\check{s}(1)$ and the relations

$$\frac{\check{s}(i)}{\check{s}(1)} = \frac{\chi_{H_{i-1}}(\theta)}{\prod_{l=1}^{i-1} h_{l+1,l}} \quad \forall\ i \in \underline{m},$$

is (up to scaling) the unique left eigenvector of H to eigenvalue θ.

Theorem: Let $H \in \mathcal{H}(m)$. Let θ be an eigenvalue of H. Then s defined by non-zero $s(m)$ and the relations

$$\frac{s(j)}{s(m)} = \frac{\chi_{H_{j+1:m}}(\theta)}{\prod_{l=j+1}^{m} h_{l,l-1}} \quad \forall\ j \in \underline{m},$$

is (up to scaling) the unique right eigenvector of H to eigenvalue θ.

Since the polynomials remain unchanged, merely the eigenvalue moves, this helps to explain convergence behaviour (even in finite precision).

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.

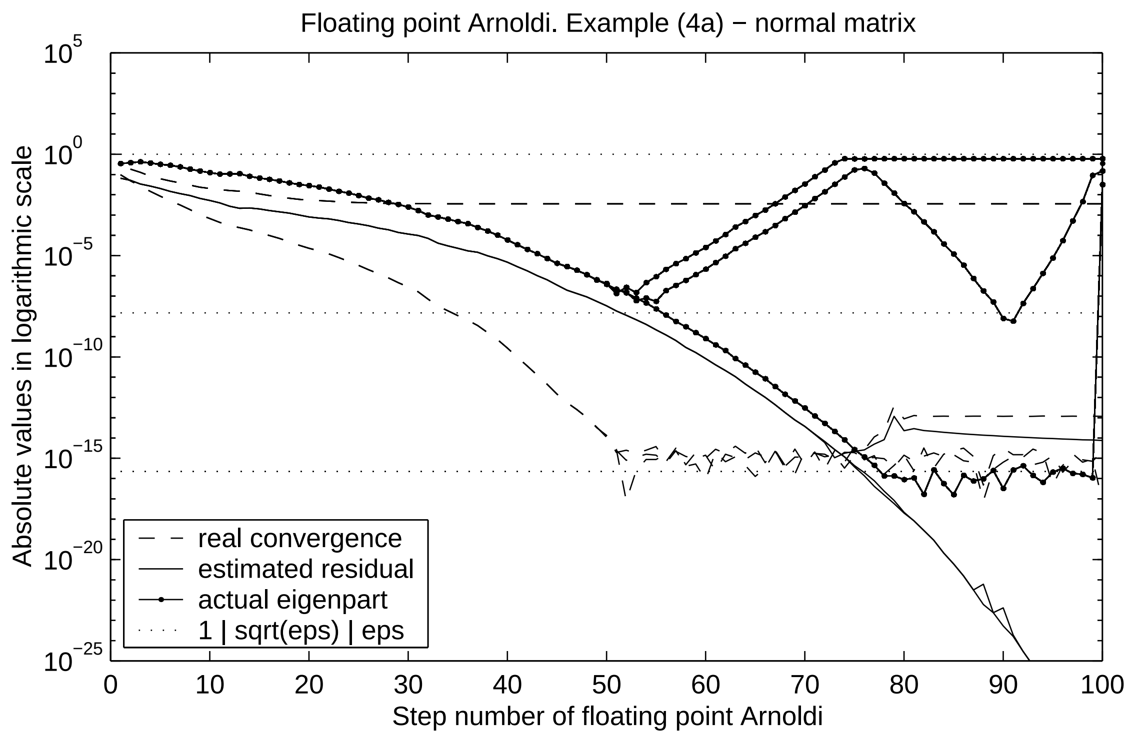
Theorem: The recurrence of the basis vectors in eigenparts is given by

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

This *local error amplification formula* consists of:

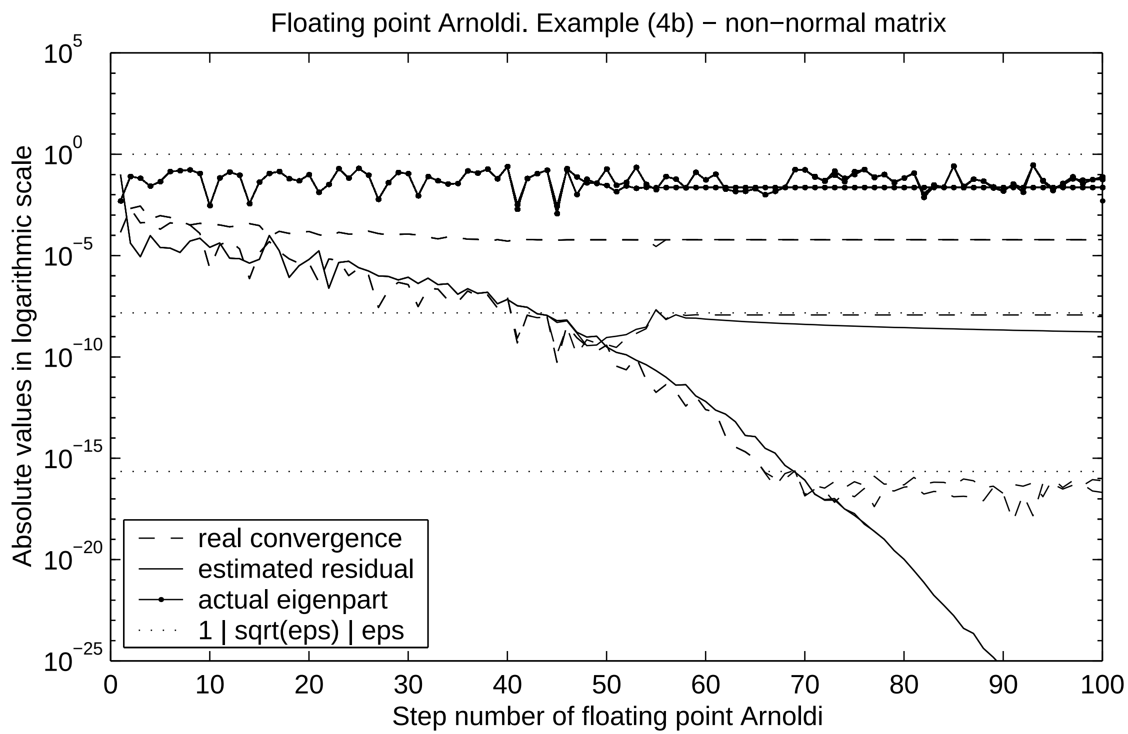
- o the left eigenpart of q_{k+1}: $\hat{v}_i^H q_{k+1}$,
- o a measure of convergence: $\left(\lambda_i - \theta_j\right) \hat{v}_i^H y_j$,
- o an error term: $\hat{v}_i^H F_k s_j$,
- o an amplification factor: $c_{k+1,k} s_{kj}$.

$A \in \mathbb{R}^{100\times 100}$ normal, eigenvalues equidistant in $[0,1]$.



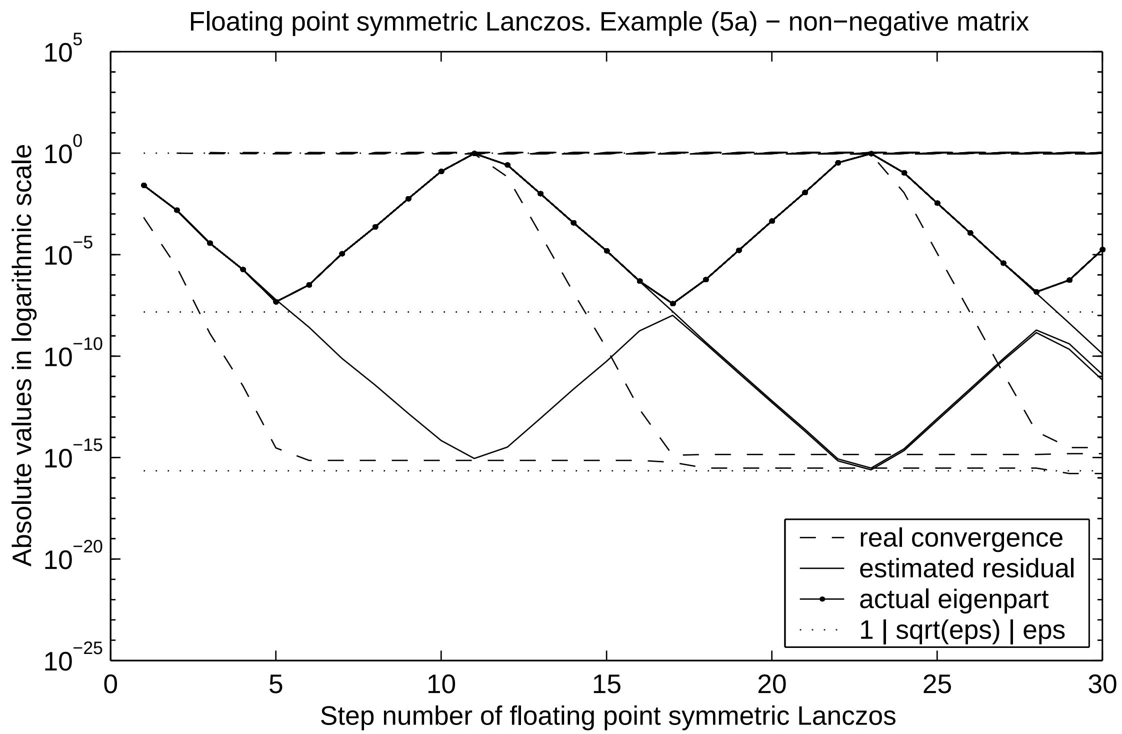
Behaviour of CGS-Arnoldi, MGS-Arnoldi, DO-Arnoldi, convergence to largest eigenvalue.

$A \in \mathbb{R}^{100\times 100}$ non-normal, eigenvalues equidistant in $[0, 1]$.



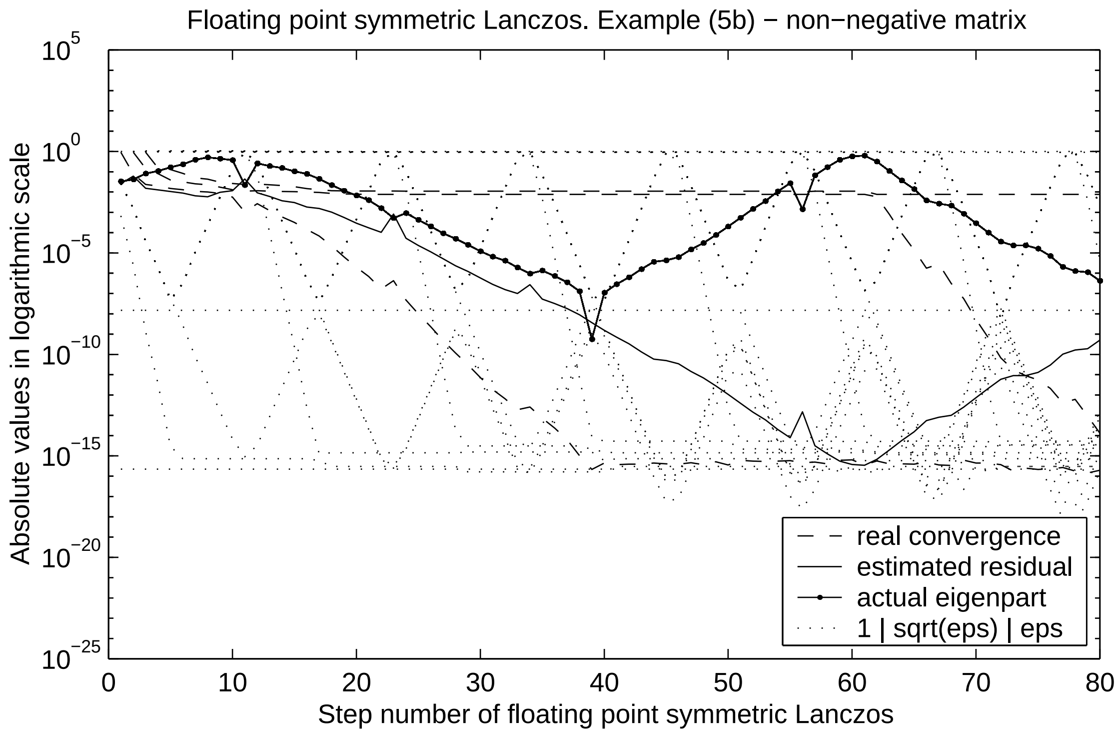
Behaviour of CGS-Arnoldi, MGS-Arnoldi, DO-Arnoldi, convergence to largest eigenvalue.

$A = A^T \in \mathbb{R}^{100\times 100}$, 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.

The formula depends on the *Ritz pair* of the actual step. Using the eigenvector basis we can get rid of the *Ritz vector*:

$$I = SS^{-1} = S\check{S}^T \quad \Rightarrow \quad e_l = S\check{S}^T e_l \equiv \sum_{j=1}^{k} \check{s}_{lj} s_j.$$

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

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

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

$$\left[\sum_{j=1}^{k} \frac{c_{k+1,k} s_{kj} \check{s}_{1j}}{\lambda_i - \theta_j}\right] \hat{v}_i^H q_{k+1} = \hat{v}_i^H q_1 + \hat{v}_i^H F_k \left[\sum_{j=1}^{k} \left(\frac{\check{s}_{1j}}{\lambda_i - \theta_j}\right) s_j\right].$$

Interpretation: The size of the deviation depends on the *size* of the *first component* of the *left* eigenvector $\widehat{s}_j$ of C_k and the *shape and size* of the *right* eigenvector s_j.

Next step: Application of the eigenvector – eigenvalue relation

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

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

$$\left[\sum_{j=1}^{k}\frac{\prod_{p=1}^{k} c_{p+1,p}}{\prod_{s\neq j}\left(\theta_s-\theta_j\right)\left(\lambda_i-\theta_j\right)}\right]\widehat{v}_i^H q_{k+1} = \widehat{v}_i^H q_1 + \widehat{v}_i^H F_k\left[\sum_{j=1}^{k}\left(\frac{\breve{s}_{1j}}{\lambda_i-\theta_j}\right)s_j\right]$$

A result from polynomial interpolation (Lagrange):

$$\sum_{j=1}^{k} \frac{1}{\prod_{l\neq j}\left(\theta_j-\theta_l\right)\left(\lambda_i-\theta_j\right)} = \frac{1}{\chi_{C_k}(\lambda_i)} \sum_{j=1}^{k} \frac{\prod_{l\neq j}(\lambda_i-\theta_l)}{\prod_{l\neq j}\left(\theta_j-\theta_l\right)} = \frac{1}{\chi_{C_k}(\lambda_i)}$$

The following theorem holds true:

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

$$\widehat{v}_i^H q_{k+1} = \frac{\chi_{C_k}(\lambda_i)}{\prod_{p=1}^{k} c_{p+1,p}} \left(\widehat{v}_i^H q_1 + \widehat{v}_i^H F_k \left[\sum_{j=1}^{k} \left(\frac{\check{s}_{1j}}{\lambda_i-\theta_j} \right) s_j \right] \right).$$

Similarly we can get rid of the eigenvectors s_j in the error term:

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

This results in the following theorem:

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

$$\begin{aligned} \widehat{v}_i^H q_{k+1} &= \frac{\chi_{C_k}(\lambda_i)}{\prod_{p=1}^{k} c_{p+1,p}} \left(\widehat{v}_i^H q_1 + \widehat{v}_i^H \sum_{l=1}^{k} \frac{\prod_{p=1}^{l} c_{p+1,p} \chi_{C_{l+1:k}}(\lambda_i)}{\chi_{C_k}(\lambda_i)} f_l \right) \\ &= \frac{\chi_{C_k}(\lambda_i)}{\prod_{p=1}^{k} c_{p+1,p}} \widehat{v}_i^H q_1 + \sum_{l=1}^{k} \left(\frac{\chi_{C_{l+1:k}}(\lambda_i)}{\prod_{p=l+1}^{k} c_{p+1,p}} \widehat{v}_i^H f_l \right). \end{aligned}$$

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 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?