Dynamic Behavior of Complex Structures
CHAPTER 3 : KRYLOV SUBSPACE METHODS

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Krylov Subspace Methods

Suppose that $A \in \mathbb{R}^{n\times n}$ is large, sparse and symmetric, and assume that some of its extremal eigenvalues are wanted. This problem can be solved by the method of Lanczos.

The Lanczos method generates a sequence of tridiagonal matrices $T_k \in \mathbb{R}^{k\times k}$ with the property that that the extremal eigenvalues of T_k are progressively better approximations to the extremal eigenvalues of A.

We assume that the eigenvalues of A are ordered by magnitude

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n,$$

and we denote by

$$R(x) = \frac{x^T Ax}{x^T x},\ x \neq 0$$

the Rayleigh quotient of A. Then by Rayleigh's principle it holds

$$\lambda_1 = \min_{x\neq 0} R(x) \quad \text{and} \quad \lambda_n = \max_{x\neq 0} R(x).$$

Krylov Subspaces

Let $\mathcal{V}_k$ be a subspace of $\mathbb{R}^n$, let $v^1, \ldots, v^k$ be an orthonormal basis of $\mathcal{V}_k$, and $V_k = [v^1, \ldots, v^k] \in \mathbb{R}^{n\times k}$.

Let μ_k be the smallest eigenvalue of the projection $V_k^T A V_k$ of A to $\mathcal{V}$ and ν_k be its largest eigenvalue. Then it follows from the minmax and maxmin characterization of eigenvalues

$$\mu_k = \min_{y\neq 0} \frac{y^T V_k^T A V_k y}{y^T y} = \min_{y\neq 0} \frac{y^T V_k^T A V_k y}{y^T V_k^T V_k y} = \min_{y\neq 0} R(V_k y) \geq \lambda_1,$$

and

$$\nu_k = \max_{y\neq 0} \frac{y^T V_k^T A V_k y}{y^T y} = \max_{y\neq 0} \frac{y^T V_k^T A V_k y}{y^T V_k^T V_k y} = \max_{y\neq 0} R(V_k y) \leq \lambda_n.$$

The Lanczos algorithm can be derived by considering how to generate the v^k so that μ_k and ν_k become increasingly better estimates to λ_1 and λ_n.

Krylov Subspaces ct.

Suppose that $u^k \in \mathcal{V}_k$ such that $R(u^k) = \mu_k$. $R(x)$ decreases most rapidly in the direction of the negative gradient

$$-\nabla R(x) = -\frac{2}{x^T x}(Ax - R(x)x)$$

and therefore $\mu_{k+1} < \mu_k$ if v^{k+1} is determined such that

$$\nabla R(u^k) \in \text{span}\{v^1, \ldots, v^k, v^{k+1}\}.$$

Likewise, if $w^k \in \mathcal{V}_k$ satisfies $\nu_k = R(w^k)$, then $\mathcal{V}_k$ should be expanded such that

$$\nabla R(w^k) \in \text{span}\{v^1, \ldots, v^k, v^{k+1}\}$$

since $R(x)$ increases most rapidly in the direction of $\nabla R(x)$. Since $\nabla R(x) \in \text{span}\{x, Ax\}$ both requirements can be satisfied simultaneously if

$$\mathcal{V}_{k+1} = \text{span}\{v^1, \ldots, v^k, v^{k+1}\} = \text{span}\{v^1, Av^1, \ldots, A^k v^1\}.$$

$\mathcal{K}_k(v^1, A) = \text{span}\{v^1, Av^1, \ldots, A^{k-1}v^1\}$ is called Krylov space.

Lanczos method

The Lanczos algorithm determines an orthonormal basis $\{v^1, \ldots, v^k\}$ of the Krylov space

$$\mathcal{K}_k(r^0, A) := \text{span}\{r^0, Ar^0, \ldots, A^{k-1}r^0\}, \; k = 1, \ldots, n,$$

such that

$$T_k := V_k^T A V_k, \quad V_k := [v^1, \ldots, v^k]$$

is tridiagonal.

The vectors v^k can be obtained by a three term recurrence.

Lanczos method ct.

Assume that we already computed the orthonormal basis $v^1, \ldots, v^k$ of the Krylov space $\mathcal{K}_k(v, A)$.

Then $A^{k-1}v \in \operatorname{span}\{v^1, \ldots, v^k\}$, and therefore, there exist $\gamma_1, \ldots, \gamma_k \in \mathbb{R}$ such that

$$A^k v = A(A^{k-1}v) = A\Big(\sum_{j=1}^{k} \gamma_k v^j\Big) = \gamma_k A v^k + A\Big(\sum_{j=1}^{k-1} \gamma_j v^j\Big).$$

The second term on the right hand side is contained in $\mathcal{K}_k(v, A)$. Hence, to obtain an orthonormal basis of $\mathcal{K}_{k+1}(v, A)$ it suffices to compute the orthonormal complement of the $u^k := Av^k$ with respect to the vectors $v^1, \ldots, v^k$.

Lanczos method ct.

Since $Av^j \in \mathcal{K}_{j+1}(v, A) \subset \mathcal{K}_{k-1}(v, A)$ for every $j < k-1$, we have

$$(v^j)^T u^k = (v^j)^T A v^k = (Av^j)^T v^k = 0.$$

Hence, $(u^k)^T v^j = 0$ for $j = 1, \ldots, k-2$, and therefore

$$Av^k = \gamma_k v^{k+1} + \alpha_k v^k + \beta_{k-1} v^{k-1}.$$

Lanczos method ct.

The coefficients are obtained from

$$\begin{aligned}\beta_{k-1} &= (v^{k-1})^T A v^k = (Av^{k-1})^T v^k \\ &= (\gamma_{k-1} v^k + \alpha_{k-1} v^{k-1} + \beta_{k-2} v^{k-2})^T v^k = \gamma_{k-1},\end{aligned}$$

i.e.

$$Av^k = \beta_k v^{k+1} + \alpha_k v^k + \beta_{k-1} v^{k-1}. \qquad (1)$$

Thus,

$$\alpha_k = (v^k)^T A v^k,$$

and the condition $\|v^{k+1}\|_2 = 1$ yields

$$\beta_k = 1/\|Av^k - \alpha_k v^k - \beta_{k-1} v^{k-1}\|_2. \qquad (2)$$

If the denominator in (2) vanishes, then $Av^k \in \mathcal{K}_k(v, A)$, and therefore, $\mathcal{K}_k(v, A)$ is a k-dimensional invariant subspace of A.

Lanczos method ct.

1: $v^0 = 0$; $k = 1$
2: $\beta_0 = \|r^0\|$
3: **while** $r^{k-1} \neq 0$ **do**
4: $\quad v^k = r^{k-1}/\beta_{k-1}$
5: $\quad r^k = Av^k$
6: $\quad r^k = r^k - \beta_{k-1} v^{k-1}$
7: $\quad \alpha_k = (v^k)^T r^k$
8: $\quad r^k = r^k - \alpha_k v^k$
9: $\quad \beta_k = \|r^k\|$
10: **end while**

Then with $T_k = \text{tridiag}\{\beta_{j-1}, \alpha_j, \beta_j\}$

$$AV_k = V_k T_k + r^k (e^k)^T, \quad r^k = Av^k - \alpha_k v^k - \beta_{k-1} v^{k-1}.$$

and $r^k = \|r^k\|_2 v^{k+1} = \beta_k v^{k+1}$

Lucky termination

The Lanczos method may terminate with $\beta_j = 0$ for some j.

Then $v^{j+1} = 0$, and therefore

$$Av^j = \alpha_j v^j + \beta_{j-1} v^{j-1} \in \mathcal{K}_j(A, v^1).$$

For $i < j$ it holds by construction

$$Av^i \in \mathcal{K}_j(A, v^1).$$

Hence, $\mathcal{K}_j(A, v^1)$ is an invariant subspace of A, and therefore every eigenvalue $\theta_i^{(j)}$ of T_j is an eigenvalue of A, and the corresponding Ritz vectors are eigenvectors of A.

Error bound

If $\theta_i^{(m)}$ are the Ritz values (eigenvalues of T_m), $s_i^{(m)}$ the corresponding eigenvectors, and $x_i^{(m)} = V_m s_i^{(m)}$ the Ritz vectors, it holds

$$\begin{aligned}(A-\theta_i^{(m)}I)x_i^{(m)} &= (A-\theta_i^{(m)}I)V_m s_i^{(m)} = AV_m s_i^{(m)} - V_m(\theta_i^{(m)} s_i^{(m)}) \\ &= V_m T_m s_i^{(m)} + \beta_m v^{m+1}(e^m)^T s_i^{(m)} - V_m T_m s_i^{(m)} = \beta_m v^{m+1}(e^m)^T s_i^{(m)},\end{aligned}$$

which implies

$$\|(A-\theta_i^{(m)}I)x_i^{(m)}\|_2 = \beta_m |s_{m,i}^{(m)}|.$$

Then by the Krylov & Bogoliubov Theorem there exists an eigenvalue $\tilde{\lambda}$ of A such that

$$|\tilde{\lambda} - \theta_i^{(m)}| \le \beta_m |s_{m,i}^{(m)}|.$$

Notice, that this error bound can be computet without determining the Ritz vector $x_i^{(m)} = V_m s_i^{(m)}$.

Convergence

The Lanczos method is a generalization of the power method where approximations to eigenvectors are obtained from the last iterate only.

As for the power method we therefore can expect fast convergence to the eigenvalue which is maximal in modulus and to the corresponding eigenvector.

One can influence the convergence of the power method by shifts, either to separate the wanted eigenvalue more from the remaining spectrum or to enforce convergence to a different eigenvalue.

The Lanczos method is independent of shifts since

$$\mathcal{K}_m(v^1, A) = \mathcal{K}_m(v^1, A + \alpha I) \quad \text{for all } \alpha \in \mathbb{R}.$$

Hence, we can expect convergence of the Lanczos method to extreme eigenvalues first.

Monotonicity

Assume that the eigenvalues of A and the Ritz values with respect to $\mathcal{K}_m$ are ordered by magnitude:

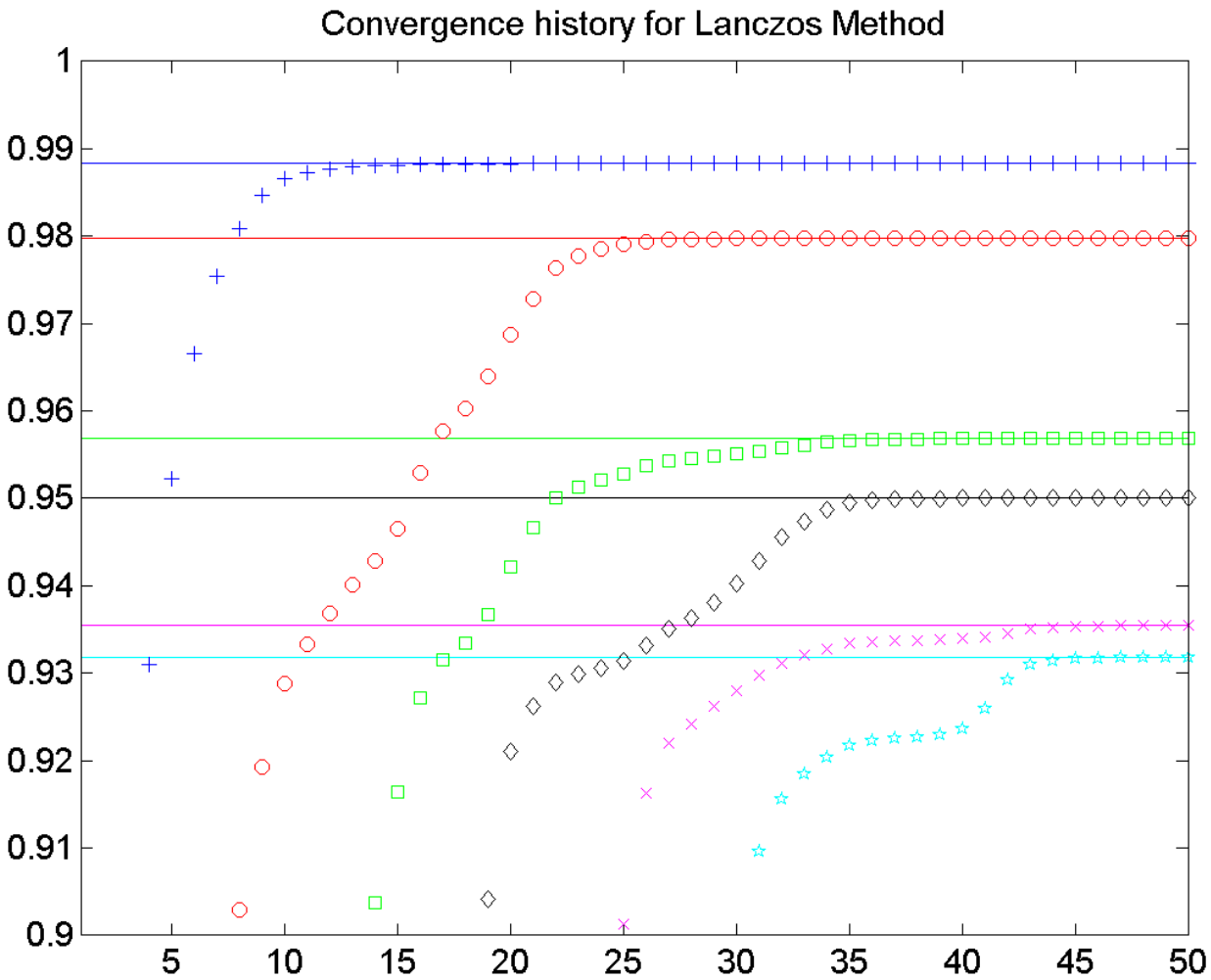
$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n, \qquad \theta_1^{(m)} \le \theta_2^{(m)} \le \cdots \le \theta_m^{(m)},$$

Then the minmax principle yields (S denotes a subspace of $\mathbb{C}^m$ and $\tilde{S}$ a subspace of $\mathbb{C}^n$)

$$\begin{aligned}
\theta_j^{(m)} &= \min_{\dim S=j} \max_{y\in S} \frac{y^H T_m y}{y^H y} = \min_{\dim S=j} \max_{y\in S} \frac{y^H V_m^H A V_m y}{y V_m^H V_m y} \\
&= \min_{\dim \tilde{S}=j,\ \tilde{S}\subset\mathcal{K}_m} \max_{x\in\tilde{S}} \frac{x^H A x}{x^H x} \ge \min_{\dim \tilde{S}=j,\ \tilde{S}\subset\mathcal{K}_{m+1}} \max_{x\in\tilde{S}} \frac{x^H A x}{x^H x} \\
&= \theta_j^{(m+1)} \ge \min_{\dim \tilde{S}=j} \max_{x\in\tilde{S}} \frac{x^H A x}{x^H x} = \lambda_j.
\end{aligned}$$

Each (finite) sequence $\{\theta_j^{(m)}\}_{m=j,j+1,j+2}$ therefore is monotonically decreasing and bounded below by λ_j.
Likewise the sequence of the j-largest eigenvalues of T_m are monotonically increasing and bounded above by the j-largest eigenvalue of A.

Example


Convergence history for Lanczos Method
1
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
0.91
0.9
5
10
15
20
25
30
35
40
45
50

Convergence

Before getting results about the speed of convergence of the Lanczos method we first prove a bound for the angle between an eigenvector of A and a Krylov space $\mathcal{K}_m(v^1, A)$. Denote by u^i a system of orthonormal eigenvectors corresponding to the eigenvalues λ_i.

LEMMA 10.1
Let P_i be the orthogonal projector onto the eigenspace corresponding to λ_i. If $P_i v^1 \neq 0$ then

$$\tan \delta(u^i, \mathcal{K}_m) = \min_{p \in \Pi_{m-1},\ p(\lambda_i)=1} \|p(A)y^i\|_2 \tan \delta(u^i, v^1),$$

where

$$y^i = \begin{cases} \frac{(I-P_i)v^1}{\|(I-P_i)v^1\|_2} & \text{if } (I-P_i)v^1 \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

Proof

The Krylov space $\mathcal{K}_m(v^1, A)$ consists of all vectors which can be written as $x = q(A)v^1$ where $q \in \Pi_{m-1}$ is any polynomial of degree $m-1$.
With the orthogonal decomposition

$$x = q(A)v^1 = q(A)P_i v^1 + q(A)(I - P_i)v^1$$

it holds for the angle $\delta(x, u^i)$ between x and u^i

$$\tan\delta(x,u^i) = \frac{\|q(A)(I-P_i)v^1\|_2}{\|q(A)P_i v^1\|_2} = \frac{\|q(A)y^i\|_2}{|q(\lambda_i)|}\frac{\|(I-P_i)v^1\|_2}{\|P_i v^1\|_2},$$

and the scaling $p(\lambda) := q(\lambda)/q(\lambda_i)$ yields

$$\tan\delta(x,u^i) = \|p(A)y^i\|_2 \tan\delta(v^1,u^i)$$

from which we get the statement by minimizing over all $x \in \mathcal{K}(v^1, A)$.□

Convergence ct.

Inserting any polynomial of degree $m-1$ which satisfies $p(\lambda_i)=1$ one obtains an upper bound for $\tan\delta(u_i,\mathcal{K}_m(v^1,A))$ from the last lemma.

We already have

THEOREM 10.2
Let $\alpha,\beta,\gamma\in\mathbb{R}$ with $\alpha<\beta$ and $\gamma\notin(\alpha,\beta)$. Then the minimization problem

$$\min_{p\in\Pi_m,\ p(\gamma)=1}\ \max_{t\in[\alpha,\beta]}\ |p(t)|$$

has a unique solution, and is solved by the scaled Chebyshev polynomial

$$\tilde{c}_m(t):=\begin{cases} c_m(1+2\frac{t-\beta}{\beta-\alpha})/c_m(1+2\frac{\gamma-\beta}{\beta-\alpha}) & \text{für } \gamma>\beta \\ c_m(1+2\frac{\alpha-t}{\beta-\alpha})/c_m(1+2\frac{\alpha-\gamma}{\beta-\alpha}) & \text{für } \gamma<\alpha \end{cases}$$

THEOREM 10.3

The angle $\delta(u^j, \mathcal{K}_m(v^1, A))$ between the exact eigenvector u^j and the m-th Krylov space satisfies the inequality

$$\tan\delta(u^j, \mathcal{K}_m) \le \frac{\kappa_j}{c_{m-j}(1+2\rho_j)} \tan\delta(u^j, v^1) \qquad (1)$$

where

$$\kappa_1 = 1,\ \kappa_j = \prod_{j=1}^{i-1} \frac{\lambda_n - \lambda_j}{\lambda_i - \lambda_j} \text{ für } i > 1 \qquad (2)$$

and

$$\rho_i = \frac{\lambda_{i+1} - \lambda_i}{\lambda_n - \lambda_{i+1}}. \qquad (3)$$

In particular for $i = 1$ one gets the estimate

$$\tan\delta(u^1, \mathcal{K}_m(v^1, A)) \le \frac{1}{c_{m-1}(1+2\rho_1)} \tan\delta(v^1, u^1) \quad \text{where } \rho_1 = \frac{\lambda_2 - \lambda_1}{\lambda_n - \lambda_2}.$$

Crucial for the convergence is the distance of the two smallest eigenvalues relative to the width of the entire spectrum.

Proof

We consider the case $i = 1$ first.

Expanding the vector y^i in the basis $\{u^i\}$ of eigenvectors yields

$$y^i = \sum_{j=1}^{n} \alpha_j u^j, \quad \text{where} \sum_{j=1}^{n} |\alpha_j|^2 = 1$$

from which we get

$$\|p(A)y^1\|_2 = \sum_{j=2}^{n} |p(\lambda_j)\alpha_j|^2 \le \max_{j=2,\dots,n} |p(\lambda_j)|^2 \le \max_{\lambda\in[\lambda_2,\lambda_n]} |p(\lambda)|^2,$$

and the statement follows from Theorem 10.2.

Proof ct.

For $i > 1$ we consider in Lemma 10.1 polynomials of the form

$$p(\lambda) := \frac{(\lambda - \lambda_1) \cdot \cdots \cdot (\lambda - \lambda_{i-1})}{(\lambda_i - \lambda_1) \cdot \cdots \cdot (\lambda_i - \lambda_{i-1})} q(\lambda)$$

with $q \in \Pi_{m-i}$ and $q(\lambda_i) = 1$.

Then one gets as before

$$\begin{aligned} \|p(A)y^i\|_2 &\leq \max_{\lambda \in [\lambda_{i+1}, \lambda_n]} \left| \prod_{j=1}^{i-1} \frac{\lambda - \lambda_j}{\lambda_i - \lambda_j} q(\lambda) \right| \\ &\leq \prod_{j=1}^{i-1} \frac{\lambda_n - \lambda_j}{\lambda_i - \lambda_j} \max_{\lambda \in [\lambda_{i+1}, \lambda_n]} |q(\lambda)|. \end{aligned}$$

The result follows by minimizing this expression over all polynomials q satisfying the constraint $q(\lambda_i) = 1$.□

THEOREM 10.4 (Kaniel & Paige; 1. eigenvalue)

Let $A \in \mathbb{C}^{n\times n}$ be Hermitean with eigenvalues $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$ and corresponding orthonormal eigenvectors $u^1, \ldots, u^n$.

If $\theta_1^{(m)} \le \cdots \le \theta_m^{(m)}$ denote the eigenvalues of the matrix T_m obtained after m steps of Lanczos' method, then

$$0 \le \theta_1^{(m)} - \lambda_1 \le (\lambda_n - \lambda_1)\left(\frac{\tan\delta(u^1, v^1)}{c_{m-1}(1+2\rho_1)}\right)^2,$$

where $\rho_1 = (\lambda_2 - \lambda_1)/(\lambda_n - \lambda_2)$.

Crucial for the speed of convergence is the growth of $c_{j-1}(1+2\rho_1)$, i.e. the separation of the first two eigenvalues relative to the width of the entire spectrum of A.

Proof

The left inequality follows from Rayleigh's principle.

We have

$$\theta_1^{(m)} = \min_{x \in \mathcal{K}_m(v^1, A), x \neq 0} \frac{x^H A x}{x^H x},$$

and, since each $x \in \mathcal{K}_m(v^1, A)$ can be represented as $x = q(A)v^1$ for some $q \in \Pi_{m-1}$, it follows

$$\begin{aligned} \theta_1^{(m)} - \lambda_1 &= \min_{x \in \mathcal{K}_m(v^1, A), x \neq 0} \frac{x^H (A - \lambda_1 I) x}{x^H x} \\ &= \min_{q \in \Pi_{m-1}, q \neq 0} \frac{(v^1)^H q(A)^H (A - \lambda_1 I) q(A) v^1}{(v^1)^H q(A)^2 v^1}. \end{aligned}$$

Proof ct.

With $v^1 = \sum_{j=1}^n \alpha_j u^j$ it holds

$$\begin{aligned}
\theta_1^{(m)} - \lambda_1 &= \min_{q\in\Pi_{m-1}, q\neq 0} \frac{\sum_{j=2}^n (\lambda_j - \lambda_1)|\alpha_j q(\lambda_j)|^2}{\sum_{j=1}^n |\alpha_j q(\lambda_j)|^2} \\
&\leq (\lambda_n - \lambda_1) \min_{q\in\Pi_{m-1}, q\neq 0} \frac{\sum_{j=2}^n |\alpha_j q(\lambda_j)|^2}{|\alpha_1 q(\lambda_1)|^2} \\
&\leq (\lambda_n - \lambda_1) \min_{q\in\Pi_{m-1}, q\neq 0} \max_{j=2,\ldots,n} \frac{|q(\lambda_j)|^2}{|q(\lambda_1)|^2} \cdot \frac{\sum_{j=2}^n |\alpha_j|^2}{|\alpha_1|^2}
\end{aligned}$$

Defining $p(\lambda) = q(\lambda)/q(\lambda_1)$, and observing that the set of all p:s when q passes through the set Π_{m-1} is the set of all polynomials of degree not exceeding $m-1$ and satisfying the constraint $p(\lambda_1) = 1$ we get

$$\theta_1^{(m)} - \lambda_1 \leq (\lambda_n - \lambda_1) \tan^2 \delta(u^1, v^1) \min_{p\in\Pi_{m-1}, p(\lambda_1)=1} \max_{\lambda\in[\lambda_2,\lambda_n]} |p(\lambda)|^2$$

and the statement follows from Theorem 10.2.□

Example

Matrix A has eigenvalue $\lambda_1 = 1$ and 99 eigenvalues uniformly distributed in $[\alpha, \beta]$.

it.	$[\alpha,\beta]$=[20,100]		$[\alpha,\beta]$=[2,100]	
	error	bound	error	bound
2	3.3890e+001	3.4832e+003	1.9123e+001	1.1385e+005
3	1.9708e+001	1.0090e+002	1.0884e+001	7.5862e+004
4	6.6363e+000	1.5083e+001	5.8039e+000	5.5241e+004
5	1.5352e+000	2.2440e+000	4.1850e+000	3.8224e+004
10	7.9258e-005	1.6293e-004	1.8948e+000	4.2934e+003
15	4.3730e-009	1.1827e-008	1.0945e+000	4.1605e+002
20	2.9843e-013	8.5861e-013	1.6148e-001	3.9725e+001
25			1.4843e-002	3.7876e+000
30			1.6509e-003	3.6109e-001
35			2.0658e-004	3.4423e-002
40			5.8481e-006	3.2816e-003
45			9.5770e-007	3.1285e-004
50			3.0155e-009	2.9824e-005
55			8.0487e-012	2.8432e-006
60			3.1530e-014	2.7105e-007

THEOREM 10.5 (Kaniel & Paige; higher eigenvalues)

Under the conditions of Theorem 10.4 it holds

$$0 \le \theta_j^{(m)} - \lambda_j \le (\lambda_n - \lambda_1) \left(\frac{\kappa_j^{(m)} \tan \delta(v^1, u^j)}{c_{m-j}(1 + 2\rho_j)} \right)^2$$

with

$$\rho_j = (\lambda_{j+1} - \lambda_j)/(\lambda_n - \lambda_{j+1}),$$

and

$$\kappa_1^{(m)} \equiv 1, \ \kappa_j^{(m)} = \prod_{i=1}^{j-1} \frac{\lambda_n - \theta_i^{(m)}}{\lambda_j - \theta_i^{(m)}}.$$

The general case $j > 1$ can be proved by using the maxmin characterization of $\theta_j^{(m)}$ of Courant and Fischer.

Analogous results hold for the largest eigenvalues and Ritz values.

Orthogonality of basis vectors

In exact arithmetic the Lanczos method generates an orthonormal basis of the Krylov space $\mathcal{K}_m(v^1, A)$. In the algorithm only the orthogonality with respect to two basis vectors v^j and v^{j-1} obtained in the last two steps is enforced, with respect to the previous v^i:s it follows from the symmetry of A.

It can be shown that in floating point arithmetic the orthogonality is destroyed when a sequence $\theta_i^{(j)}$, $j = 1, 2, \ldots$, of Ritz values has converged to an eigenvalue $\tilde{\lambda}$ of A, i.e. if the residual $\beta_j s_{j,i}^{(j)}$ has become small.

Thereafter all v^j:s obtain a component in the direction of the eigenspace of the converged eigenvalue, and a duplicate copy of that eigenvalue will show up in the spectrum of the tridiagonal matrix T_m.

This effect was first observed and studied by Paige (1971). A detailed discussion is contained in the monograph of Parlett (1998).

Orthogonality of basis vectors ct.

Note that these multiple Ritz values have nothing to do with possible multiple eigenvalues of a given matrix, they occur simply as a result of a converged eigenvalue.

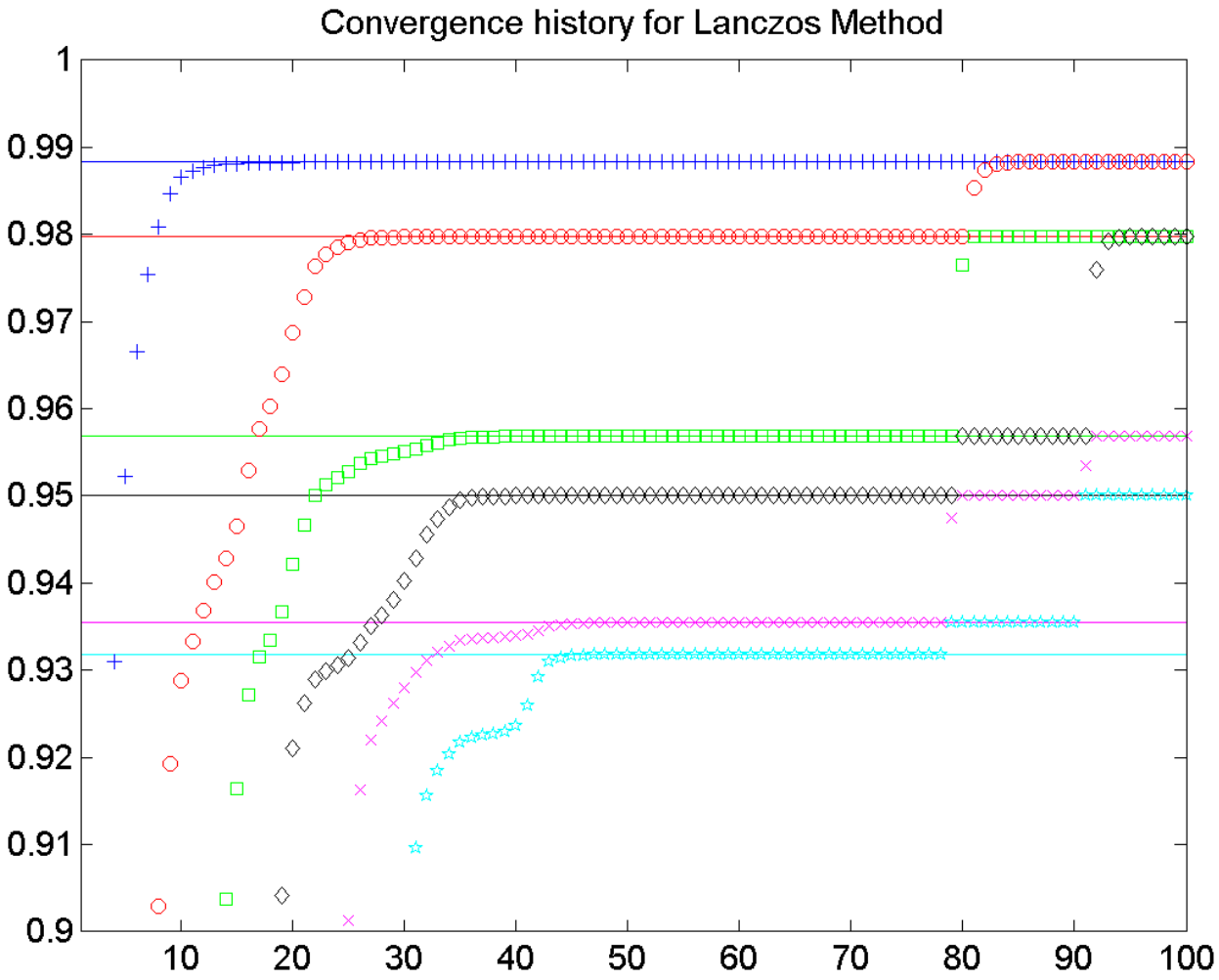
For multiple eigenvalues the Lanczos (and Arnoldi) method in exact arithmetic can only detect one eigenvector, namely the projection of the initial vector v^1 to the corresponding eigenspace. Further eigenvectors can only be obtained restarting with a different initial vector or by a block Lanczos (Arnoldi) method.

A simple trick to detect duplicate copies of an eigenvalue advocated by Cullum & Willoughby (1986) is the following.

Compute the eigenvalues of the reduced matrix $\hat{T}_m \in \mathbb{R}^{m-1\times m-1}$ obtained from T_m by detracting the first row and column. Those eigenvalues that differ less than a small multiple times machine precision from the eigenvalues of T_m are the unwanted eigenvalues, i.e. the ones due to loss of orthogonality.

Example

Convergence of the Lanczos process for $A = \text{diag}\,(\text{rand}(100,1))$



Complete reorthogonalization

In each step the new vector v^{j+1} is reorthogonalized against all previous vectors v^i.

With classical Gram–Schmidt this means: v^{j+1} is replaced by

$$\tilde{v}^{j+1} = v^{j+1} - V_j V_j^H v^{j+1}.$$

If the norm is decreased by a nontrivial amount, say

$$\|\tilde{v}^{j+1}\| < \frac{1}{\sqrt{2}} \|v^{j+1}\|,$$

the reorthogonalization will have to be repeated.

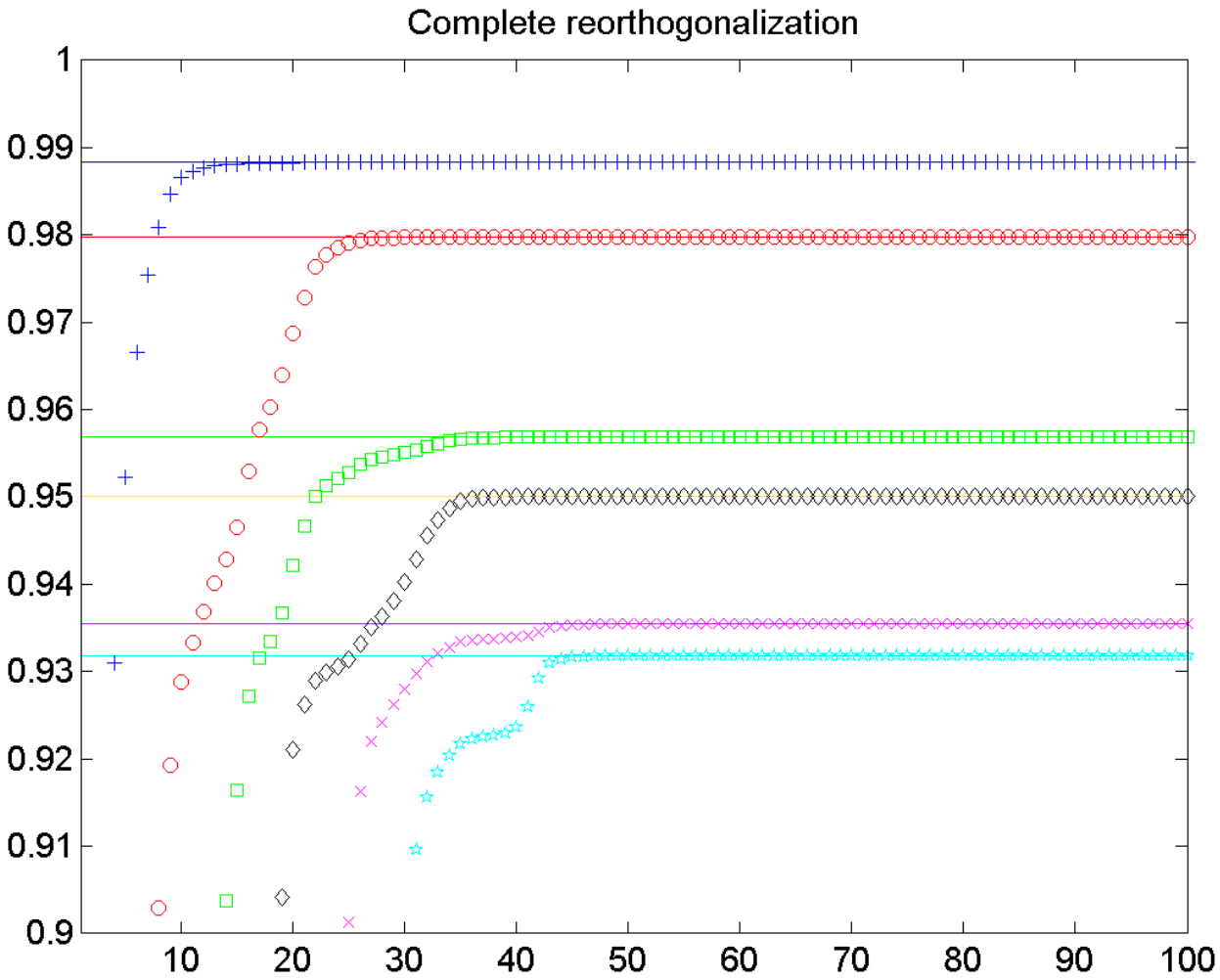
Complete reorthogonalization is very reliable, but very expensive.

Lanczos with complete reorthogonalization

1: Choose initial vector v^1 with $\|v^1\| = 1$
2: Set $v^0 = 0$; $\beta_0 = 0$; $V = [v^1]$
3: **for** $j = 1, 2, \ldots$ **do**
4: $\quad v^{j+1} = Av^j - \beta_{j-1} v^{j-1}$
5: $\quad \alpha_j = (v^j)^H v^{j+1}$
6: $\quad v^{j+1} = v^{j+1} - \alpha_j v^j$
7: $\quad v^{j+1} = v^{j+1} - VV^H v^{j+1}$
8: $\quad \beta_j = \|v^{j+1}\|$
9: $\quad v^{j+1} = v^{j+1}/\beta_j$
10: $\quad V = [V, v^{j+1}]$
11: $\quad$ Solve projected eigenproblem $T_j s = \theta s$
12: $\quad$ Test for convergence
13: **end for**

Example

Convergence of the Lanczos process with complete reorthogonalization for $A =$ diag (rand(100,1))



THEOREM 10.8 (Paige)

Let $V_k = [v^1, \ldots, v^k]$ be the matrix of vectors actually obtained in the Lanczos algorithm, $\Theta_k = \mathrm{diag}\{\theta_1, \ldots, \theta_k\}$ and $S_k = [s^1, \ldots, s^k]$ such that $T_k S_k = S_k \Theta_k$ and $S_k^H S_k = I_k$.

Let $y^{k,i} = V_k s^i$ be the corresponding Ritz vectors. Then it holds

$$(y^{k,i})^H v^{k+1} = \frac{O(\varepsilon \|A\|_2)}{\beta_k |s_{k,i}|}.$$

Hence, the component $(y^{k,i})^H v^{k+1}$ of the computed Lanczos vector v^{k+1} in the direction of the Ritz vector $y^{k,i}$ is proportional to the reciprocal of the error bound for the Ritz value θ_i

Selective reorthogonalization

By Paige's theorem the $v^j : s$ lose orthogonality since the vector v^{j+1} obtained in the final step has a large component with respect to the Ritz vector $y = [v^1, \ldots, v^j] * s$ corresponding to the converged Ritz value θ (measured by the error bound $\beta_j |s_j|$).

This suggests to monitor the error bounds $\beta_j |s_j|$ for all eigenvectors s of T_j in every iteration step, and to reorthogonalize v^{j+1} against the Ritz vector y:

$$v^{j+1} = v^{j+1} - (y^H v^{j+1}) y.$$

This so called selective reorthogonalization is applied if

$$\beta_j |s_j| < \sqrt{\varepsilon} \|T_j\|$$

(actually $\|A\|$ would have been needed on the right hand side, but $\|A\|$ is not available).

Selective reorthogonalization

1: Choose initial vector v^1 with $\|v^1\| = 1$
2: Set $v^0 = 0$; $\beta_0 = 0$; $V = [v^1]$
3: **for** $j = 1, 2, \ldots$ **do**
4: $\quad v^{j+1} = Av^j - \beta_{j-1} v^{j-1}$
5: $\quad \alpha_j = (v^j)^H v^{j+1}$
6: $\quad v^{j+1} = v^{j+1} - \alpha_j v^j$
7: $\quad \beta_j = \|v^{j+1}\|$
8: $\quad$ Solve tridiag$\{\beta_{i-1}, \alpha_i, \beta_i\} S = S\Theta$
9: $\quad$ **for** $i = 1, \ldots, j$ **do**
10: $\quad\quad$ **if** $\beta_j |s_j^{(i)}| < \sqrt{\varepsilon}\, \max(\text{diag}\Theta)$ **then**
11: $\quad\quad\quad y = [v^1, \ldots, v^j] s$
12: $\quad\quad\quad v^{j+1} = v^{j+1} - (y^H v^{j+1}) y$
13: $\quad\quad$ **end if**
14: $\quad$ **end for**
15: $\quad \beta_j = \|v^{j+1}\|$
16: $\quad v^{j+1} = v^{j+1} / \beta_j$
17: $\quad V = [V, v^{j+1}]$
18: **end for**

Partial reorthogonalization

It can be shown (Simon (1984)) that the properties of the Lanczos method are widely retained as long as the basis is semiorthogonal, i.e.

$$V_j^H V_j = I_j + E \quad \text{with} \quad \|E\|_2 = \sqrt{\varepsilon},$$

where ε denotes the rounding unit.

If the tridiagonal matrix T_j is determined using a semiorthogonal basis V_j then there exists an orthonormal basis N_j of span V_j such that

$$T_j = V_j^H A V_j = N_j^H A N_j + G \quad \text{with} \quad \|G\|_2 = O(\varepsilon \|A\|_2).$$

Hence, the eigenvalues of the problem projected to span V_j are obtained with full precision.

Partial reorthogonalization

1: Choose initial vector v^1 with $\|v^1\| = 1$
2: Set $v^0 = 0$; $\beta_0 = 0$; $V = [v^1]$
3: **for** $j = 1, 2, \ldots$ **do**
4: $\quad v^{j+1} = Av^j - \beta_{j-1} v^{j-1}$
5: $\quad \alpha_j = (v^j)^H v^{j+1}$
6: $\quad v^{j+1} = v^{j+1} - \alpha_j v^j$
7: $\quad \beta_j = \|v^{j+1}\|$
8: $\quad v^{j+1} = v^{j+1} / \beta_j$
9: $\quad$ **if** $\|[V, v^{j+1}]^H [V, v^{j+1}] - I_{j+1}\| > \sqrt{\varepsilon}$ **then**
10: $\quad\quad v^{j+1} = v^{j+1} - VV^H v^{j+1}$
11: $\quad\quad \beta_j = \|v^{j+1}\|$
12: $\quad\quad v^{j+1} = v^{j+1} / \beta_j$
13: $\quad$ **end if**
14: $\quad V = [V, v^{j+1}]$
15: **end for**

Arnoldi Method

One way to extend the Lanczos process to non-symmetric matrices is due to Arnoldi (1951). Consider the Hessenberg reduction $V^T AV = H$ with $V^T V = I$.

If $V = [v^1, \ldots, v^n]$, then the kth column in $AV = VH$ reads

$$Av^{k+1} = \sum_{j=1}^{k+1} h_{jk} v^j, \quad 1 \le k \le n-1.$$

Isolating the last term in the summation gives

$$h_{k+1,k} v^{k+1} = Av^k - \sum_{j=1}^{k} h_{jk} v^j =: r^k,$$

from which we obtain $h_{jk} = (v^j)^T Av^k$ for $j = 1, \ldots, k$, and if $r^k \neq 0$, then v^{k+1} is defined as

$$v^{k+1} = r^k / h_{k+1,k}.$$

Arnoldi method

choose initial vector v^1 with $\|v^1\| = 1$, $V_1 = [v^1]$
compute $w = Av^1$, $h = (v^1)^T w$, $r = w - v^1 h$, $H_1 = [h]$, $\beta = \|r\|_2$
for $j = 1, 2, \ldots$ **do**
  $v^{j+1} = r/\beta$
  $V_{j+1} = [V_j, v^{j+1}], \quad \hat{H}_j = \begin{bmatrix} H_j \\ \beta e_j^T \end{bmatrix}$
  $w = Av^{j+1}$
  $h = V_{j+1}^T w, \quad r = w - V_{j+1} h$
  if $\|r\|_2 < \eta \|h\|_2$ **then**
    $s = V_{j+1}^T r, \quad r = r - V_{j+1} s$
    $h = h + s$
  end if
  $H_{j+1} = [\hat{H}_j, h]$, $\beta = \|r\|_2$
  compute approximate eigenvalues of H_{j+1}
  test for convergence
end for

The v^k are called Arnoldi vectors. They obviously define an orthonormal basis of the Krylov space $\mathcal{K}_k(v^1, A) = \text{span}\{v^1, Av^1, \ldots, A^{k-1}v^1\}$.

Arnoldi method; compact form

In compact form the Arnoldi method can be written as

$$AV_m = V_m H_m + h_{m+1,m} v^{m+1} e_m^T$$

$$V_m^T V_m = I_m, \quad V_m^T v^{m+1} = 0,$$

$$V_m^T A V_m = H_m = \begin{pmatrix} h_{11} & h_{12} & h_{13} & \dots & \dots & h_{1m} \\ h_{21} & h_{22} & h_{23} & \dots & \dots & h_{2m} \\ 0 & h_{32} & h_{33} & \dots & \dots & h_{3m} \\ & & \ddots & \ddots & & \vdots \\ & & & \ddots & \ddots & \vdots \\ & & & & h_{m,m-1} & h_{mm} \end{pmatrix}$$

The eigenvalue problem

$$H_m s = \theta s$$

can be solved inexpensively by the QR algorithm.

Cost

For large matrices the Arnoldi method becomes costly, both in terms of computation and storage.

We need to keep m vectors of length n plus an $m \times m$ Hessenberg matrix.

For the arithmetic costs, we need to multiply v^{j+1} by A, at the cost of $2N_z$, where N_z is the number of nonzero elements of A, and then orthogonalize the result against j basis vectors, at the cost of $4(j+1)n$.

Thus, an m-dimensional Arnoldi costs $\approx nm + 0.5m^2$ in storage and $\approx 2nN_z + 2nm^2$ in arithmetic operations.

In the symmetric case only the last two basis vectors v^j are needed when determining the projection H_m. The previous vectors are not even needed to determine an error bound, and can be stored on secondary storage until the Ritz vectors are computed.

Backward Error

For symmetric A the theorem of Krylov and Bogoliubov immediately yielded an error bound. Simmilarly, we obtain for general A the backward error from the compact form of the Arnoldi recurrence

$$h_{m+1,m}|s^T e^m| = \min \|E\|_2 \quad \text{such that } (A+E-\theta I)x = 0,\ x := V_m s.$$

$$\begin{aligned} Ex &= (A-\theta I)V_m s = V_m H_m s + h_{m+1,m} v^{m+1}(e^m)^T s - V_m H_m s \\ &= h_{m+1,m} v^{m+1}(e^m)^T s, \end{aligned}$$

from which we obtain

$$\|E\|_2 = \max_{y\neq 0} \frac{\|Ey\|_2}{\|y\|_2} \geq \frac{\|Ex\|_2}{\|x\|_2} = h_{m+1,m}|s^T e^m|.$$

Conversely, for $\hat{E} = -h_{m+1,m} v^{m+1} x^T \cdot s^T e^m$ one gets

$(A+\hat{E}-\theta I)V_m s = 0$ and $\|\hat{E}\|_2 = h_{m+1,m}\|v^{m+1}\|_2 \|x\|_2 |s^T e^m| = h_{m+1,m}|s^T e^m|.$

Convergence

The Arnoldi method is a generalization of the power method where approximations to eigenvectors are obtained from the last iterate only (or the two last iterates in case of a complex eigenvalue).

As for the power method we therefore can expect fast convergence to the eigenvalue which is maximal in modulus and to the corresponding eigenvector.

One can influence the convergence of the power method by shifts, either to separate the wanted eigenvalue more from the remaining spectrum or to enforce convergence to a different eigenvalue.

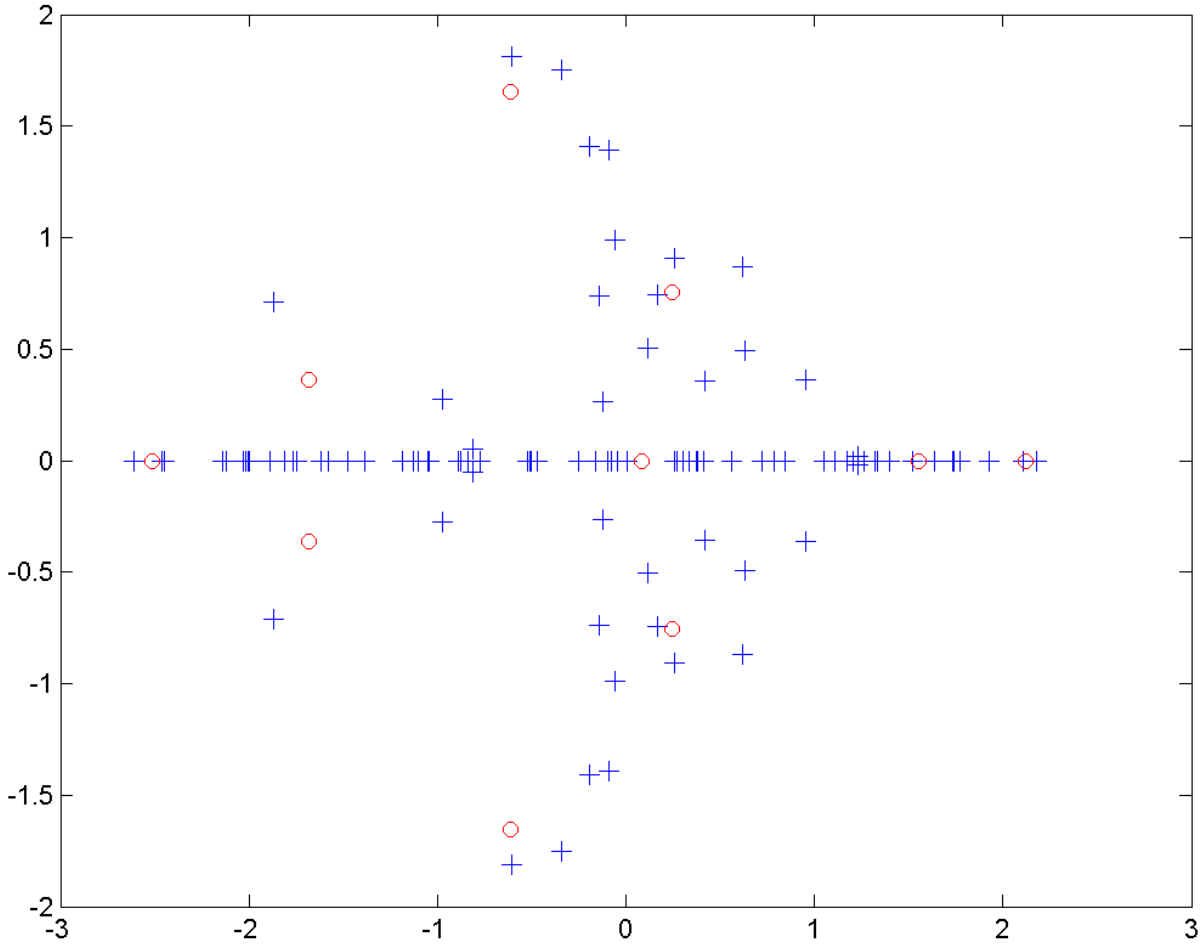
The Arnoldi method is independent of shifts since

$$\mathcal{K}_m(v^1, A) = \mathcal{K}_m(v^1, A + \alpha I) \quad \text{for all } \alpha \in \mathbb{C}.$$

Hence, we can expect convergence of the Arnoldi method to extreme eigenvalues first.

Example

Eigenvalues (blue plus) of a random tridiagonal $(100, 100)$ matrix and approximations (red circle) after 10 steps of Arnoldi:



Convergence of Arnoldi Method

For nonsymmetric matrices and the Arnoldi process the speed of convergence was analyzed by Saad (1983).

This was done by considering the distance of a particular eigenvector u^1 of A from the subspace $\mathcal{K}_m(v^1, A)$.

Let

$$\varepsilon^{(m)} := \min_{p \in \Pi^*_{m-1}} \max_{\lambda \in \sigma(A) \setminus \{\lambda_1\}} |p(\lambda)|$$

where $\sigma(A)$ is the spectrum of A, and Π^*_{m-1} denotes the set of polynomials of maximum degree $m-1$ such that $p(\lambda_1) = 1$.

The following lemma relates the distance of this quantity to $\|(I - \mathcal{P}_m)u^1\|$ where $\mathcal{P}_m$ denotes the projector onto $\mathcal{K}_m(v^1, A)$.

Convergence of Arnoldi Method ct.

LEMMA 10.6
Assume that A is diagonalizable and that the initial vector v^1 of Arnoldi's method has the expansion $v^1 = \sum_{j=1}^{n} \alpha_j u^j$ with respect to an eigenbasis $u^1, \ldots, u^n$ of A where $\|u^j\| = 1$ and $\alpha_1 \neq 0$. Then the following inequality holds

$$\|(I - \mathcal{P}_m)u^1\| \leq \xi \varepsilon^{(m)} \quad \text{where } \xi = \sum_{j=2}^{n} |\alpha_j|/|\alpha_1|.$$

Hence, upper bounds of $\varepsilon^{(m)}$ estimate the speed of convergence of the Arnoldi method.

THEOREM 10.7
Assume that all eigenvalues of A but λ_1 are lying in an ellipse with center c, focal points $c - e$ and $c + e$ and large semiaxis a. Then it holds

$$\varepsilon^{(m)} \leq \frac{c_{m-1}\left(\frac{a}{c}\right)}{\left|c_{m-1}\left(\frac{\lambda_1 - c}{e}\right)\right|},$$

where c_{m-1} denotes the Chebyshev polynomial of degree $m-1$.
The relative difference between the right and left hand side converges to 0.

Refined Ritz vector

After a Ritz pair (θ, y) has been determined, the approximation y to the eigenvector can be improved solving the optimization problem

$$\|Az - \theta z\|_2 = \min!,\ z \in \mathcal{K}_m(v^1, A),\ \|z\|_2 = 1,$$

This improvement was introduced by Jia (1997) and was called refined Ritz vector although a solution in general is not a Ritz vector corresponding to θ.

Given a Ritz pair the refined Ritz vector can be obtained from the augmented Hessenberg matrix

$$\tilde{H}_m = \begin{pmatrix} h_{11} & h_{12} & h_{13} & \dots & \dots & h_{1m} \\ h_{21} & h_{22} & h_{23} & \dots & \dots & h_{2m} \\ 0 & h_{32} & h_{33} & \dots & \dots & h_{3m} \\ & & \ddots & \ddots & & \vdots \\ & & & \ddots & \ddots & \vdots \\ & & & & h_{m,m-1} & h_{mm} \\ & & & & & h_{m+1,m} \end{pmatrix} \in \mathbb{R}^{(m+1)\times m}$$

Refined Ritz vector ct.

$z \in \mathcal{K}_m(v^1, A)$ can be written as $z = V_m t$, and $\|z\|_2 = 1$ holds if and only if $\|t\|_2 = 1$.

Hence,

$$\begin{aligned} \|(AV_m - \theta V_m)t\|_2 &= \|(V_{m+1}\tilde{H}_m - \theta V_m)t\|_2 \\ &= \|V_{m+1}(\tilde{H}_m - \theta I_{m+1,m})t\|_2 \\ &= \|(\tilde{H}_m - \theta I_{m+1,m})t\|_2 \end{aligned}$$

and this expression attains its minimum under the constraint $\|t\|_2 = 1$ for the right singular vector of $\tilde{H}_m - \theta I_{m+1,m}$ corresponding to the smallest singular value.

Explicit restarts

The growing storage and arithmetic cost may make restarts of the Arnoldi algorithm necessary.

Since the Arnoldi method naturally starts with one vector, one of the most straightforward restarting schemes is to reduce the whole basis into one vector and start the new Arnoldi iteration with it.

If only one eigenvalue is required (for instance the one with the largest real part), we can choose to restart with the corresponding Ritz vector.

If more than one eigenvalue is wanted, we may add all Ritz vectors together to form one starting vector, or use a block version of the Lanczos algorithm that has the same block size as the number of wanted eigenvalues.

These options are simple to implement but not nearly as effective as the more sophisticated ones such as the implicit restarting scheme and the thick restart scheme.

Implicit restarts (Sorensen 1992)

With $m = k + p$ steps of the Arnoldi method one determines a factorization

$$AV_m = V_m H_m + r^m (e^m)^H.$$

With p steps of the QR algorithm with implicit shifts for H_m one gets

$$AV_m^+ = V_m^+ H_m^+ + r^m (e^m)^H Q \qquad (*)$$

where $Q = Q_1 Q_2 \cdot \ldots \cdot Q_p$, and Q_j are the orthogonal matrices from the p QR–steps, and $V_m^+ = V_m Q$, $H_m^+ = Q^H H_m Q$.

The leading $k-1$ components of $(e^m)^H Q$ are 0. Hence, the leading k columns of (*) have the form

$$AV_k^+ = V_k^+ H_k^+ + (r^k)^+ (e^k)^H$$

with the updated residual $(r^k)^+ = V_m^+ e^{k+1} h_{k+1,k} + r^m Q(m,k)$.

Implicitly restarted Arnoldi method (IRA)

Choose initial vector v^1 with $\|v^1\| = 1$
Determine $AV_m = V_m H_m + r^m (e^m)^T$ for $m = k + p$
while $\max_{j=1,\ldots,k} |t_{j+1,j}| > \text{tol}$ **do**
  Determine eigenvalues of H_m and choose shifts $\mu_1, \ldots, \mu_p$
  $Q = I_m$
  for $j = 1, \ldots, p$ **do**
    Compute QR factorization $Q_j R_j = T_m - \mu_j I$;
    $H_m = Q_j^H H_m Q_j$
    $Q = Q Q_j$
  end for
  $V_k^+ = V_m Q(:, 1:k)$;
  $H_k^+ = H_m(1:k, 1:k)$;
  $(r^k)^+ = V_m^+ e^{k+1} h_{k+1,k} + r^m Q(m, k)$
  Determine $AV_m = V_m H_m + r^m (e_m)^H$ by p Arnoldi steps
  starting with $AV_k^+ = V_k H_k^+ + (r^k)^+ (e^k)^H$
end while

Advantages

From the standpoint of numerical stability the updating scheme has several advantages:

(i) Orthogonality can be maintained since the value k is modest.

(ii) There is no question of spurious solutions

(iii) There is a fixed storage requirement

(iv) Deflation techniques similar to those associated with the QR iteration for dealing with numerically small diagonal elements of H_k (or T_k in the symmetric case) may be taken advantage of directly.

Choice of shifts

Applying one QR–step with shift μ is equivalent to multiplying v^1 by $A - \mu I$ (actually multiplying $e^1 \in \mathbb{R}^m$ by $H_m - \mu I_m$), p QR steps with shifts $\mu_1, \ldots, \mu_p$ therefore corresponds to a multiplication

$$v^1 \leftarrow \psi(A)v^1 \quad \text{mit} \quad \psi(\lambda) = \prod_{j=1}^{p}(\lambda - \mu_j).$$

If for instance $\lambda(A)$ is known to be contained in $D \subset \mathbb{C}$, and if the eigenvalues in $\tilde{D} \subset D$ are wanted, then it is reasonable to chose the shifts as roots of a polynomial ψ the modulus of which is as large as possible on $\tilde{D}$ and as small as possible on D.

This suggests for instance the roots of a

- Chebyshev polynomial with respect to $D \setminus \tilde{D}$ (Saad (1984))
- least squares polynomial (Saad (1987))
- Leja polynomial for $D \setminus \tilde{D}$ (Baglama, Calvetti & Reichel (1998))

Leja polynomial

Definition: Let $K \subset \mathbb{C}$ be a compact set, and let $w : K \to \mathbb{R}^+$ be a continuous weight function.

Let a sequence of points z_k be defined recursively by

(i) $z_1 \in K : w(z_1)|z_1| = \max_{z\in K} w(z)|z|$

(ii) $z_k \in K : w(z_k)\prod_{j=1}^{k-1}|z_k - z_j| = \max_{z\in K} w(z)\prod_{j=1}^{k-1}|z - z_j|,\ k = 2, 3, \ldots$

Then z_k are called Leja points, and the polynomial

$$\psi(\lambda) = \prod_{k=1}^{p}(\lambda - z_k)$$

is called Leja polynomial of degree p with respect to w.

There is no easy way to determine Leja points. However, Baglama, Calvetti & Reichel (1998) contains a method to determine approximations (called fast Leja points) in an efficient way.

Exact shifts

Lehoucq & Sorensen (1996) suggested exact shifts, i.e. $\lambda(T_m)$ is decomposed into k *wanted* and p *unwanted* eigenvalues, and the unwanted eigenvalues are chosen as shifts.

Possible wanted eigenvalues are

- the k largest / smallest eigenvalues
- the k largest / smallest eigenvalues in modulus
- the k right most eigenvalues
- the k eigenvalues with largest/smallest imaginary part
- the k eigenvalues which are closest to an excitation frequency

Other strategies include

- refined shifts (Jia 1998)
- harmonic Ritz values (Morgan 1991)

Locking and Purging

It may happen that a Ritz pair converged $(\theta_i^{(m)}, V_m s_i^{(m)})$ without $h_{j+1,j}$ or β_j having become small.

If $\theta_i^{(m)}$ is a wanted eigenvalue, then in the next step of the Arnoldi (or Lanczos) method the factorization can be curtailed to

$$\begin{aligned} Av^1 &= \theta_1 v^1 + \text{“small perturbation”}, \ (v^1 := V_m s_i^{(m)}) \\ AV_2 &= V_2 T_2 + h_{k+1,k} r (e^{k-1})^H. \end{aligned}$$

with $V_2^H v^1 = 0$. (θ_1, v_1) then is “locked” and will not be changed in the subsequent steps.

If $\theta_i^{(m)}$ is unwanted it may happen that the the influence of $\theta_i^{(m)}$ can not be removed by the QR iteration. This situation can be handled by a special deflation technique called “purging” (cf. Lehoucq & Sorensen 1996).

Software

Implementations of the Arnoldi method with implicit shifts by Lehoucq, Sorensen & Yang (1998) are freely available

- ARPACK (Fortran 77)
- P_ARPACK (Fortran 77, parallel version)
- eigs (MATLAB) (which calls ARPACK)

For symmetric eigenvalue problems Wu and Simon (2000) proposed an alternative restarted version of Lanczos (called thick restarts) which is mathematically equivalent to the implicitly restarted Lanczos method with exact shifts. An implementation

- TRLAN (Fortran 90)

is also freely available.
The code can run on a single address machine or in a distributed parallel environment, which requires MPI.

Thick restart

IRA projects $Ax = \lambda x$ to the Krylov space $\mathcal{K}_m(A, V_m Q(:,1))$, and with exact shifts μ_j this subspace is

$$\text{span}\{y^1, \ldots, y^k, v^{k+1}, Av^{k+1}, \ldots, A^{p-1}v^{k+1}\} \qquad (*)$$

where y^j denotes the Ritz vector corresponding to the kept Ritz values.

It was shown by Morgan (1996) that the subspace (*) is equal to

$$\text{span}\{y^1, \ldots, y^k, Ay^i, A^2y^i, \ldots, A^p y^i\}$$

for every $i \in \{1, \ldots, k\}$. This helps to explain the efficiency of IRA, since for each Ritz vector y^j the IRA subspace contains a Krylov subspace $\mathcal{K}_{p+1}(y^j, A)$ with starting vector y^j.

Wu and Simon (2000) developed an alternative restarted version of the Lanczos method (called thick restarts) which is equivalent to IRA with exact shifts. Instead of using the QR algorithm they orthonormalize the vectors $y^1, \ldots, y^k, v^{k+1}, Av^{k+1}, \ldots, A^{p-1}v^{k+1}$ in order to generate an orthonormal basis of the subspace (*).

Generalized Hermitean eigenproblem

There are several variants of the Lanczos algorithm for the generalized Hermitean eigenvalue problem

$$Ax = \lambda Bx, \quad A = A^H,\ B = B^H,\ B \text{ positive definite} \qquad (*).$$

They all correspond to a reformulation as a standard eigenproblem $Cy = \theta y$

Problem (*) can be transformed to a symmetric eigenproblem

$$Cy := R^{-H} A R^{-1} y = \lambda y, \quad x = R^{-1} y$$

where R denotes the Cholesky factor $B = R^H R$.

Alternatively the problem $Cx = B^{-1}Ax = \lambda x$ is symmetric with respect to the scalar product $\langle x, y\rangle_B := y^H Bx$. Hence, one can construct by the Lanczos process a B–orthogonal basis of the Krylov space $\mathcal{K}_m(C, v)$ such that the projected problem is tridiagonal.

Obviously in each step we have to multiply a vector by C, i.e. we have to solve one linear system.

Lanczos method for $C := B^{-1}A$

The Lanczos method for $C := B^{-1}A$ computes a basis V_j of $\mathcal{K}_j(v^1, C)$ and a real symmetric tridiagonal matrix T_j such that

$$AV_j = BV_jT_j + r(e^j)^H$$

$$\text{with} \quad V_j^HBV_j = I_j, \quad V_j^HAV_j = T_j, \quad V_j^HBr = 0.$$

Ritz pairs $(\theta_i^{(j)}, x^{i,(j)})$ are obtained from the tridiagonal eigenproblem

$$T_js^{i,(j)} = \theta_i^{(j)}s^{i,(j)}, \quad x^{i,(j)} = V_js^{i,(j)}.$$

For the residual it holds

$$\begin{aligned} r^{i,(j)} &= Ax^{i,(j)} - Bx^{i,(j)}\theta_i^{(j)} = AV_js^{i,(j)} - BV_js^{i,(j)}\theta_i^{(j)} \\ &= (AV_j - BV_jT_j)s^{i,(j)} = r(e^j)^Hs^{i,(j)} = Bv^{j+1}\beta_js_j^{i,(j)} \end{aligned}$$

from which we obtain

$$\|r^{i,(j)}\|_{B^{-1}}^2 = (r^{i,(j)})^HB^{-1}r^{i,(j)} = |\beta_js_j^{i,(j)}|^2$$

Theorem 10.9

Let $A, B \in \mathbb{C}^{n\times n}$ Hermitean and B positive definite, and denote by λ_j, $j = 1, \ldots, n$ the eigenvalues of $Ax = \lambda Bx$. Then it holds

$$\min_{j=1,\ldots,n} |\lambda_j - \theta| \leq \frac{\|Ax - \theta Bx\|_{B^{-1}}}{\|x\|_B}.$$

Proof: Let u^j be a set of B-orthonormal eigenvalues corresponding to λ_j and $x = \sum_{j=1}^n \alpha_j u^j$. Then it holds $\|x\|_B^2 = \sum_{j=1}^n |\alpha_j|^2$, and

$$\|Ax - \theta Bx\|_{B^{-1}} = \|\sum_{j=1}^n \alpha_j (Au^j - \theta Bu^j)\|_{B^{-1}} = \|\sum_{j=1}^n \alpha_j (\lambda_j - \theta) Bu^j\|_{B^{-1}}$$

$$= \sum_{j,k=1}^n \overline{\alpha_k(\lambda_k - \theta)} \alpha_j (\lambda_j - \theta)(Bv^k)^H B^{-1} Bv^j = \sum_{j=1}^n |\alpha_j(\lambda_j - \theta)|^2$$

$$\geq \min_{j=1,\ldots,n} |\lambda_j - \theta|^2 \|x\|_B^2. \qquad \square$$

As in the standard case we only have to monitor the subdiagonal elements β_j of T_j and the last component $s_j^{i,(j)}$ of its eigenvectors to control the errors of the Ritz values.

Lanczos method for $C := B^{-1}A$

1: Start with $q = x$, determine $r = Bq$, $\beta_0 = \sqrt{q^H r}$
2: **for** j=1,2,... until convergence **do**
3: $v^j = q/\beta_{j-1}$
4: $w^j = r/\beta_{j-1}$
5: $r = Av^j$
6: $r = r - \beta_{j-1} w^{j-1}$
7: $\alpha_j = (v^j)^H r$
8: $r = r - \alpha_j w^j$
9: reorthogonalize if necessary
10: solve $Bq = r$ for q
11: $\beta_j = \sqrt{q^H r}$
12: solve eigenproblem $T_j = S\Theta_j S^H$
13: test for convergence
14: **end for**
15: compute approximate eigenvectors $X = V_j S$

Comments

To simplify the description of the B-orthogonalization we introduce an auxiliary basis $W_j := BV_j$, which is B^{-1}-orthogonal, i.e. $W_j^H B^{-1} W_j = I_j$, and for which $W_j^H V_j = I_j$.

In step 9 we only have to reorthogonalize one of the bases V_j and W_j where we can use (as for the standard eigenproblem) complete or selective or partial reorthogonalization.

The complete reorthogonalization obtains the form

$$r = r - B(V_j(V_j^H r)),$$

and this step is repeated if the new residual r and V_j are not yet orthogonal.

The additional multiplication by B in the reorthogonalization step can be avoided if both bases, V_j and W_j are stored. Then the reorthogonalization can be performed by

$$r = r - W_j V_j^H r.$$

Comments ct.

The algorithm is stopped when the Ritz values $\theta_i^{(j)}$ are sufficiently good approximations of the wanted eigenvalues of the pencil $Ax = \lambda Bx$.

The estimate $|\beta_j s_j^{i,(j)}|$ may be too optimistic if the basis V_j is not fully B-orthogonal. Then the Ritz vector $x^{i,(j)}$ may have its norm smaller than 1, and we have to replace the estimate by

$$\|r^{i,(j)}\|_{B^{-1}} \approx |\beta_j s_j^{i,(j)}| / \|V_j s^{i,(j)}\|_B.$$

The Ritz vectors of the original matrix pencil are computed only when the test in step 13 has indicated that the wanted eigenvalues have been converged.

Shift-and-invert

Under general conditions an eigenvalue problem

$$Lu(x) = \lambda Mu(x),\ x \in \Omega, \quad Bu(x) = 0,\ x \in \partial\Omega,$$

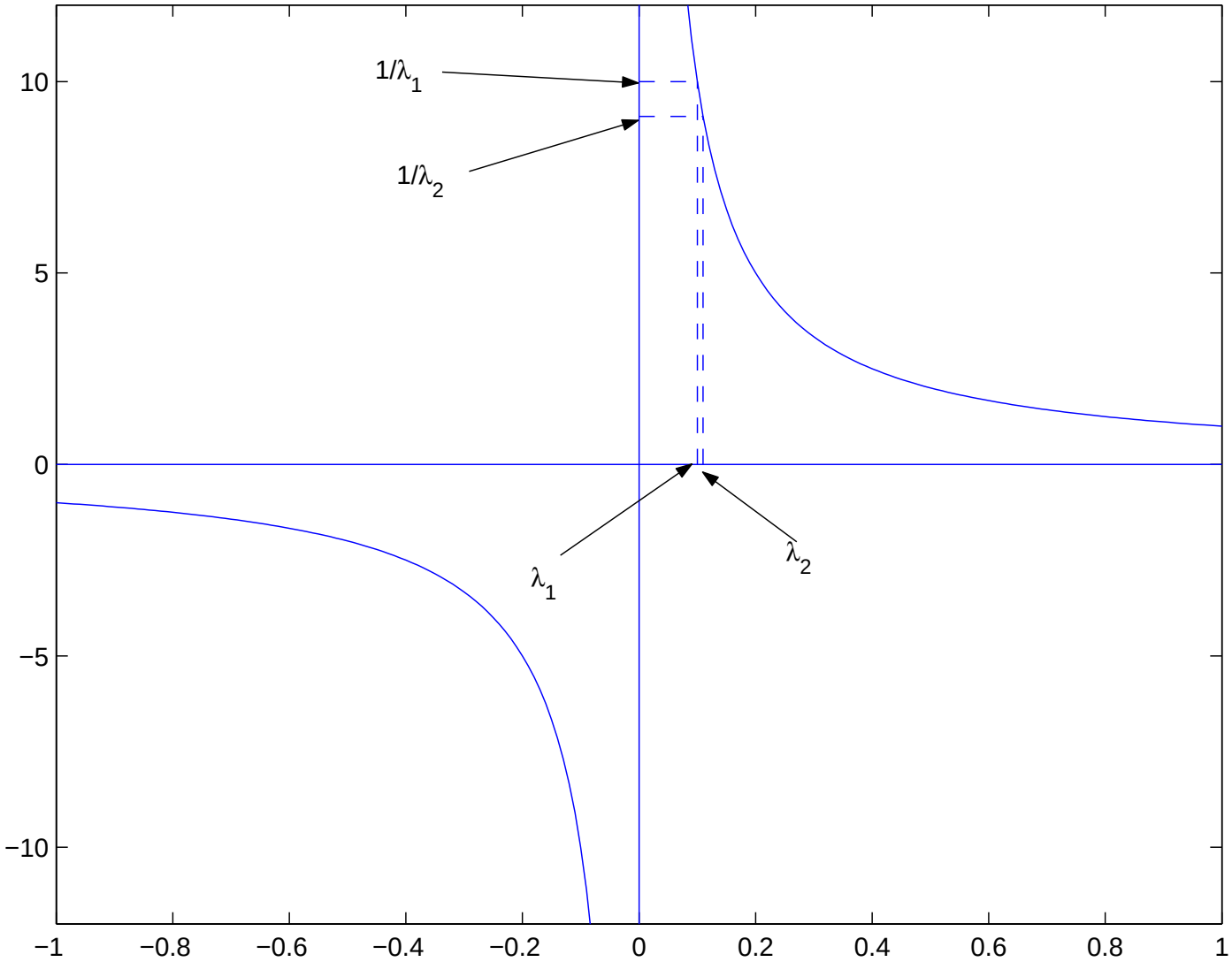
with elliptic operators L and M has a countable set of eigenvalues λ_n, which are clustered only at ∞.

For instance, for an ordinary differential operator L of second order and $M = I$ it holds $\lambda_n = \mathcal{O}(n^2)$. Hence the small eigenvalues are relatively close to each other whereas for large eigenvalues the distances will grow.

Therefore, for a discretization by the Rayleigh–Ritz method the spectrum will be very widely extended, in the lower part the eigenvalues will be clustered (relatively to the width of the spectrum) and higher eigenvalues will be well separated.

Usually one is interested in small eigenvalues. Therefore, the Lanczos method is applied to $A^{-1}B$ or to $(A - \sigma B)^{-1}B$ if eigenvalues in the vicinity of a fixed parameter σ are of interest.

Shift-and-invert



Shift–and–invert Lanczos method

The shift-and-invert variant corresponds to the application of the Lanczos method to $C := B(A - \sigma B)^{-1}$ for some shift σ.

It gives eigenvalues close to σ, and usually one gets convergence after a small number of steps. Even if systems with the shifted matrix $A - \sigma B$ are more laborious to solve than those with B needed in the direct variant, the smaller number of required steps will very often compensate for this.

The basic recursion of the shift-and-invert method is

$$B(A - \sigma B)^{-1} V_j = V_j T_j + r(e^j)^H. \qquad (*)$$

If V_j is chosen to be B^{-1}-orthogonal, i.e. $V_j^H B^{-1} V_j = I_j$ then multiplying $(*)$ by $V_j^H B^{-1}$ one gets

$$V_j^H (A - \sigma B)^{-1} V_j = T_j,$$

and the Lanczos process yields $V_j^H B^{-1} r = 0$.

Shift–and–invert Lanczos method ct.

An eigenvalues $\theta_i^{(j)}$ of the tridiagonal matrix T_j is an approximate eigenvalue of

$$C := B(A - \sigma B)^{-1},$$

and therefore

$$\lambda_i^{(j)} = \sigma + \frac{1}{\theta_i^{(j)}}$$

is an approximate eigenvalue of the original pencil $Ax = \lambda Bx$.

If $s^{i,(j)}$ is a corresponding eigenvector, then the Ritz vector

$$x^{i,(j)} := B^{-1} V_j s^{i,(j)}$$

is an approximation to the corresponding eigenvector of $Ax = \lambda Bx$.

Let W_j be the auxiliary basis for which $V_j = BW_j$. Then W_j is B-orthogonal, V_j and W_j are biorthogonal, i.e. $W_j^H V_j = I_j$, and the Ritz vectors are

$$x^{i,(j)} := W_j s^{i,(j)}.$$

Shift–and–invert Lanczos method ct.

Multiplying the basic recursion by $B^{-1}(A-\sigma B)$ from the left and $s^{i,(j)}$ from the right, one gets

$$V_j s^{i,(j)} = (A-\sigma B)B^{-1}V_j T_j s^{i,(j)} + \beta_j (A-\sigma B)B^{-1} v^{j+1} s_j^{i,(j)},$$

and it follows for the residual of a Ritz pair

$$\begin{aligned} r^{i,(j)} &= Ax^{i,(j)} - \lambda_i^{(j)} Bx^{i,(j)} = (A-\sigma B)x^{i,(j)} - \frac{1}{\theta_i^{(j)}} Bx^{i,(j)} \\ &= \frac{1}{\theta_i^{(j)}} \left((A-\sigma B)B^{-1} V_j s^{i,(j)} \theta_i^{(j)} - V_j s^{i,(j)} \right) \\ &= -\frac{1}{\theta_i^{(j)}} (A-\sigma B)B^{-1} v^{j+1} \beta_j s_j^{i,(j)}. \end{aligned}$$

In this case we do not obtain an error bound for the Ritz values from the residual (but only for the harmonic Ritz values). Nevertheless, $|\beta_j s_j^{i,(j)}|$ is an error indicator and is used in termination conditions.

Shift–and–invert Lanczos algorithm

1: Start with $r = x$, compute $q = Br$, $\beta_0 = \sqrt{q^H r}$
2: **for** j=1,2,... until convergence **do**
3: $v^j = q/\beta_{j-1}$
4: $w^j = r/\beta_{j-1}$
5: Solve $(A - \sigma B)r = v^j$ for r
6: $r = r - \beta_{j-1} w^{j-1}$
7: $\alpha_j = (v^j)^H r$
8: $r = r - \alpha_j w^j$
9: reorthogonalize if necessary
10: $q = Br$
11: $\beta_j = \sqrt{q^H r}$
12: solve eigenproblem $T_j = S\Theta_j S^H$
13: test for convergence
14: **end for**
15: compute approximative eigenvectors $X = W_j S$

Shift–and–invert Lanczos algorithm

Since for the shift-and-invert method we can expect rapid convergence to eigenvalues close to the shift one usually applies complete reorthogonalization

$$r = r - W_j(W_j^H(Br))$$

or

$$r = r - W_j(V_j^H r)$$

until r and the basis W_j are B-orthogonal.

The linear system in step 5 one uses a factorization

$$LDL^H = P^T(A - \sigma B)P$$

for an appropriate sparsity preserving permutation P, which is determined in the beginning using sparse Gaussian elimination. Then r in step 5 is obtained as

$$r = P(L^{-H}(D^{-1}(L^{-1}(P^T v^j)))).$$

If all eigenvalues are on one side of the shift then $A - \sigma B$ is definite, and one can use (sparse) Cholesky, otherwise the matrix $A - \sigma B$ is indefinite, and one has to use a symmetric indefinite factorization.

Shift–and–invert Arnoldi

The shift-and-invert idea can be used for non-Hermitean eigenvalue problems and regular pencils $Ax = \lambda Bx$ (i.e. $\det(A - \lambda B) \not\equiv 0$) to determine eigenvalues in the vicinity of a given shift σ.

Since B is no longer definite the Arnoldi method constructs an orthogonal basis (with respect to the Euclidean inner product) of $\mathcal{K}_m(v_1, C)$ where $C := (A - \sigma B)^{-1} B$ such that

$$(A - \sigma B)^{-1} B V_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T$$

The method converges to eigenvalues close to the shift first, and the convergence is faster, the better these eigenvalues are separated from the rest of the spectrum.

ARPACK has driver routines for the generalized eigenvalue problem and uses shift-and-invert.

Rational Krylov subspace method

If one is interested in eigenvalues in a large interval $[\alpha, \beta] \subset \sigma(A)$ or an extended region of the complex plane then one can apply the shift-and-invert method in several runs with several parameters $\sigma_j \in [\alpha, \beta]$.

The cost can be reduced considerably if the eigenproblem is projected to a rational Krylov space

$$\{v, (A-\sigma_1 B)^{-1}Bv, \ldots, (A-\sigma_1 B)^{-i_1}Bv, (A-\sigma_2 B)^{-1}Bv, \ldots, (A-\sigma_2 B)^{-i_2}Bv, \ldots, (A-\sigma_k B)^{-1}Bv, \ldots, (A-\sigma_k B)^{-i_k}Bv\}$$

and the projected eigenproblem is solved.
In the Arnoldi method the eigenproblem is projected onto a subspace of the form

$$V_m = \{\psi((A-\sigma B)^{-1}B)v \,:\, \psi \in \Pi_{m-1},\ \psi(0) = 1\}.$$

For the rational Krylov method the subspace can be written as

$$V = \{\rho(A)v \,:\, \rho \text{ a suitable rational function},\ \rho(0) = 1\}.$$

It can be shown (Ruhe 1998) that the rational Krylov method can be interpreted as a shift-and-invert Lanczos method with shift σ_k and a modified initial vector $\tilde{v}^1$.

Rational Krylov subspace method ct.

Rational Krylov starts as shift-and-invert Arnoldi method with shift σ_1 and initial vector v^1, and determines an Arnoldi recursion

$$(A - \sigma_1 B)^{-1} B V_m = V_{m+1} H_{m+1,m}. \qquad (1)$$

If m is big enough then accurate approximations to eigenvalues in the vicinity of σ_1 are obtained from extreme eigenvalues of $H_m = H_{m+1,m}(1:m, 1:m)$.

To obtain further eigenvalue approximations we choose a new shift σ_2 and continue the Arnoldi process without throwing away the information gathered in the basis of the Krylov space $\mathcal{K} := \mathcal{K}_m((A - \sigma_1 B)^{-1} B, v^1)$.

This is indeed possible if we are able to determine an Arnoldi recursion

$$(A - \sigma_2 B)^{-1} B W_m = W_{m+1} \tilde{H}_{m+1,m}. \qquad (2)$$

corresponding to the shift σ_2 and the initial vector w^1 such that $\tilde{H}_{m+1,m}$ has the same trapezoidal form as $H_{m+1,m}$ (i.e. $\tilde{h}_{ij} = 0$ for $i > j + 1$), and $\text{span}(V_{m+1}) = \text{span}(W_{m+1})$.

Rational Krylov subspace method ct.

Rewrite the recursion (1) as

$$BV_m = (A - \sigma_1 B) V_{m+1} H_{m+1,m},$$

which is equivalent to

$$(\sigma_1 - \sigma_2) BV_{m+1} H_{m+1,m} + BV_m = (A - \sigma_2 B) V_{m+1} H_{m+1,m},$$

and to

$$BV_{m+1}(I_{m+1,m} + (\sigma_1 - \sigma_2) H_{m+1,m}) = (A - \sigma_2 B) V_{m+1} H_{m+1,m},$$

where the matrix

$$K_{m+1,m} := I_{m+1,m} + (\sigma_1 - \sigma_2) H_{m+1,m}$$

is trapezoidal of the same form as $H_{m+1,m}$.

Rational Krylov subspace method ct.

From

$$(A-\sigma_2 B)^{-1}BV_{m+1}K_{m+1,m} = V_{m+1}H_{m+1,m}$$

we obtain the desired Arnoldi recursion if we get rid of the factor $K_{m+1,m}$ on the left.

If

$$K_{m+1,m} = Q_{m+1}\begin{bmatrix} R_m \\ 0 \end{bmatrix}$$

denotes the QR factorization of $K_{m+1,m}$, then R_m is regular (otherwise a subdiagonal element of $H_{m+1,m}$ would have been 0, and the Arnoldi process would have stopped with an invariant subspace), and it follows

$$(A-\sigma_2 B)^{-1}BV_{m+1}Q_{m+1}\begin{bmatrix} R_m \\ 0 \end{bmatrix} = V_{m+1}H_{m+1,m},$$

and multiplication by R_m^{-1} from the right yields

Rational Krylov subspace method ct.

$$(A-\sigma_2 B)^{-1}BV_{m+1}Q_{m+1,m} = V_{m+1}Q_{m+1}Q_{m+1}^H H_{m+1,m}R_m^{-1}. \qquad (3)$$

Hence, with the orthogonal basis $V_{m+1}Q_{m+1}$ of the Krylov space $\mathcal{K}$ the projection of $(A-\sigma_2 B)^{-1}B$ is represented by the full matrix

$$L_{m+1,m} = Q_{m+1}^H H_{m+1,m}R_m^{-1}$$

which can be transformed to trapezoidal form by applying Householder matrices from bottom upwards

$$L_{m+1,m} = \begin{bmatrix} P_m & 0 \\ 0 & 1 \end{bmatrix} \tilde{H}_{m+1,m}P_m^H.$$

Multiplying equation (3) by P_m from the right one gets

Rational Krylov subspace method ct.

$$(A-\sigma_2 B)^{-1}BV_{m+1}Q_{m+1,m}P_m = V_{m+1}Q_{m+1}\begin{bmatrix} P_m & 0 \\ 0 & 1 \end{bmatrix}\tilde{H}_{m+1,m},$$

i.e. an Arnoldi recursion

$$(A-\sigma_2 B)^{-1}BW_m = W_{m+1}\tilde{H}_{m+1,m}$$

with the new shift σ_2, the new orthogonal basis

$$W_{m+1} = V_{m+1}Q_{m+1}\begin{bmatrix} P_m & 0 \\ 0 & 1 \end{bmatrix},$$

and the upper Hessenberg matrix $\tilde{H}_{m+1,m}$.

Rational Krylov subspace method ct.

Notice that all transformations are done without performing operations with the large matrices A and B, and that it can even be avoided to form the matrix W explicitly, thus avoiding all work on large vectors.

In practical implementations the rational Krylov method is combined with locking, purging, and implicit restarts.

Implicitly restarted shift-and-invert Arnoldi with shift σ_1 is run until an appropriate number of eigenvalues around σ_1 have converged. Then these eigenvalues are locked, and eigenvalues outside the interesting region are purged leaving an Arnoldi recursion of dimension m. Then a new shift σ_2 is introduced, W_{m+1} and $\tilde{H}_{m+1,m}$ are determined, and the implicitly restarted shift-and-invert Arnoldi process with shift σ_2 is continued without touching the locked Ritz pairs. The same procedure is repeated until all interesting eigenvalues have converged.

Block Arnoldi method

Block methods are used mainly for reliably determining multiple and/or clustered eigenvalues.

Let A be a matrix of order n, and let b be th block size.

$$AV_{[m]} = V_{[m]}H_{[m]} + F_m\tilde{E}_m \qquad (1)$$

is a block Arnoldi reduction of order m if $V_{[m]}^H AV_{[m]} = H_{[m]}$ is a band upper Hessenberg matrix of order mb, $V_{[m]}^H V_{[m]} = I_{mb}$, $V_{[m]}^H F_m = 0$, and $\tilde{E}_m = [O, \ldots, O, I_b] \in \mathbb{R}^{mb\times b}$.

Here, a band upper Hessenberg matrix is an upper triangular matrix with b subdiagonals. The columns of $V_{[m]}$ form an orthonormal basis of the block Krylov space

$$\mathcal{K}_m(A, V_1) := \text{span}\{V_1, AV_1, \ldots, A^{m-1}V_1\}.$$

Extending a block Arnoldi reduction

1: compute the QR factorization $V_{m+1}H_{m+1,m} = F_m$ using iterated classical Gram Schmidt process

2: $V_{[m+1]} = \left[V_{[m]}, V_{m+1}\right]$

3: $W = AV_{m+1}$

4: $H_{m+1,m+1} = V_{m+1}^H W$

5: $H_{[m+1]} = \begin{bmatrix} H_{[m]} & V_{[m]}^H W \\ H_{m+1,m}\tilde{E}_m & H_{m+1,m+1} \end{bmatrix}$

6: $F_{m+1} = W - V_{[m+1]} \begin{bmatrix} V_{[m]}^H W \\ H_{m+1,m+1} \end{bmatrix}$

Comments

1. The classical Gram Schmidt method can be performed using the BLAS2 matrix-vector multiplication subroutine.

Moreover, this scheme gives a simple way to fill out a rank deficient F_m. For instance, if a third step of orthogonalization is needed when computing column j of V_{m+1} then the corresponding column of F_m depends linearly on the previous columns of V_{m+1}. The j-th diagonal element of $H_{m+1,m}$ then is set ot zero, and random vector is orthogonalized against $V_{[m]}$ and the first $j-1$ columns of V_{m+1}.

2. Application of A to a group of vectors might prove essential if accessing A is expensive.

3. Allows to use BLAS3 matrix-matrix multiplication subroutine

Block implicitly restarted Arnoldi method

1: **for** $i = 1, 2, \ldots$ until convergence **do**
2: extend the length r block Arnoldi reduction by p blocks:

$$AV_{[r+p]} = V_{[r+p]}H_{[r+p]} + F_{r+p}\tilde{E}_{r+p}$$

3: check whether the k wanted Ritz values are sufficiently accurate
4: lock Ritz values that satisfy the convergence tolerance
5: implicitly restart with p shifts and retain a length r block Arnoldi reduction
6: **end for**

Band Lanczos method (Ruhe (1979), Freund (1997))

The Lanczos algorithm is not able to detect the multiplicity of a multiple eigenvalue and to compute a basis of the corresponding eigenspace. It has problems with clusters of eigenvalues.

Way out: Use several initial vectors $w_1, \ldots, w_p$ and consider the block Krylov sequence

$$w_1, \ldots, w_p, Aw_1, \ldots, Aw_p, \ldots, A^{m-1}w_1, \ldots, A^{m-1}w_p, \ldots, \tag{1}$$

construct an orthonormal basis $v_1, \ldots, v_j$ of the space which is spanned by the first j linear independent vectors of the sequence (1), and solve the projection of the eigenproblem to this subspace.

Band Lanczos method ct.

For the Lanczos method $v_{m+1} = 0$, $v_j \neq 0$, $j = 1, \ldots, m$, means that $\mathcal{K}_m(A, v_1)$ within the sequence $\mathcal{K}_j(A, v_1)$, $j = 1, 2, \ldots$, is the first invariant subspace of A. Then all eigenvalues of T_m are eigenvalues of A as well, and the Ritz vectors are eigenvectors of A.

For $p > 1$ the occurrence of the first linear dependent vector does not mean that an invariant subspace has been detected but only that some newly obtained vector $A^k v_i$ can be combined linearly by the previous vectors and hence does not contain new information. The same holds for the subsequent vectors $A^{k+1} v_i$, $A^{k+2} v_i$, ... Therefore, the vector $A^k v_i$ is removed from the further construction. Particularly inconvenient is the fact that the linear dependence has to be detected in finite precision.

The projected problem is a banded matrix with bandwidth $2p + 1$, where the effective bandwidth diminishes by 2 for every deflation.

Lanczos method for non-Hermitean problems

Disadvantages of the Arnoldi method are high arithmetic cost (orthonormalization with respect to all previous basis elements and reorthogonalization) and high (unpredictable) storage requirements.

The arithmetic cost can be reduced essentially by using oblique projections and a two sided Gram–Schmidt procedure. To this end two Krylov sequences $p_1, p_2, \ldots$ and $q_1, q_2, \ldots$ are constructed according to

$$\begin{aligned} \beta_{j+1} q_{j+1} &= A q_j - \alpha_j q_j - \gamma_j q_{j-1} \\ \gamma_{j+1} p_{j+1} &= A^H p_j - \alpha_j p_j - \beta_j p_{j-1}. \end{aligned}$$

$q_1, \ldots, q_m$ is a(non orthogonal) basis of $\mathcal{K}_m(A, q_1)$ and $p_1, \ldots, p_m$ is a (non orthogonal) basis of $\mathcal{K}_m(A^H, p_1)$. The bases are biorthogonal, i.e. $p_j^H q_k = \delta_{kl}$.

Lanczos method for non-Hermitan problems ct.

With $Q_m = [q_1, \ldots, q_m]$, $P_m = [p_1, \ldots, p_m]$, $T_m = \text{tridiag}\{\beta_j, \alpha_j, \gamma_{j+1}\}$ a compact form of the two-sided Lanczos method reads

$$\begin{aligned} AQ_m &= Q_m T_m + \beta_{m+1} q_{m+1} e_m^T \\ A^H P_m &= P_m T_m^H + \gamma_{m+1} p_{m+1} e_m^T \\ P_m^H Q_m &= I_m,\ P_m^H q_{m+1} = 0,\ p_{m+1}^H Q_m = 0 \\ T_m &= P_m^H A Q_m \end{aligned}$$

The Ritz values $\theta_i^{(m)}$ of

$$T_m z_i^{(m)} = \theta_i^{(m)} z_i^{(m)} \quad \text{and} \quad T_m^H w_i^{(m)} = \theta_i^{(m)} w_i^{(m)}$$

are approximations to eigenvalues of A, and the right Ritz vectors $x_i^{(m)} = Q_m z_i^{(m)}$ and left Ritz vectors $y_i^{(m)} = P_m w_i^{(m)}$ are approximations to corresponding left and right eigenvectors.

Lanczos method for non-Hermitean problems ct.

The residuals

$$\begin{aligned} r_i^{(m)} &= Ax_i^{(m)} - \theta_i^{(m)} x_i^{(m)} = \beta_{m+1} q_{m+1} e_m^T x_i^{(m)} \\ s_i^{(m)} &= A^H y_i^{(m)} - \theta_i^{(m)} y_i^{(m)} = \gamma_{m+1} p_{m+1} e_m^T y_i^{(m)} \end{aligned}$$

and their norms again can be determined without computing the Ritz vectors.

If $\beta_{m+1} = 0$ or $\gamma_{m+1} = 0$, then the algorithm terminates which is called lucky breakdown. In this case $\mathcal{K}_m(A, q_1)$ is an invariant subspace of A or $\mathcal{K}_m(A^H, p_1)$ is an invariant subspace of A^H, the Ritz values $\theta_i^{(m)}$ are eigenvalues of A, and the right and left Ritz vectors are right and left eigenvectors of A, respectively.

Lanczos method for non-Hermitean problems ct.

The method also terminates if $p_{m+1}^H q_{m+1} = 0$ for some m which is called an (essential breakdown). In this case one very often can construct vectors $q_{m+1}, \ldots, q_{m+k} \in \mathcal{K}_{m+k}(A, q_1)$ and $p_{m+1}, \ldots, q_{m+1} \in \mathcal{K}_{m+k}(A^H, p_1)$ for some $k > 1$ such that $p_j^H q_i = 0$ and $p_i^H q_j = 0$ for $j = 1, \ldots, m$ and $i = m+1, \ldots, m+k$, and it is possible to construct bi-orthogonal bases of subsequent Krylov spaces by the Lanczos algorithm. The obliquely projected eigenvalue problem then has tridiagonal form which is perturbed by a full block in columns and rows $m, \ldots, m+k$.

This construction is called look ahead Lanczos method. It is implemented in the (public domain) software QMRPACK by Freund and Nachtigal (1996). If the construction (in very rare cases) is not possible then the breakdown is called incurable.

Inexact Arnoldi method (Simoncini 2005)

Assume that A can not be applied exactly, but at each iteration the operation $y = Av$ is replaced by the inexact evaluation

$$y = Av + f$$

where f can change in each iteration and $\|f\|$ can be monitored.

For example, let $A = (B - \sigma I)^{-1}$ be a shift-and-invert operator, and in the kth step of the Arnoldi method solve

$$(B - \sigma I)y = v$$

by a (preconditioned) Krylov method iterating until

$$\|f\| = \|(B - \sigma I)y - v\| \leq \varepsilon_k$$

for a given ε_k.

Inexact Arnoldi method ct.

Aim: Given $\varepsilon > 0$, determine $\varepsilon_k > 0$, $k = 1, 2, \ldots, m$ such that for an eigenpair (θ, u) of H_m it holds

$$\|(AV_m u - \theta V_m u) - r_m\| \leq \varepsilon \quad \text{(at least asymptotically)}$$

where

$$r_m = h_{m+1,m} v_{m+1} e_m^T u$$

is the computet residual of the Ritz pair $(\theta, V_m u)$.

Suggestion of Simoncini justified by a THEOREM which contains unavailable terms: Assume that a maximum of m inexact Arnoldi steps are to be carried out.
Require that

$$\|f_k\| \leq \begin{cases} \frac{1}{m}\varepsilon & \text{for } k = 1 \\ \frac{\min\{\alpha, \delta_{k-1}\}}{2m\|r_{k-1}\|}\varepsilon & \text{for } k > 1 \end{cases}$$

where

$$\delta_{k-1} := \min_{\theta \in \Lambda(H_{k-1}) \setminus \{\theta^{(k-1)}\}} |\theta_{k-1} - \theta|,$$

α is an estimate of $\|A\|$ and r_{k-1} is the computed residual in step $k-1$.