The Arnoldi and Lanczos methods for approximating the eigenpairs of a matrix

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The Arnoldi and Lanczos methods for approximating the eigenpairs of a matrix

Reinier Torenbeek and Kees Vuik

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Chapter 1

Introduction

Solving the eigenvalue problem for large linear systems, which is often required in engineering problems, is still a difficult task. In many cases, only a part of the eigenvalue spectrum is asked for, and some of the most popular methods for approximating a part of the eigenvalue spectrum are given by so called projection methods. The best known versions of these projection methods are the Arnoldi method and the Bi-Lanczos method, or, in the case of a Hermitian problem, the Lanczos method.

Unfortunately, many aspects of these methods are not (yet) very well understood, especially for the non-Hermitian problem. Some convergence properties and minimization characteristics are known, but in practice, these are not very useful.

The aim of this report is to give an impression of the current state of the art for both the Arnoldi and the Lanczos methods. First, some basic linear algebra aspects, necessary to understand the complete report, will be briefly mentioned. After that, a description of the general projection method is given, and the Arnoldi method, the Bi-Lanczos method and the Lanczos method are explained. This is followed by a summary of known relevant properties of orthogonal projection methods, of which the Arnoldi and Lanczos methods are special versions. Finally, some open questions about the methods are given, as well as an impression of what further investigation I want to do .

Most of the information gathered in this report is based on [1].

Chapter 2

Basics

This chapter covers some basic subjects from linear algebra, mainly concerning the eigenvalue problem.

2.1 Eigenvalues and eigenvectors

The linear eigenvalue problem consists of finding so-called eigenpairs $\lambda_i \in \mathbb{C}$ and $u_i \in \mathbb{C}^n$, with $u_i \neq 0$, which satisfy the following equation for $A \in \mathbb{C}^{n \times n}$

$$Au_i = \lambda_i u_i$$

The λ_i are called eigenvalues, the set of eigenvalues of A is called the (eigenvalue) spectrum of A. The u_i are called eigenvectors, or sometimes right eigenvectors. The eigenvectors of A^H are called left eigenvectors.

For each eigenvalue λ, the matrix $A-\lambda I$ must be singular, since $(A-\lambda I)u = 0$, with u the eigenvector corresponding to λ. Therefore, the determinant of $A - \lambda I$, which is called the characteristic polynomial of A, must vanish for each eigenvalue λ. So the eigenvalues of A can be defined as the roots of the characteristic polynomial of A. The corresponding eigenvectors are those vectors which are mapped by $A - \lambda I$ onto the zero vector. It can be proved that the characateristic polynomial of A applied to the matrix A itself results in the zero matrix.

It is possible that the characteristic polynomial has some multiple roots. An eigenvalue λ of A is said to have algebraic multiplicity μ if it is a root of multiplicity μ of the characteristic polynomial. An eigenvalue λ of A is said to have geometric multiplicity γ if the maximum number of independent eigenvectors associated with it is γ. The geometric multiplicity is equal to the dimension of $\mathcal{N}(A-\lambda I)$. The index l of an eigenvalue λ is equal to the smallest integer l for which $\mathcal{N}((A-\lambda I)^l) = \mathcal{N}((A-\lambda I)^{l+1})$.

If A is a Hermitian matrix, the eigenvalues are known to be real and the eigenvectors can be chosen such that they are an orthogonal basis of $\mathbb{C}^n$.

A change of basis does not affect the eigenvalues. This means that for all invertible matrices X, the spectrum of $X^{-1}AX$ is equal to that of A. The eigenvectors of $X^{-1}AX$ are equal to those of A, multiplied by X^{-1}.

An interesting article about the linear algebra of eigenvalues and eigenvectors is [2]. Its fresh approach to the eigenvalueproblem gives a good insight in the meaning of eigenvectors and eigenvalues.

2.2 The conditioning of eigenvalues

The eigenvalues of A^H are equal to those of A, the eigenvectors, however, are different. If u_i is an eigenvector of A and v_i is an eigenvector of A^H, both associated with eigenvalue λ_i, then u_i and v_i can be scaled such that $(u_i, v_j) = \delta_{ij}$, that is, the u's and the v's are biorthogonal.

Now consider the family of matrices $A(t) = A + tE$, where E is an arbitrary matrix of the same order as A. If λ is an eigenvalue of A with algebraic multiplicity one, then the eigenvalue $\lambda(t)$ of $A(t)$ is a continuous differentiable function of t, for t small enough. It can be shown ([1], p.92) that

$$\lambda'(0) \leq \frac{\|Eu\|_2\|v\|}{|(u,v)|} \leq \|E\|_2 \frac{\|u\|_2\|v\|_2}{|(u,v)|}$$

in which u and v are right and left eigenvectors associated with λ.

The factor by which $\|E\|_2$ is multiplied in the upper bound is called the condition number of the eigenvalue. This condition number can be rewritten as

$$\mathrm{Cond}(\lambda) = \frac{1}{\cos\theta(u,v)}$$

where $\theta(u,v)$ denotes the angle between u and v. For normal matrices, $u_i = v_i$ for all i, which means that the condition of each eigenvalue equals 1 in that case. If A is highly non-normal, the angle between u_i and v_i can be large, which implies a high condition number for the corresponding eigenvalues.

2.3 Error bounds on approximate eigenpairs

Suppose that an approximate eigenvalue $\tilde{\lambda}$ and a corresponding approximate eigenvector $\tilde{u}$ of the matrix A have been found by some algorithm. What can be said about the error made on these approximations?

A possible criterion used to determine the accuracy of an approximate eigenpair is the norm of the residual vector $r = A\tilde{u} - \tilde{\lambda}\tilde{u}$. An iterative method, for instance, is repeated until $\|r\|_2 \leq \varepsilon$, where ε is a prescribed tolerance. Unfortunately, this stopping criterion does not guarantee a good eigenvalue approximation. The best thing that can be said about the residual vector is that if $\tilde{u}$ is of 2-norm unity and A is diagonalizable with eigenvector matrix X, then there exists an eigenvalue λ of A such that

$$|\lambda - \tilde{\lambda}| \leq \|X\|_2\|X^{-1}\|_2\|r\|_2$$

(See [1],p.77). In general, this bound is of no practical use since the condition number of X is usually not known. If A is Hermitian, however, then $\|X\|_2 = \|X^{-1}\|_2 = 1$ and we have

$$|\lambda - \tilde{\lambda}| \leq \|r\|_2$$

Another stopping criterion is based on the backward error, this is used, for example, in [4]. The normwise backward error associated with the approximate eigenpair $\tilde{\lambda}, \tilde{u}$ is defined to be

$$\eta = \min\{\delta : \exists \Delta A \text{ with } \|\Delta A\|_2 \leq \delta \|A\|_2, (A + \Delta A)\tilde{u} = \tilde{\lambda}\tilde{u}\}$$

The backward error gives a measure of the shortest distance between the original problem with computed solution $\tilde{u}$ and a perturbed problem with exact solution $\tilde{u}$. It can be shown(see [5]) that if $\|\tilde{u}\|_2 = 1$, then

$$\eta = \frac{\|A\tilde{u} - \tilde{\lambda}\tilde{u}\|_2}{\|A\|_2}$$

The stopping criterion is given by $\eta \leq \varepsilon$. Since it is usually hard to compute the 2-norm of A, $\|A\|_2$ is replaced by $\|A\|_F/\sqrt{n}$, the Frobenius norm of A divided by the square root of the order of A. This results in a lower bound on the backward error, since $\|A\|_F \leq \sqrt{n}\|A\|_2$.

For Hermitian A, it is possible to give an upperbound for the sine of the angle between the exact eigenvector u and the approximate eigenvector $\tilde{u}$. If $\tilde{u}$ is of norm unity, $\tilde{\lambda} = (A\tilde{u}, \tilde{u})$ and $r = A\tilde{u} - \tilde{\lambda}\tilde{u}$, then

$$\sin\theta(u, \tilde{u}) \leq \frac{\|r\|_2}{\delta}$$

where δ is the second smallest distance from $\tilde{\lambda}$ to any eigenvalue λ (see [1],p.82).

2.4 Min-max principles for Hermitian matrices

For Hermitian matrices, the eigenvalues can be expressed by a min-max principle. Since the eigenvalues of a Hermitian matrix are real, we can label them decreasingly, that is, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. With this notation, the Courant-Fisher min-max principle is formulated as follows:

$$\lambda_k = \max_{S, \dim(S)=k} \min_{x \in S, x \neq 0} \frac{(Ax, x)}{(x, x)}$$

Making use of the fact that the eigenvectors of a Hermitian matrix are orthogonal, this principle can be rewritten in the form of the Courant characterization: the eigenvalues λ_i and the corresponding eigenvectors q_i of a Hermitian matrix are such that

$$\lambda_1 = \frac{(Aq_1, q_1)}{(q_1, q_1)} = \max_{x \in \mathbb{C}^n, x \neq 0} \frac{(Ax, x)}{(x, x)}$$

and for $k > 1$:

$$\lambda_k = \frac{(Aq_k, q_k)}{(q_k, q_k)} = \max_{x \neq 0, q_1^H x = \ldots = q_{k-1}^H x = 0} \frac{(Ax, x)}{(x, x)}$$

2.5 Projectors

Projectors play an important role in the analysis done in this report. A projector P is a linear transformation from $\mathbb{C}^n$ to $\mathbb{C}^n$ which satisfies

$$P^2 = P,$$

When P is a projector then so is $I - P$ and we have $\mathcal{N}(P) = \mathcal{R}(I - P)$. The two subspaces $\mathcal{N}(P)$ and $\mathcal{R}(P)$ have only the zero element in common. Since they also span $\mathbb{C}^n$, we have

$$\mathbb{C}^n = \mathcal{N}(P) \oplus \mathcal{R}(P)$$

Conversely, every pair of subspaces $\mathcal{M}$ and $\mathcal{S}$ that form a direct sum of $\mathbb{C}^n$ define a unique projector P such that $\mathcal{R}(P) = \mathcal{M}$ and $\mathcal{N}(P) = \mathcal{S}$. The projector P is said to be the projector onto $\mathcal{M}$ along $\mathcal{S}$. Every vector x can be uniquely decomposed into the sum of a vector $x_1 \in \mathcal{M}$ and $x_2 \in \mathcal{S}$, given by $x_1 = Px$, $x_2 = (I - P)x$.

2.5.1 Orthogonal projectors

A projector P is said to be orthogonal if

$$\mathcal{N}(P) = \mathcal{R}(P)^\perp$$

In this case, we have

$$Px \in \mathcal{M} \qquad \text{and} \qquad (I - P)x \perp \mathcal{M}$$

Without proof, we mention that a projector is orthogonal if and only if it is Hermitian.

If an orthonormal basis of $\mathcal{M}$ is given by $\{v_1, \ldots, v_m\}$, then the orthogonal projection onto $\mathcal{M}$ is given by $P = VV^H$, where V is the $n \times m$ matrix which has $v_1, \ldots, v_m$ as its columns. This can easily be seen by recalling that the projection onto $\mathcal{M}$ is equal to the sum of the projections onto the seperate vectors v_i. The projection of x onto v_i is given by $(v_i, x)v_i = v_i v_i^H x$. This is equal to multplication of the i-th column of V by the i-th element of $V^H x$.

Since the orthogonal projector onto $\mathcal{M}$ is unique, we must have $V_1 V_1^H = V_2 V_2^H$ for all orthonormal bases V_1 and V_2 of $\mathcal{M}$.

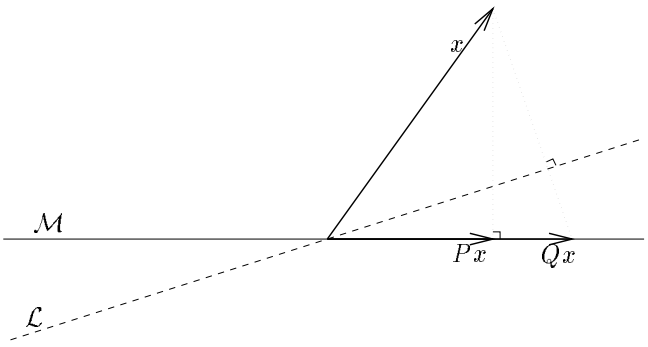

Figure 2.1: Visualization of an orthogonal projector P onto $\mathcal{M}$ and and oblique projector Q onto $\mathcal{M}$ along $\mathcal{L}^\perp$.

2.5.2 Oblique projectors

A projector that is not orthogonal is said to be oblique. An oblique projector Q is uniquely determined by the two subspaces $\mathcal{M}$ and $\mathcal{L}$ such that

$$Qx \in \mathcal{M} \qquad \text{and} \qquad (I - Q)x \perp \mathcal{L}$$

This is a projector onto $\mathcal{M}$ along $\mathcal{L}^\perp$. Note that $\mathcal{R}(Q^T)$ is equal to $\mathcal{L}$. This means that Q^T is a projector onto $\mathcal{L}$ along $\mathcal{M}^\perp$. A visualization of both an orthogonal and an oblique projector onto $\mathcal{M}$ is given in figure 2.1.

A projector onto $\mathcal{M}$ along $\mathcal{L}^\perp$ can exist only in the case that two biorthogonal bases V of $\mathcal{M}$ and W of $\mathcal{L}$ exist, this is the multidimensional analogue to the condition in two dimensions that $\mathcal{M}$ and $\mathcal{L}^\perp$ are not parallel. In that case, with $V^H W = I$, the oblique projector Q onto $\mathcal{M}$ along $\mathcal{L}^\perp$ is given by the matrix $Q = VW^H$.

2.6 The Jordan canonical form and spectral projectors

The Jordan canonical form of a square matrix A gives a similarity transformation, or in other words a change of basis, such that the new representation J has a special block diagonal structure. In words, the Jordan form can be described as follows: any square matrix A can be reduced to a block diagonal matrix consisting of p diagonal blocks, each associated with a distinct eigenvalue. Each diagonal block number i has itself a block diagonal structure consisting of γ_i subblocks, where γ_i is the geometric multiplicity of the eigenvalue λ_i. Each of the subblocks, referred to as a Jordan block, is an upper bidiagonal matrix of size not exceeding l_i, where l_i is the index of λ_i, with the constant λ_i on the diagonal and the constant one on the superdiagonal.

In other words, for any square matrix A there exists a non-singular matrix X

such that

$$X^{-1}AX = J = \begin{pmatrix} J_1 & & & & & \\ & J_2 & & & & \\ & & \ddots & & & \\ & & & J_i & & \\ & & & & \ddots & \\ & & & & & J_p \end{pmatrix}$$

where

$$J_i = \begin{pmatrix} J_{i1} & & & \\ & J_{i2} & & \\ & & \ddots & \\ & & & J_{i\gamma_i} \end{pmatrix}$$

with

$$J_{ik} = \begin{pmatrix} \lambda_i & 1 & & \\ & \ddots & \ddots & \\ & & \lambda_i & 1 \\ & & & \lambda_i \end{pmatrix}$$

When A is considered with respect to the basis X, the nature of the transformation is very clear: Since J is block-diagonal, with p blocks, $\mathbb{C}^n$ can be divided into p subspaces, say $M_1, \ldots, M_p$, which are invariant under A. This means that every vector x can be written as

$$x = x_1 + x_2 + \ldots + x_i + \ldots + x_p$$

The linear transformation which is defined by $P_i : x \rightarrow x_i$ is a projector onto M_i along the direct sum of the subspaces $M_i, i \neq j$, it is called a spectral projector. Since the invariant subspaces M_i together span $\mathbb{C}^n$, we must have $P_1 + \ldots + P_p = I$.

2.7 The Schur canonical form

For any square matrix A there exists a unitary matrix Q such that $Q^H AQ = R$, with R upper triangular. This means that a unitary change of basis is possible, such that the transformation A can be represented by an upper triangular matrix, with respect to the basis Q. This is called the Schur canonical form. It is clear that the diagonal elements of R are equal to the eigenvalues of A, since R is upper triangular and similar to A. Writing the relation as $AQ = QR$, we see that the first i columns of Q span an invariant subspace under A.

The Schur decomposition is not unique, the eigenvalues can for example appear in any order on the diagonal of R, depending on the choice for Q.

2.8 Krylov subspaces

The Krylov subspace $\mathcal{K}_m(A, v)$ is a subspace given by

$$\mathcal{K}_m(A, v) \equiv \text{span}\{v, Av, A^2v, \ldots, A^{m-1}v\}$$

As can be seen from this definition, the Krylov subspaces $\mathcal{K}_m(A, v)$, $\mathcal{K}_m(A - \alpha I, v)$, $\mathcal{K}_m(\alpha A, v)$ and $\mathcal{K}_m(A, \alpha v)$ are the same.

The Krylov subspace can be defined in a alternative way: $\mathcal{K}_m(A, v)$ is the subspace of all vectors x in $\mathbb{C}^n$ which can be written as $x = p(A)v$, where p is a polynomial of degree not exceeding $m - 1$.

Chapter 3

Projection methods

An important class of algorithms for approximating the eigenvalues and eigenvectors of large matrices is given by the so-called projection methods. This chapter describes the general projection method.

3.1 The general projection method

The eigenvalue problem consists of finding the eigenvectors and eigenvalues of a certain $n \times n$ matrix A, which means that we want to find $u \in \mathbb{C}^n$ and $\lambda \in \mathbb{C}$ such that

$$Au = \lambda u$$

The general projection methods essentially consist of restricting the approximation $\tilde{u}$ of the eigenvector u to be an element of some subspace $\mathcal{K}$, called the right subspace. Usually, the dimension of $\mathcal{K}$ will be substantially lower than n, which means that the amount of work required for finding an approximate eigenpair is much lower than the amount of work required for finding an exact eigenpair: if $\dim\mathcal{K} = m$ then the approximate eigenvectors will turn out to be the exact eigenvalues of a certain $m \times m$ matrix.

An approximate eigenpair is given by those $\tilde{\lambda}$ and $\tilde{u}$ which result in a residual vector orthogonal to another subspace $\mathcal{L}$, called the left subspace. So the approximants $\tilde{\lambda} \in \mathbb{C}$ and $\tilde{u} \in \mathcal{K}$ must satisfy the condition

$$A\tilde{u} - \tilde{\lambda}\tilde{u} \perp \mathcal{L}$$

It is clear that the results of this method are determined by the choices for the subspaces $\mathcal{K}$ and $\mathcal{L}$. Since the approximate eigenvectors are taken from the subspace $\mathcal{K}$, a good approximation of any eigenvector is possible only for certain choices for $\mathcal{K}$. The special case $\mathcal{K} = \mathcal{L}$ results in an orthogonal projection method, of which the Arnoldi method is an example. If $\mathcal{K} \neq \mathcal{L}$, the method is called an oblique projection method, like the Bi-Lanczos method. These two classes of methods will be treated separately in the following two sections.

3.2 Orthogonal projection methods

In the case that $\mathcal{K} = \mathcal{L}$, the method consists of solving the following problem: find $\tilde{\lambda} \in \mathbb{C}$ and $\tilde{u} \in \mathcal{K}$ such that

$$A\tilde{u} - \tilde{\lambda}\tilde{u} \perp \mathcal{K}$$

If we define $\mathcal{P}_{\mathcal{K}}$ to be the orthogonal projector onto the subspace $\mathcal{K}$, then this condition is equivalent to

$$\mathcal{P}_{\mathcal{K}} A\tilde{u} = \tilde{\lambda}\tilde{u}, \qquad \tilde{\lambda} \in \mathbb{C}\,, \tilde{u} \in \mathcal{K} \tag{3.1}$$

This means that the approximate eigenpairs found by the orthogonal projection method are exact eigenpairs of the transformation given by $A_p = \mathcal{P}_{\mathcal{K}} A_{|\mathcal{K}}$, where $A_{|\mathcal{K}}$denotes the transformation A restricted to the subspace $\mathcal{K}$.

Since this linear transformation is from $\mathcal{K}$ to $\mathcal{K}$, it is useful to translate the problem into a basis of $\mathcal{K}$. Let $\{v_1, \ldots, v_m\}$ be an orthonormal basis of $\mathcal{K}$ and let V be the $n \times m$ matrix which has $v_1, \ldots, v_m$ as its columns. A change of basis can be achieved by introducing $y \in \mathbb{C}^m$ and setting $\tilde{u} = Vy$. With this, the orthogonality condition can be rewritten as

$$(AVy - \tilde{\lambda}Vy, Vz) = 0 \qquad \forall z \in \mathbb{C}^m$$

which is equal to

$$(V^H AVy - \tilde{\lambda}y, z) = 0 \qquad \forall z \in \mathbb{C}^m$$

This condition can be satisfied only if $V^H AVy - \tilde{\lambda}y = 0$, or

$$V^H AVy = \tilde{\lambda}y$$

So in order to find the approximate eigenpairs of A we need to find the exact eigenpairs of the operator $V^H AV$, which is called the Ritz-matrix. It represents the transformation $A_p = \mathcal{P}_{\mathcal{K}} A_{|\mathcal{K}}$ with respect to the basis $\{v_1, \ldots, v_m\}$, which can be seen by inspecting the product $V^H AVy$: Vy indicates a change of basis from $\{v_1, \ldots, v_m\}$ to the standard basis, this change of basis is followed by the transformation A and finally, the result is orthogonally projected onto $\mathcal{R}(V) = \mathcal{K}$ and expressed in terms of the basis $\{v_1, \ldots, v_m\}$.

So in order to find the approximate eigenpair $\tilde{\lambda}, \tilde{u}$ which satisfy condition 3.1, we need to generate the matrix $A_p = V^H AV$, where V has an orthonormal basis of $\mathcal{K}$ as its columns, and compute its eigenpairs $\tilde{\lambda}_i, y_i$. The approximate eigenpairs of A are then given by $\tilde{\lambda}_i, Vy_i$.

3.3 Oblique projection methods

If $\mathcal{K} \neq \mathcal{L}$ we have to find $\tilde{\lambda} \in \mathbb{C}$ and $\tilde{u} \in \mathcal{K}$ such that

$$A\tilde{u} - \tilde{\lambda}\tilde{u} \perp \mathcal{L}$$

We now have to introduce a projector $\mathcal{Q}_\mathcal{L}$ along the subspace $\mathcal{L}^\perp$ onto the subspace $\mathcal{K}$ which is an oblique projector. The orthogonality condition can be written as

$$\mathcal{Q}_\mathcal{L}(A\tilde{u} - \tilde{\lambda}\tilde{u}) = 0$$

Since $\mathcal{Q}_\mathcal{L}$ is a projection onto $\mathcal{K}$, we have $\mathcal{Q}_\mathcal{L}\tilde{u} = \tilde{u}$, so the condition above is equal to

$$\mathcal{Q}_\mathcal{L}A\tilde{u} = \tilde{\lambda}\tilde{u}$$

We see that, analogously to the orthogonal method, the approximate eigenpairs are given by exact eigenpairs of the transformation $\mathcal{Q}_\mathcal{L}A_{|\mathcal{K}}$.

Again, a change of basis is useful. We assume that it is possible to find two biorthogonal bases $\{v_1, \ldots, v_m\}$ and $\{w_1, \ldots, w_m\}$ of $\mathcal{K}$ and $\mathcal{L}$, which means that $(v_i, w_j) = \delta_{ij}$. By V and W we denote the $n \times p$ matrices which have these bases as their columns. With $\tilde{u} = Vy$ the orthogonality condition can be written as

$$(AVy - \tilde{\lambda}Vy, Wz) = 0 \qquad \forall z \in \mathbb{C}^m$$

Since $W^HV = I$, this is equal to

$$(W^HAVy - \tilde{\lambda}y, z) = 0 \qquad \forall z \in \mathbb{C}^m$$

In this case, we see that an approximate eigenpair satisfies

$$W^HAVy = \tilde{\lambda}y$$

which means that it is an exact eigenpair of the matrix W^HAV, again called Ritz-matrix. This Ritz-matrix indeed represents $\mathcal{Q}_\mathcal{L}A_{|\mathcal{K}}$ with respect to the basis V: multiplication by V represents a change of basis from $\mathcal{K}$ to the standard basis, this is followed by the transformation A and finally, multiplication by W^H represents projection onto $\mathcal{K}$ along $\mathcal{L}$ with respect to the basis V, since $W^HV = I$.

3.4 A special situation: the right subspace is invariant under A

It is possible that the right subspace $\mathcal{K}$ is chosen such that it is invariant under A. If this is the case, then all approximate eigenpairs found by the projection method are eigenpairs of the original matrix A. If $\mathcal{K}$ is invariant under A, then the Ritz-matrix is equal to A restricted to $\mathcal{K}$, and since the Ritz-matrix then represents exactly the same transformation as A, but with a restricted domain, the eigenpairs found are exact eigenpairs of A. Since $\mathcal{K}$ is invariant, it must be spanned by m of the eigenvectors of A, where m is the dimension of $\mathcal{K}$, these are exactly those eigenvectors which are found by the method, together with the corresponding eigenvalues.

3.5 The usual procedure in practice

The methods desribed above require choices for $\mathcal{K}$ and $\mathcal{L}$, and these choices result in some approximate eigenpairs. In practice, however, the method is used in an iterative way: in each step, the subspaces $\mathcal{K}$ and $\mathcal{L}$ used in the previous step are expanded by one extra dimension, and again the approximate eigenvectors are calculated. This procedure is repeated until a satisfactory result is obtained. If too many iteration steps are required, the process is restarted with a new starting choice for the left and right subspaces.

The most popular projection methods use Krylov subspaces as their left and right subspaces. These methods are described in the following section

3.6 Examples of projection methods: Krylov-based methods.

In this section we take a closer look at the most important examples of projection methods: the Arnoldi method (an orthogonal projection method) and the Bi-Lanczos method (an oblique projection method), which in the case of a Hermitian matrix both degenerate to the well-known Lanczos method. Only the the most important properties of each method are given; the following chapter will treat the Arnoldi and Lanczos methods extensively.

In this section, $\mathcal{K}_m(A, v)$ denotes the m-th Krylov subspace generated by the matrix A and the vector v: $\mathcal{K}_m(A, v) = \text{span}\{v, Av, A^2v, \ldots, A^{m-1}v\}$. If no ambiguity is possible, then the arguments (A, v) are omitted.

3.6.1 The Arnoldi method

The Arnoldi method is an orthogonal projection method which has the Krylov-space $\mathcal{K}_m(A, v)$ as its right subspace, where the vector v can be any element of $\mathbb{C}^n$. This particular choiche for $\mathcal{K}$ results in a Ritz-matrix that is an $m \times m$ upper-Hessenberg matrix. This is a slight advantage over methods which produce a full Ritz-matrix, since the computation of eigenpairs takes less effort for Hessenberg matrices than for full matrices. Another advantage is given by the fact that storing a Hessenberg matrix requires less memory. However, in comparison with projection methods which result in an even sparser Ritz-matrix, like for example a tri-diagonal matrix, the same arguments result in disadvantages of Arnoldi.

3.6.2 The Bi-Lanczos method

Bi-Lanczos is an example of an oblique projection method. It uses the choices $\mathcal{K} = \mathcal{K}_m(A, v)$ and $\mathcal{L} = \mathcal{K}_m(A^H, w)$, where v and w are elements of $\mathbb{C}^n$ such that $v^H w = 1$. So like Arnoldi, approximate eigenvectors are taken from $\mathcal{K}_m(A, v)$, these approximants are those vectors which result in a residual vector orthogonal to $\mathcal{K}_m(A^H, w)$. This method can be used to approximate the left eigenvectors

as well. Switching the roles of $\mathcal{K}$ and $\mathcal{L}$, which is the same as approximating eigenpairs of A^H, leads to a Ritz-matrix which is the transposed of the original Ritz-matrix. In other words, calculating the left eigenvectors of the Ritz-matrix results in approximations of the left eigenvectors of A. The main advantage of Bi-Lanczos, however, is the sparsity of the resulting Ritz-matrix, which is a tri-diagonal $m \times m$ matrix.

Disadvantages of Bi-Lanczos are possible loss of orthogonality due to the three-term recursion used to compute the entries of the Ritz-matrix and the risks of a breakdown of the algorithm.

3.6.3 The Lanczos method

If A is Hermitian, then both Arnoldi and Bi-Lanczos result in the same symmetric tri-diagonal Ritz-matrix. In this special case, the method is called the Lanczos method.

In order to get a better insight in orthogonal projection methods, the Arnoldi method and its Hermitian version, the Lanczos method, the next chapter extensively treats some of the known properties of these methods.

Chapter 4

Properties of orthogonal projection methods

This chapter gives a summary of the most important porperties of orthogonal projection methods, especially the Arnoldi method and its Hermitian version, the Lanczos method.

4.1 An overview of known convergence properties of orthogonal projection methods

This section gives an indication of the known properties of orthogonal projection methods, for both the non-Hermitian and the Hermitian problem. Of course, everything said for the non-Hermitian case also applies to the Hermitian case.

4.1.1 The non-Hermitian problem

First, it is interesting to note that an orthogonal projection method applied to the matrix A with a right subspace $\mathcal{K}$ which has V as its basis gives the same results as an orthogonal projection method applied to $Q^H AQ$ with a left subspace $\mathcal{K}'$ which has $Q^H V$ as its basis, where Q is a unitary matrix. This observation will be used when analyzing the Arnoldi and Lanczos methods.

Since the approximate eigenvectors are all taken from the subspace $\mathcal{K}$, the best possible approximation, with respect to the two-norm, for an eigenvector u is given by the projection of this eigenvector onto $\mathcal{K}$, which is given by $\mathcal{P}_{\mathcal{K}} u$. Therefore, the quantity $\|(I - \mathcal{P}_{\mathcal{K}})u\|_2$, which is the distance between $\mathcal{K}$ and the eigenvector u, plays an important role in the analysis of projection methods. If this quantity is not small, a good approximation of u is not possible, since $\|\tilde{u} - u\|_2 \geq \|(I - \mathcal{P}_{\mathcal{K}})u\|_2$ for all $\tilde{u} \in \mathcal{K}$. Since the norm of u is assumed to be 1, $\|(I - \mathcal{P}_{\mathcal{K}})u\|_2$ can be seen as the sine of the angle between u and $\mathcal{K}$. This quantity can be used to give the following inequality: the residual norm

of the pair $\lambda, \mathcal{P}_{\mathcal{K}} u$, which are the exact eigenvalue and the corresponding best approximating eigenvector, satisfies for the linear operator $A_p = \mathcal{P}_{\mathcal{K}} A_{|\mathcal{K}}$ (see [1], p.130):

$$\|(A_p - \lambda I)\mathcal{P}_{\mathcal{K}} u\|_2 \leq \gamma \|(I - \mathcal{P}_{\mathcal{K}})u\|_2,$$

with $\gamma = \|\mathcal{P}_{\mathcal{K}} A(I - \mathcal{P}_{\mathcal{K}})\|_2$. The exact eigenpair λ, u satisfies

$$\|(A_p - \lambda I)u\|_2 \leq \sqrt{\lambda^2 + \gamma^2}\|(I - \mathcal{P}_{\mathcal{K}})u\|_2$$

With V the orthogonal matrix which has a basis of $\mathcal{K}$ as its columns and $y_u = V^H u / \|V^H u\|_2$, the first inequality can be rewritten to

$$\|(V^H A V - \lambda I)y_u\|_2 \leq \gamma \frac{\|(I - \mathcal{P}_{\mathcal{K}})u\|_2}{\|\mathcal{P}_{\mathcal{K}} u\|_2} \equiv \gamma \tan\theta(u, \mathcal{K})$$

The parameter $\gamma = \|\mathcal{P}_{\mathcal{K}} A(I - \mathcal{P}_{\mathcal{K}})\|_2$, which appears in the inequalities above, can be seen as a measure of invariance of the subspace $\mathcal{K}$ under the transformation A. If $\gamma = 0$ then the subspace $\mathcal{K}$ is invariant under A, a small value for γ indicates that $\mathcal{K}$ is "almost invariant" under A.

4.1.2 The Hermitian problem

The eigenvalues of a Hermitian matrix A are real and the eigenvectors are an orthogonal basis of $\mathbb{C}^n$. These properties make the Hermitian case much easier to analyse than the non-Hermitian case. Since the eigenvalues are real, it is possible to label them decreasingly, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. This gives the possibility of making quantitative comparisons between exact eigenvalues and approximate eigenvalues, which are real as well.

For the approximate eigenvalues of A, which are the eigenvalues of $\mathcal{P}_{\mathcal{K}} A_{|\mathcal{K}}$, a min-max formulation can be given: the i-th largest approximate eigenvalue of a Hermitian matrix A, obtained from an orthogonal projection onto a subspace $\mathcal{K}$, satisfies

$$\tilde{\lambda}_i = \max_{S \ \mathcal{K}, \dim(S)=i} \min_{x \in S, x \neq 0} \frac{(Ax, x)}{(x, x)},$$

which can be seen as a Courant-Fisher principle restricted to the subspace $\mathcal{K}$. Comparison with the original Courant-Fisher principle results in the following inequality:

$$\lambda_i \geq \tilde{\lambda}_i, \quad i = 1, 2, \ldots, m$$

The Courant characterisation can also be rewritten in a restricted version: the approximate eigenvalue $\tilde{\lambda}_i$ and the corresponding eigenvector $\tilde{u}_i$ are such that

$$\tilde{\lambda}_1 = \frac{(A\tilde{u}_1, \tilde{u}_1)}{(\tilde{u}_1, \tilde{u}_1)} = \max_{x \in \mathcal{K}, x \neq 0} \frac{(Ax, x)}{(x, x)}$$

and for $k > 1$:

$$\tilde{\lambda}_k = \frac{(A\tilde{u}_k, \tilde{u}_k)}{(\tilde{u}_k, \tilde{u}_k)} = \max_{x \in \mathcal{K}, x \neq 0, \tilde{u}_1^H x = \ldots = \tilde{u}_{k-1}^H x = 0} \frac{(Ax, x)}{(x, x)}$$

The approximate eigenvectors give an orthogonal basis of $\mathcal{K}$. Since for Hermitian A the Ritz-matrix is Hermitian as well, these restricted versions of the Courant-Fisher principle and the Courant characterisations are not too surprising. They can be used, however, to give a rather general upper boundary for the difference between an exact and an approximate eigenvalue (see [1],p.135): let $\tilde{Q}_i$ be the sum of the spectral projectors associated with the approximate eigenvalues $\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_{i-1}$, then the error between the i-th exact and approximate eigenvalues λ_i and $\tilde{\lambda}_i$ is such that

$$0 \leq \lambda_i - \tilde{\lambda}_i \leq \|A - \lambda_i I\| \frac{\|\tilde{Q}_i u_i\|_2^2 + \|(I - \mathcal{P}_\mathcal{K}) u_i\|_2^2}{\|(I - \tilde{Q}_i)\mathcal{P}_\mathcal{K} u_i\|_2^2}$$

Unfortunately, this inequality is not of any immediate practical use since it contains many unknown quantities.

It is also possible to give an upperbound for the sine of the angle between the exact eigenvector u and the approximate eigenvector $\tilde{u}$ for the Hermitian case: let $\gamma = \|\mathcal{P}_\mathcal{K} A (I - \mathcal{P}_\mathcal{K})\|_2$, and consider any eigenvalue λ_i of A. Then there is an eigenvector $\tilde{u}$ associated with the approximate eigenvalue $\tilde{\lambda}$ such that

$$\sin\theta(u_i, \tilde{u}) \leq \sqrt{1 + \frac{\gamma^2}{\delta_i^2}} \sin\theta(u_i, \mathcal{K})$$

where δ_i is the distance between λ_i and the set of approximate eigenvalues other than $\tilde{\lambda}$. This shows that in the Hermitian case, a good result is guaranteed if the angle between the exact eigenvector and the subspace $\mathcal{K}$ is sufficiently small.

4.2 Properties of the Arnoldi and Lanczos methods

As mentioned earlier, the choice of a Krylov-subspace as the left subspace for an orthogonal projection method results in a method called the Arnoldi method, or the Lanczos method in the Hermitian case. This section gives some properties which are specific for the Arnoldi and Lanczos methods. First, algorithms for both methods are derived.

4.2.1 An Arnoldi algorithm

As explained in the previous chapter, the Arnoldi method applied to the $n \times n$ matrix A consists of computing the eigenpairs of the Ritz-matrix $A_p = V^H A V$. Here, V satisfies $V^H V = I$ and $\mathcal{R}(V) = \mathcal{K}_m(A, v)$, with v arbitrary. So for given A and v, the product $V^H A V$ needs to be computed. First we will show that A_p is upper-Hessenberg, which simplifies the determination of its coefficients substantially.

Define B to be the $n \times m$ matrix which has $v, Av, \ldots, A^{m-1}v$ as its columns. This matrix B satisfies

$$AB = B \begin{pmatrix} 0 & & & & & & 0 \\ 1 & 0 & & & & & 0 \\ & 1 & \ddots & & & & \vdots \\ & & \ddots & \ddots & & & \vdots \\ & & & \ddots & 0 & & \vdots \\ & & & & 1 & 0 & 0 \\ & & & & & 1 & 0 \end{pmatrix} + A^m v e_m^T$$

Suppose that B has full column-rank, then its QR-factorization exists, say $B = QR$, where Q is $n \times m$ and $Q^H Q = I$ and R is $m \times m$, upper-triangular and non-singular. With this, we have $Q^H AQ = Q^H AQRR^{-1} = Q^H ABR^{-1}$, and with the equality above, this is equal to

$$Q^H AQ = R \begin{pmatrix} 0 & & & & & & \vdots & \\ 1 & 0 & & & & & \vdots & \\ & 1 & \ddots & & & & \vdots & \\ & & \ddots & \ddots & & & R^{-1}Q^H A^m v & \\ & & & \ddots & 0 & & \vdots & \\ & & & & 1 & 0 & \vdots & \\ & & & & & 1 & \vdots & \end{pmatrix} R^{-1}$$

Clearly, this product is upper-Hessenberg and with the choice $V = Q$, $Q^H AQ$ is equal to the Ritz-matrix.

Since we now know that A_p is upper-Hessenberg, it is possible to build the matrix V columnwise and simultaneously compute the entries of A_p, also columnwise. Suppose that we have found the first i columns of V, then all we have to do is compute Av_i and orthogonalise it to $v_1, \ldots, v_i$, and after that normalize the resulting vector. This is achieved by the following algorithm:

Choose a starting vector v_1 of norm 1
for $j = 1, 2, \ldots, m$ do
begin
  for $i = 1, 2, \ldots, j$ do
    $h_{ij} = (Av_j, v_i)$
  $w_j = Av_j - \sum_{i=1}^{j} h_{ij} v_i$
  $h_{j+1,j} = \|w_j\|_2$

$v_{j+1} = w_j / h_{j+1,j}$

end

The coefficients h_{ij} resulting from this algorithm satisfy

$$Av_j = \sum_{i=1}^{j+1} h_{ij} v_i$$

When the h_{ij} are written as the entries of the matrix H, then this equation is exactly the column-wise version of an equation of the form $AV = VH + C$ where the columns of C are orthogonal to those of V. Pre-multiplying this equation by V^H shows that the matrix H satisfies $V^H AV = H$, in other words, H is equal to the matrix A_p which we were looking for.

From this algorithm we see that we need not only store all the coefficients h_{ij}, but also all of the vectors v_i. In some cases this can require a huge amount of memory.

4.2.2 A Lanczos algorithm

If A is Hermitian, the Arnoldi algorithm substantially simplifies. This is due to the fact that the Ritz-matrix is then upper-Hessenberg and Hermitian and therefore tridiagonal. Translated to the Arnoldi algorithm, this means that $h_{ij} = 0$ for $i \neq j-1, i \neq j, i \neq j+1$ and the Gram-Schmidt process turns into a three-term recursion. Using the notation $\alpha_j = h_{jj}$ and $\beta_j = h_{j-1,j}$ the algorithm becomes

Choose a starting vector v_1 of norm 1.
Set $\beta_1 = 0, v_0 = 0$
for $j = 1, 2, \ldots, m$ do
begin
$w_j = Av_j - \beta_j v_{j-1}$
$\alpha_j = (w_j, v_j)$
$w_j = w_j - \alpha_j v_j$
$\beta_{j+1} = \|w_j\|_2$
$v_{j+1} = w_j / \beta_{j+1}$
end

Both the number of entries in the Ritz-matrix and the number of vectors which have to be stored is considerably less than in the non-Hermitian case.

4.2.3 Changes of basis and convergence speed

A special property of the Krylov-subspace $\mathcal{K}_m(A, v)$ is the fact that $\mathcal{K}_m(A, v) = \mathcal{K}_m(A - \alpha I, v)$. The approximate eigenvalues of A are the exact eigenvalues

of $V^H AV$, the approximate eigenvalues of $A - \alpha I$ are the exact eigenvalues of $V^H(A - \alpha I)V = V^H AV - \alpha V^H IV = V^H AV - \alpha I$,where the columns of V are an orthonormal basis of $\mathcal{K}_m(A, v)$. From this, we see that the approximate eigenvalues $\hat{\lambda}_i$ of $A - \alpha I$ are equal to $\tilde{\lambda}_i - \alpha$. So a translation of origin does not change the rate of convergence of the method, it is shift invariant. Therefore, only gaps between eigenvalues seem to influence the rate of convergence. Since we also have $\mathcal{K}_m(A, v) = \mathcal{K}_m(\alpha A, v)$, multiplication of A by a scalar α results in multiplication of the approximate eigenvalues by α, so a scaling of the problem does not affect the rate of convergence. Therefore, not the gaps between the eigenvalues determine the rate of convergence, but the ratios of the gaps between the eigenvalues.

4.2.4 A closer look at the Ritz-matrix

As explained earlier, the Ritz-matrix, for the Arnoldi method applied to A, represents the transformation A restricted to the subspace $\mathcal{K}$, followed by the projection onto $\mathcal{K}$, all of this expressed in a basis of $\mathcal{K}$. Since a change of basis does not affect the eigenvalues of a matrix, the Ritz values are equal to the eigenvalues of the Ritz matrix expressed with respect to a basis of $\mathcal{K}$. If we choose the basis $v, Av, \ldots, A^{m-1}v$, the Ritz matrix can be expressed as follows:

$$A'_p = \begin{pmatrix} 0 & & & & & & \alpha_0 \\ 1 & 0 & & & & & \alpha_1 \\ & 1 & \ddots & & & & \vdots \\ & & \ddots & \ddots & & & \vdots \\ & & & \ddots & 0 & & \vdots \\ & & & & 1 & 0 & \alpha_{m-2} \\ & & & & & 1 & \alpha_{m-1} \end{pmatrix}$$

The last column in A'_p represents the orthogonal projection of $A^m v$ onto the Krylov subspace, expressed in terms of the basis $\{v, Av, \ldots, A^{m-1}v\}$. So $\mathcal{P}_{\mathcal{K}} A^m v = \alpha_0 + \alpha_1 v + \ldots + \alpha_{m-1} A^{m-1} v$. This means that $\alpha_0 v + \alpha_1 Av + \ldots + \alpha_{m-1} A^{m-1} v$ is the best possible approximation for $A^m v$ taken from the Krylov subspace $\text{span}\{v, Av, \ldots, A^{m-1}v\}$. Since this Krylov subspace can also be defined as the set of all vectors $p(A)v$ where $p(A)$ is any polynomial of degree $\leq m-1$, we see that $\alpha_0 + \alpha_1 v + \ldots + \alpha_{m-1} A^{m-1} v - A^m v$ is the unique monic polynomial of degree m which has a minimum norm over all monic polynomials of degree m.

Taking a closer look at A'_p, however, we see that it is of a companion form, which means that its characteristic polynomial equals $p_c(z) = \alpha_0 + \alpha_1 z + \ldots + \alpha_{m-1} z^{m-1} - z^m$. For $p_c(A)v$ we have $p_c(A)v = \alpha_0 v + \alpha_1 Av + \ldots + \alpha_{m-1} A^{m-1} v - A^m v$. We have just mentioned that this is the unic monic polynomial of degree m which has a minimum norm over all monic polynomials of degree m and therefore we can conclude that the characteristic polynomial p_c of the Ritz matrix minimizes $\|p(A)v\|$ over all monic polynomials of degree m. Some consequences of this conclusion are given in the following section.

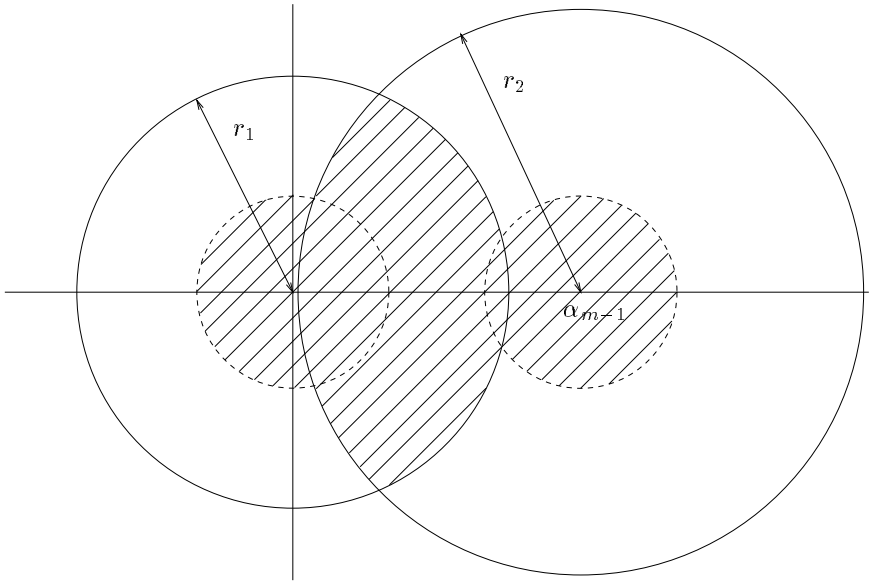

Figure 4.1: An example of the Gershgorin-circles. The Ritz-values are in the shaded area. The dashed circles have unit radius. As explained in the text, $r_1 = \max\{1 + \max_{1 \leq i \leq m-2} |\alpha_i|, |\alpha_0|\}$ and $r_2 = \sum_{k=0}^{k=m-2} |\alpha_k|$

Applying the Gershgorin theorem to the matrices A'_p and $(A'_p)^T$ results in a region in which the Ritz-values can be found. First, looking at A'_p, we see that all Ritz-values are situated in the union of the unit circle in the complex plane which has α_{m-1} as its center and the circle which has the origin as its center and a radius equal to $\max\{1+\max_{1 \leq i \leq m-2} |\alpha_i|, |\alpha_0|\}$. If these two circles are disjunct, then exactly one Ritz-value is situated in the unit circle around α_{m-1}, the others are in the other circle. Gershgorin applied to $(A'_p)^T$ shows that all Ritz-values are situated in the union of the unit circle around the origin and the circle which has α_{m-1} as its center and $\sum_{k=0}^{k=m-2} |\alpha_k|$ as its radius. If these to circles are disjunct, then one of the Ritz-values is situated in the circle around α_{m-1} and the others all lie in the unit circle around the origin. Finally, the intersection of these two unions (this is the intersection of the union of two circles) gives an area which encloses all Ritz-values. An example is visualized in figure 4.1.

4.2.5 The methods as a polynomial approximation problem

As explained in the prevoius section, the Arnoldi method can be formulated in a different way: if $\hat{p}_m$ is the characteristic polynomial of the Ritz-matrix when an orthogonal projection method onto a Krylov subspace is applied to A then $\hat{p}_m$ minimizes the norm $\|p(A)v\|_2$ over all monic polynomials of degree m. In other

words, the Arnoldi method solves the problem of finding the best approximation for $A^m v$ in the subspace $\text{span}\{v, Av, \ldots, A^{m-1}v\}$.

This section gives a selection of the results of the different formulation of the Krylov subspace, these are taken from [1], section 4.7.

Let P_i be the spectral projector associated with the eigenvalue λ_i (see section 2.6) for Hermitian A. Then, if $P_i v_i \neq 0$, we have

$$\tan\theta(u_i, \mathcal{K}_m) = \min_{p \in \mathbb{P}_{m-1}, p(\lambda_i)=1} \|p(A)y_i\|_2 \tan\theta(u_i, v)$$

in which $\mathbb{P}_{m-1}$ represents the set of polynomials of degree $\leq m-1$ and

$$y_i = \begin{cases} \dfrac{(I-P_i)v}{\|(I-P_i)v\|_2} & \text{if } (I-P_i)v \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

With the Chebyshev polynomials of the first kind, written as C_k for the Chebyshev polynomial of degree k, this minimization property results in the following inequality:

$$\tan\theta(u_i, \mathcal{K}_m) \leq \frac{\kappa_i}{C_{m-i}(1+2\gamma_i)} \tan\theta(u_i, v),$$

where

$$\kappa_1 = 1, \qquad \kappa_i = \prod_{j=1}^{i-1} \frac{\lambda_j - \lambda_n}{\lambda_j - \lambda_i} \quad \text{for } i > 1$$

and

$$\gamma_i = \frac{\lambda_i - \lambda_{i+1}}{\lambda_{i+1} - \lambda_n}$$

A two-sided inequality for the difference between the i-th exact and the approximate eigenvalues is given by

$$0 \leq \lambda_i - \lambda_i^{(m)} \leq (\lambda_1 - \lambda_n)\Big(\frac{\kappa_i^{(m)} \tan\theta(u_i, v)}{C_{m-i}(1+2\gamma_i)}\Big)^2$$

where

$$\kappa_1^{(m)} \equiv 1, \qquad \kappa_i^{(m)} = \prod_{j-1}^{i-1} \frac{\lambda_j^{(m)} - \lambda_n}{\lambda_j^{(m)} - \lambda_i}, \quad \text{for } i > 1$$

and γ_i is given in the previous result.

For the sine of the angle between the i-th exact and approximate eigenvector the following inequality holds:

$$\sin\theta(u_i, \tilde{u}_i) \leq \frac{\kappa_i \sqrt{1 + \beta_{m+1}^2/\delta_i^2}}{C_{m-i}(1+2\gamma_i)} \tan\theta(u_i, v)$$

For Arnoldi, the following inequality is the most important result of convergence analysis: assume that A is diagonalizable and that the initial vector v in

Arnoldi's method has the expansion $v = \sum_{k=1}^{k=n} \alpha_k u_k$ with respect to the eigenbasis $\{u_1, \ldots, u_n\}$ in which $\|u_k\|_2 = 1$ and $\alpha_i \neq 0$. Then the following inequality holds:

$$\|(I - \mathcal{P}_m)u_i\|_2 \leq \xi_i \varepsilon_i^{(m)}$$

where

$$\xi_i = \sum_{k=1, k\neq i}^{n} \frac{|\alpha_j|}{|\alpha_i|}$$

Here, $\varepsilon_i^{(m)}$ is defined by

$$\varepsilon_i^{(m)} \equiv \min_{p \in \mathbb{P}^*_{m-1,i}} \max_{\lambda \in \sigma(A) - \lambda_i} |p(\lambda)|,$$

where $\mathbb{P}^*_{m-1,i}$ represents the set of all polynomials of degree not exceeding $m-1$ such that $p(\lambda_i) = 0$.

The quantity ε_i is an important parameter in this inequality. For ε_1, it is known that if $m < n$, then there exist m eigenvalues of A which can be labeled $\lambda_2, \lambda_3, \ldots, \lambda_{m+1}$ such that

$$\varepsilon_1^{(m)} = \Big(\sum_{j=2}^{m+1} \prod_{k=2, k\neq j}^{m+1} \frac{|\lambda_k - \lambda_1|}{|\lambda_k - \lambda_j|} \Big)^{-1}$$

4.2.6 Ideal Arnoldi

The polynomial interpretation as given in section 4.2.4 implies that the Arnoldi method solves the problem of finding the best approximation for $A^m v$ in the subspace $\text{span}\{v, Av, \ldots, A^{m-1}v\}$. Intuitively, this is not the most natural minimisation problem for approximation of the eigenvalues. The exact characteristic polynomial p_c of A satisfies $p_c(A) = 0$ and therefore a better approximating problem might be given by minimizing $\|p(A)\|$ over all monic polynomials of degree m and then finding the roots of that polynomial. This method, however, is useful for theoretical purposes only. It is proposed by Greenbaum and Trefethen in [3], they have given it the name "ideal Arnoldi". Ideal Arnoldi consists of finding the best approximation for A^n in the linear span of $I, A, \ldots, A^{n-1}$.

Chapter 5

Open questions

Many questions about the behaviour of both the Arnoldi and Lanczos methods are still unanswered. The aim of this chapter is to give a selection of these questions, especially those concerning the Arnoldi methods, and to give an impression of further work that could be done.

5.1 A list of open questions

- Is it possible to extend the convergence analysis from the previous chapter to a somewhat more practical convergence analysis?
- If an approximate eigenpair $\tilde{\lambda}, \tilde{u}$ is found, what can be said about the error in this approximation? In the chapter about linear algebra basics, we have seen that if A is diagonalisable, with X the eigenvector matrix, then there exists an eigenvalue λ of A such that $|\lambda - \tilde{\lambda}| \leq \|X\|_2 \|X^{-1}\|_2 \|r\|$. Assumed that nothing about X is known, is it possible to approximate the condition of X by using the approximate eigenvectors? What can be said about the average quality of this approximation if the starting vector is chosen randomly?
- How does the starting vector v affect the results given by the methods? If we see the starting vector $v \in \mathbb{C}^n$ as an input parameter for the Arnoldi method and a vector $l \in \mathbb{C}^m$ which contains the m approximating eigenvalues, as output, then the method can be seen as a continuous, non-linear mapping from $\mathbb{C}^n$ to $\mathbb{C}^m$. A simple dimension argument shows that there must be many starting vectors v which result in exactly the same m Ritz-values, for a certain m. Scaling the vector v, for example , does not affect the results at all. What can be concluded about these observations? Analogously, what can be said about pairs A, v which give the same results? Is it possible to make choices which result in exactly the same results for all iteration steps?

- It might be interesting to study the convergence behaviour of certain matrices with a special eigenvalue distribution. Examples are matrices with no complex eigenvalues or with only one pair of complex eigenvalues. What can be said about convergence behaviour for these simplified cases?
- For ideal Arnoldi (see [3]) Greenbaum and Trefethen have given five open questions which might give more insight in the usual Arnoldi methods as well.

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