Chapter XI

# Polynomial and Constrained Eigenproblems

## 55 Introduction

In theory and practical applications one may encounter eigenproblems that are more complicated than the standard and generalized eigenproblems discussed in previous chapters. In this chapter we will discuss a particular class of eigenproblems: polynomial eigenproblems, with focus on the quadratic case. Furthermore, we will discuss briefly a so-called *constrained* eigenproblem.

In Section 56 we will pay attention to the important class of quadratic eigenproblems, with a small sidestep to higher order polynomial eigenproblems. These quadratic eigenproblems are of the form

$$(\lambda^2 M + \lambda C + K)x = 0, \tag{55.1}$$

where $M$, $C$, and $K$ are given square matrices of order $n$. Solutions $\lambda, x$, with $\lambda$ a scalar and $x \neq 0$ an $n$-vector, are the eigenvalues and eigenvectors of the given problem.

There are three basic approaches for the solution of a quadratic eigenproblem:

- Rewrite the problem as a generalized eigenvalue problem of order $2n$, see Section 56. A drawback of this approach is that the dimension of the problem is doubled, which may complicate things if $n$ is not small.
- For larger values of $n$, the problem (55.1) can first be reduced to a low-dimensional problem of the form

  $$(\theta^2 Q^* M P + \theta Q^* C P + Q^* K P)z = 0,$$

  for properly defined $n$ by $m$ matrices $Q$ and $P$. The trick is to select and expand these projection matrices so that the eigenpairs $\theta, Pz$ form good approximations to desired eigenpairs of the original problem. This approach has its own problems, for instance, a wrong selection of $\theta$ and $z$ may lead to misconvergence. The low-dimensional problem may be solved by Newton's method.

- Treat (55.1) directly as a nonlinear equation and apply, for instance, Newton's method for its solution. Potential danger here are slow convergence, or convergence to undesired eigenpairs. This makes this approach feasable for relatively small $n$ only, but it can be combined with the dimension reduction technique.

## 56 Quadratic eigenvalue problems

**Introduction** In this section, we consider the quadratic eigenvalue problem (QEP) of the form

$$(\lambda^2 M + \lambda C + K)x = 0 \quad \text{and} \quad y^*(\lambda^2 M + \lambda C + K) = 0, \tag{56.1}$$

where $M, K$ and $C$ are given matrices of size $n \times n$. The nontrivial $n$-vectors $x$, $y$, and the corresponding scalars $\lambda$ are the right, left eigenvectors, and eigenvalues, respectively.

The matrix-function $L(\lambda) := \lambda^2 M + \lambda C + K$ is a special case of a matrix polynomial, or a $\lambda$-matrix, see, for example, GANTMACHER [1959], LANCASTER [1969]. In this case, it is a $\lambda$-matrix of degree 2. The matrix-function $L(\lambda)$ is said to be *regular* if $\det(L(\lambda))$ is not identical to zero for all $\lambda$. Otherwise, it is called *singular*.

An important special case of the quadratic eigenvalue problem is when

$$M^* = M > 0, \quad C^* = C \quad \text{and} \quad K^* = K > 0. \tag{56.2}$$

These matrices are sometimes called mass, damping and stiffness matrices, respectively, referring to their origin in mechanical engineering models, see, for instance, DUFFIN [1955].

One of the factors that makes the QEP different from standard eigenproblems $Ax = \lambda x$, or generalized eigenproblems $Ax = \lambda Bx$, is that there are $2n$ eigenvalues for QEP, with at most $2n$ right (and left) eigenvectors. Of course, in an $n$-dimensional space the right (and left) eigenvectors do no longer form an independent set. This is illustrated by the following simple example, in which we have taken some of the matrices as unsymmetric, in order to make some phenomena more clearly visible. The triplet

$$M = \begin{pmatrix} 5 & 2 \\ 1 & 4 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & 1 \\ 0 & 7 \end{pmatrix}, \quad K = \begin{pmatrix} 2 & 0 \\ 0 & 12 \end{pmatrix}.$$

has 4 different (but pairwise conjugate) eigenvalues (rounded to 5 decimals):

$$\lambda_1 = -0.9396 + 1.5749\imath, \quad \lambda_2 = -0.9396 - 1.5749\imath,$$
$$\lambda_3 = -0.0049 + 0.6296\imath, \quad \lambda_4 = -0.0049 - 0.6296\imath.$$

The associated eigenvectors (normalized so that the first coordinate is equal to one) are:

$$x_1 = (1, -2.4756 - 0.9779\imath)^T, \quad x_2 = (1, -2.4756 + 0.9779\imath)^T,$$
$$x_3 = (1,\ 0.0326 - 0.0132\imath)^T, \quad x_4 = (1,\ 0.0326 + 0.0132\imath)^T.$$

The four eigenvectors are obviously dependent, but, in actual problems, each of them may represent a relevant state of the system.

One has to be careful with Rayleigh quotients for quadratic eigenproblems. Indeed, given $x$ as a right eigenvector for the QEP (56.1), i.e.,

$$(\lambda^2 M + \lambda C + K)x = 0,$$

one can form a *quadratic Rayleigh quotient*:

$$\lambda^2(x^* M x) + \lambda(x^* C x) + (x^* K x) = 0. \qquad (56.3)$$

However, this equation has two roots, and one of the roots is an eigenvalue, the other root may be a spurious one. For instance, if we compute the quadratic Rayleigh quotient for our example, with $(\lambda_1, x_1)$, then clearly, the pair $(\lambda_1, x_1)$ satisfies equation (56.3). If we solve equation (56.3), then we find the two roots $\mu_1 = -0.9396 + 1.5749\imath$, $\mu_2 = -0.8776 - 1.6057\imath$. We see that $\lambda_1$ is recovered (by $\mu_1$), the other root has no meaning for the given QEP.

In an effort to decide which of the two is the desired one and which is the spurious one, one could compute the residual vector

$$r_\mu := (\mu^2 M + \mu C + K)x_1,$$

and this leads to $\|r_{\mu_1}\|_2 \approx 8.4 \times 10^{-14}$, $\|r_{\mu_2}\|_2 \approx 12.5$, which, in this case, clearly indicates that $\mu_2$ is not an eigenvalue. We can not exclude that in contrived examples, one might make a wrong choice, which may lead to a delay in a specific iterative solution method.

For more general matrices, we can have defectiveness, as for the standard eigenproblems, which means that there is not necessarily a complete set of eigenvectors. In the next section, we will relate the QEP to a generalized standard problem, which helps to shed more light on this matter.

**Reduction to Linear Form** It is easy to see that the QEP in (56.1) is equivalent to the following generalized "linear" eigenvalue problem:

$$Az = \lambda Bz \quad \text{and} \quad w^* A = \lambda w^* B \tag{56.4}$$

where

$$A = \begin{pmatrix} 0 & I \\ -K & -C \end{pmatrix}, \quad B = \begin{pmatrix} I & 0 \\ 0 & M \end{pmatrix} \tag{56.5}$$

and

$$z = \begin{pmatrix} x \\ \lambda x \end{pmatrix}, \quad w = \begin{pmatrix} (\lambda M + C)^* y \\ y \end{pmatrix}. \tag{56.6}$$

The generalized eigenvalue problem (56.4) is commonly called the linearization of the QEP (56.1). It can be shown that for any matrices $A$ and $B$ of the above forms, the right and left eigenvectors $z$ and $w$ have the structures described in (56.6).

From the factorization

$$A - \lambda B = \begin{pmatrix} 0 & I \\ -I & -\lambda M - C \end{pmatrix} \begin{pmatrix} \lambda^2 M + \lambda C + K & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -\lambda I & I \end{pmatrix}, \tag{56.7}$$

it follows that the pencil $A - \lambda B$ is *equivalent* to the matrix

$$\begin{pmatrix} \lambda^2 M + \lambda C + K & 0 \\ 0 & I \end{pmatrix} \tag{56.8}$$

and

$$\det(A - \lambda B) = \det(\lambda^2 M + \lambda C + K),$$

This means that the eigenvalues of the original QEP (56.1) coincide with the eigenvalues of the generalized eigenvalue problem (56.4). Furthermore, we have

- $L(\lambda)$ is regular if and only if $A - \lambda B$ is regular.
- If $M$ (hence $B$) is nonsingular, then $L(\lambda)$ is regular.
- If $K$ (hence $A$) is nonsingular, then $L(\lambda)$ is regular.

For theory on regular pencils $(A, B)$, see for instance Stewart and Sun [1990, Chapter VI]. We will assume that $M$ is nonsingular throughout this section.

A disadvantage of the above reduction to generalized form is that if the matrices $M$, $C$ and $K$ are all Hermitian, then this is not reflected in the reduced form (56.5), where $A$ is non-Hermitian. This can be repaired as follows.

In fact, the matrix pair $(A, B)$ in (56.4) can be chosen in a more general form

$$A = \begin{pmatrix} 0 & W \\ -K & -C \end{pmatrix}, \quad B = \begin{pmatrix} W & 0 \\ 0 & M \end{pmatrix},$$

where $W$ can be any arbitrary nonsingular matrix. Note that now the matrix pencil $A - \lambda B$ is equivalent to the matrix polynomial (56.8) if and only if $W$ is nonsingular, and because of (56.7)

$$\det(A - \lambda B) = \det(W) \cdot \det(\lambda^2 M + \lambda C + K).$$

For example, if the matrices $M$, $K$ and $C$ are all Hermitian, as in the special case (56.2), and $K$ is nonsingular, then we may choose $W = -K$, which leads to the following symmetric generalized "linear" eigenvalue problem

$$Az = \lambda Bz \quad \text{and} \quad w^* A = \lambda w^* B \tag{56.9}$$

where

$$A = \begin{pmatrix} 0 & -K \\ -K & -C \end{pmatrix}, \quad B = \begin{pmatrix} -K & 0 \\ 0 & M \end{pmatrix}, \tag{56.10}$$

and

$$z = \begin{pmatrix} x \\ \lambda x \end{pmatrix}, \quad w = \begin{pmatrix} y \\ \bar{\lambda} y \end{pmatrix}. \tag{56.11}$$

Both $A$ and $B$ are Hermitian, but may be indefinite.

The linearized problems can be treated with techniques that we have discussed in Chapter X. For more sophisticated reduction techniques for the quadratic eigenproblem, see Bai *et al* [2000].

## 57 Higher order polynomial eigenvalue problems

Some applications lead to higher order polynomial problems

$$\Psi(\lambda)x = 0 \qquad y^* \Psi(\lambda) = 0, \tag{57.1}$$

where

$$\Psi(\lambda) := \lambda^\ell C_\ell + \lambda^{\ell-1} C_{\ell-1} + \ldots + \lambda C_1 + C_0,$$

in which the $C_j$ are $n$ by $n$ matrices. In order to make this problem well defined, these matrices have to satisfy certain properties, in particular $C_\ell$

should be nonsingular. Similar to the quadratic problem, these problems can also be linearized to

$$Az = \lambda Bz,$$

where

$$A := \begin{bmatrix} 0 & I & 0 & \cdots & 0 \\ 0 & 0 & I & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & I \\ -C_0 & -C_1 & -C_2 & \cdots & -C_{\ell-1} \end{bmatrix},$$

$$B := \begin{bmatrix} I & & & & \\ & I & & & \\ & & \ddots & & \\ & & & I & \\ & & & & C_\ell \end{bmatrix}.$$

The relation between $x$ and $z$ is given by $z = (x^T, \lambda x^T, \ldots, \lambda^{\ell-1} x^T)^T$. The generalized eigenproblem $Az = \lambda Bz$ can be solved with one of the methods discussed in Chapter X. A disadvantage of this approach is that one has to work with larger matrices of order $n \times \ell$, and these matrices have, of course, also $n \times \ell$ eigenpairs. This implies that one has to check which of the computed eigenpairs satisfies the original polynomial equation.

Ruhe [1973] (see also Davis [1981]) discusses methods that handle directly the problem (57.1), for instance, with Newton's method. For larger values of $n$ one may expect all sorts of problems with the convergence of these techniques (Ruhe's examples are rather small). In Section 57, we will discuss a method that can be used to attack problems with large $n$. In that approach, one first projects the given problem (57.1) onto a low dimensional subspace, and obtains a similar problem of low dimension. This low dimensional polynomial eigenproblem can then be solved with one of the approaches mentioned above. Heeg [1998] has solved a fourth-order polynomial problem successfully with this reduction technique.

**The Jacobi-Davidson method** The possible disadvantage of the linearized approach is the doubling of the dimension of the problems, that is a problem with $n$-dimensional matrices $M$, $C$, and $K$, is transformed to a generalized problem with $2n$-dimensional matrices $A$ and $B$. This is avoided in the Jacobi-Davidson method to be discussed in this section. In this method, the QEP is first projected onto a low-dimensional subspace, which leads to a QEP of modest dimension. This low-dimensional projected QEP can be solved with any method of choice. Expansion of the subspace is realized by a Jacobi-Davidson correction equation. For polynomial eigenproblems this technique was first suggested and discussed in SLEIJPEN, BOOTEN *et al* [1996, Section 8].

As we will see below, this method can also be applied directly to polynomial eigenproblems

$$(C_0 + \lambda C_1 + \ldots + \lambda^{\ell} C_{\ell})x = 0, \qquad (57.2)$$

where $C_i$ for $i = 0, 1, \ldots, \ell$, are given $n \times n$ matrices, and no transformation to a generalized "linear" eigenvalue problem will be required. For simplicity, we will only present the case for $\ell = 2$.

In the first part of a Jacobi-Davidson iteration step, for solving the polynomial eigenproblem

$$\Psi(\lambda)x = 0 \qquad (57.3)$$

where

$$\Psi(\lambda) := C_0 + \lambda C_1 + \lambda^2 C_2, \qquad (57.4)$$

the projected polynomial problem

$$(V^* C_0 V + \theta V^* C_1 V + \theta^2 V^* C_2 V)s = 0 \qquad (57.5)$$

is solved. The columns $v_i$ of the $n \times m$ matrix $V$ form a basis for the search subspace. For stability reasons, the columns are constructed to be orthonormal. The projected problem has the same order as the original one, but is of much smaller dimension, typically $m \ll n$. We will assume that the solution vectors $s$ are normalized, $\|s\|_2 = 1$. First, a Ritz value $\theta$ with some desired properties, such as having the largest real part or being closest to some target $\tau$, and its associated eigenvector $s$, are selected. Then the Ritz vector $u := Vs$ and the residual $r := \Psi(\theta)u$ are computed. For expansion of the search space the vector $p$,

$$p := \Psi'(\theta)u$$

with

$$\Psi'(\theta) = C_1 + 2\theta C_2,$$

is also computed. For a motivation of this choice, see SLEIJPEN, BOOTEN *et al* [1996, Section 8].

In the second part of the Jacobi-Davidson iteration step, the search subspace $\mathrm{span}(V)$ is expanded by a vector $t \perp u$ that solves (approximately) the correction equation

$$\left(I - \frac{p\,u^*}{u^*p}\right) \Psi(\theta)\,(I - u\,u^*)\,t = -r. \tag{57.6}$$

The next column of $V$ is obtained by orthonormalizing the approximate solution against the previously computed columns $v_1, \ldots, v_m$.

This process is repeated until an eigenpair $(\lambda, x)$ has been detected, that is until the residual vector $r$ is sufficiently small. The basic form the algorithm is presented in Algorithm 40. We refer to SLEIJPEN, VAN DER VORST and VAN GIJZEN [1996], for an example of a quadratic eigenvalue problem arising from an acoustic problem, that has been solved with this reduction technique, for $n$ up to $250,000$.

(1) Choose an $n \times m$ orthonormal matrix $V$.
(2) **For** $i = 0, 1, 2$
    compute $W_i = C_i V$ and $M_i = V^* W_i$.
(3) Iterate until convergence
(4)     Compute the eigenpairs $(\theta, s)$ of
        $(M_0 + \theta M_1 + \theta^2 M_2)\,s = 0$.
(5)     Select the desired eigenpair $(\theta, s)$ with $\|s\|_2 = 1$.
(6)     Compute $u = Vs$, $p = \Psi'(\theta)u$, $r = \Psi(\theta)u$.
(7)     **If** $(\|r\|_2 < \epsilon)$, $\lambda = \theta$, $x = u$, STOP.
(8)     Solve (approximately) a $t \perp u$ from
        $\left(I - \frac{p\,u^*}{u^*p}\right) \Psi(\theta)\,(I - u\,u^*)\,t = -r$
(9)     Orthogonalize $t$ against $V$, $v = t/\|t\|_2$.
        **For** $i = 0, 1, 2$
          compute $w_i = C_i v$
          $M_i = \begin{pmatrix} M_i & V^* w_i \\ v^* W_i & v^* w_i \end{pmatrix}$, $W_i = [W_i, w_i]$
(10)    Expand $V = [V, v]$.

Figure 40: JD for quadratic eigenproblems

If the dimension of the search subspace becomes too large, if the number of columns of $V$ is equal to, say, $m = m_{\max}$, then the process can be continued with a search subspace of smaller dimension. Take for the new search subspace the space spanned by the best $m_{\min}$ Ritz pairs from the last step, that is, take $V = [u_1, \ldots, u_{m_{\min}}]$, where $u_1, \ldots, u_{m_{\min}}$ are the Ritz vectors associated with the best available $m_{\min}$ Ritz values $\theta_1, \ldots, \theta_{m_{\min}}$. Then apply modified Gram-Schmidt to orthonormalize $V$ and restart with this matrix. Note that the new search matrix $V = V_{m_{\min}}$ can be expressed in terms of the old search matrix $V = V_{m_{\max}}$ as $V_{m_{\min}} = V_{m_{\max}} T$ for some $m_{\max} \times m_{\min}$ matrix $T$. The transformation matrix $T$ can explicitly be computed, and can be used to update the auxiliary matrices $W_i$ $(= W_i T)$ and $M_i$ $(= T^* M_i T)$.

Eigenvectors that already have been detected can be kept in the search subspace (explicit deflation), if more eigenvectors are wanted. Keeping the eigenvectors in the search subspace prevents the process from reconstruction known eigenvectors.

In Sections 46 and 53, we suggested to use "implicit" deflation, since that approach is based on Schur forms and this is more stable, with better conditioned correction equations. However, in this general polynomial setting, it is not clear how to incorporate implicit deflation: the Schur form and the generalized Schur form can not easily be generalized.

**Additional references** Besides the methods discussed in this chapter, some alternative methods are available in literature, see for example LANCASTER [1969], KUBLANOVSKAJA [1970], RUHE [1973], DAVIS [1981], and GUO, LIN and WANG [1995]. Most of these methods are variants of Newton's method. They generally have good local convergence properties, and find one eigenpair at time. In GUO, LIN and WANG [1995], a proper deflation technique is presented for finding more than one eigenpair. MEERBERGEN [1999] discusses the problem of deflation and restart for projection methods for the quadratic eigenproblem, in particular with the Jacobi-Davidson method.

Recently, a backward error analysis of the quadratic eigenvalue problems, and higher degree polynomial eigenvalue problems is presented in TISSEUR [1998]. In SUN [1999], a perturbation analysis of the quadratic eigenvalue problem (56.2) is presented.

# 58 Constrained eigenproblems

In optimization problems, or in studying stability associated with Stokes problems, one may come accross so-called *constrained eigenproblems*. An example of this is the problem

$$Ax = \lambda Bx, \quad \text{with} \quad C^* x = 0, \tag{58.1}$$

where $A, B \in \mathbb{C}^{n\times n}$, and $C \in \mathbb{C}^{n\times k}$. In typical situations one has that $k \ll n$. The matrix $C$ represents the constraints on $x$.

Of course, under these constraints, it is very unlikely that (58.1) has an exact solution. This would only be the case if $C$ is orthogonal to an invariant subspace of $Ax = \lambda Bx$. In order to find meaningful solutions for the case where $C$ is not orthogonal to the invariant subspace of interest (that is the subspace to which the $x$ for the $\lambda$ of interest belongs), we reformulate the problem to a well-defined extended problem

$$\begin{bmatrix} A & C \\ C^* & 0 \end{bmatrix} \begin{bmatrix} x \\ p \end{bmatrix} = \lambda \begin{bmatrix} B & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ p \end{bmatrix}, \tag{58.2}$$

or

$$\begin{bmatrix} A - \lambda B & C \\ C^* & 0 \end{bmatrix} \begin{bmatrix} x \\ p \end{bmatrix} = 0. \tag{58.3}$$

The solutions of this system satisfy $C^* x = 0$, and therefore we consider the projector $P$ onto the orthogonal complement $C^\perp$:

$$P := I - C(C^* C)^{-1} C^*.$$

This fits in a straight forward manner in the Jacobi-Davidson framework, that is we may apply the Jacobi-Davidson approach for the problem

$$P^*(A - \lambda B)Px = 0.$$

As in the case of deflated Jacobi-Davidson, see Chapter 46, it is computationally more efficient to make a $QR$ decomposition of $C$:

$$C = QR,$$

where $Q \in \mathbb{C}^{n\times k}$ is unitary, and $R \in \mathbb{C}^{k\times k}$ is an upper triangular matrix. This leads to

$$P = I - QQ^*.$$

Chapter XII

# Related Issues

## 59 Sensitivity of Eigenproblems

Eigenvalues are used as a source of information on stability or convergence problems, and the question arises how valid the information of the mere values is. Many authors have studied the problem of sensitivity of the eigenvalues with respect to perturbations, see for instance Wilkinson [1965], Stewart and Sun [1990], and Chatelin [1988]. These studies are usually related to perturbations caused by rounding errors, and not so much by the relevance of the eigenvalues due to the particular representation of a given problem, for instance the choice of basis.

Around 1987, Trefethen and Trummer [1987] started to emphasize this aspect of eigencomputations, and he propagated the idea of inspecting the pseudospectra of a matrix as a relatively simple means for getting an idea of the significance of a particular part of the spectrum, without getting involved in complicated matters such as angles between eigenvectors or eigenspaces.
The definition of pseudospectra $\Lambda_\varepsilon(A)$ for a matrix $A$ is directly related to perturbations:

$$\Lambda_\varepsilon(A) := \{z \in \mathbb{C} : z \in \Lambda(A+E) \text{ for some } E \text{ with } \|E\| \leq \varepsilon\}.$$

The pseudospectra are usually graphically shown as a set of level curves for various values of $\varepsilon$. The level curves, or contour integrals, are more apparent from the original definition for the $\varepsilon$-pseudospectrum, in terms of the norm of the resolvent $(zI-A)^{-1}$:

$$\Lambda_\varepsilon(A) := \{z \in \mathbb{C} : \|(zI-A)^{-1}\| \geq \varepsilon^{-1}\},$$

with the convention $\|(zI-A)^{-1}\| = \infty$ for $z \in \Lambda(A)$.

For computational purposes, the following equivalent definition of pseudospectra is more convenient:

$$\Lambda_\varepsilon(A) := \{z \in \mathbb{C} \quad : \quad \sigma_{\min}(z - A) \leq \varepsilon\}, \tag{59.1}$$

in wich $\sigma_{\min}(A)$ denotes the smallest singular value of $A$. This definition implies that the pseudospectra of $A$ are the sets in the complex plane bounded by level curves of the function $\sigma_{\min}(z - A)$.

For Hermitian matrices, the pseudospectra of $A$ is a collection of discs around the eigenvalues of $A$ (note that the perturbation $E$ needs not be symmetric). For unsymmetric matrices the pseudospectra can be any collection of closed curves, containing the set of eigenvalues of $A$. These level curves may give information that is hidden by the information provided by the eigenvalues themselves. For instance, when studying stability of integration methods for systems of ODE's, or in bifurcation problems, the eigenvalues may be in a proper region, for instance, in the left-half plane, while the level curves even for rather small values of $\varepsilon$ may intersect with the right-half plane. In such cases it may be time to ask further questions about the problem. On the other hand the pseudospectra may not tell the full story. For instance, the sensitivity problems may be due to a single pair of ill-conditioned eigenvectors for which the more global level curves are too pessimistic. It may be the case that it is not realistic to assume equal perturbations for all matrix entries, but nevertheless the pseudospectra points the attention to critical places in the spectrum. A nice introduction to the relevance of pseudospectra is given in TREFETHEN [1992], where for a number of matrices pseudospectra are actually computed and discussed.

Due to the high computational costs, the use of pseudospectra is often restricted to matrices of moderate size. This poses another problem: if we study the pseudospectrum for a discretized PDE with rather course meshsize (since we have to compute the smallest singular value of $zI - A$, for various values of $z$), what does this tell us on the effects to be expected for finer meshsizes?

We have carried out some experiments, not reported here, with a simple discretized convection-diffusion operator:

$$u_{xx} - \beta u_x,$$

with homogeneous Dirichlet boundary conditions. If we discretize this operator over the interval $[0, 1]$, with central difference approximation, then for large values of $\beta$ and relatively large meshsize, we see that the spectrum is on a line parallel to the imaginary axis. If we decrease the meshsize, then the spectrum gradually shrinks to one single point on the real axis (a highly defective case), and then spreads along the real axis. It turns out that amazingly soon, after the spectrum starts to spread along the real axis, the pseudospectra gives quite accurate information on the sensitivity of the given problem, information that is not essentially different from the information that we would have obtained for very fine meshsizes. On the other hand, the information for rather crude meshsizes can be quite misleading. This illustrates that we have to be careful in interpreting the information obtained from pseudospectra, when these are obtained for lower-dimensional problems than the problems that are used in the actual large-scale scientific computations.

More recently, tools have become available for computing the pseudospectra of large sparse matrices. CARPRAUX, ERHEL and SADKANE [1994] propose an algorithm for computing the smallest singular value of $zI - A$, that is based on Davidson's method with ILU preconditioning. LUI [1997] (see also BRACONNIER and HIGHAM [1996]) suggests to use Lanczos' method in combination with continuation techniques. This is a plausible approach, since we need to do the computation for many values of $z$, well-distributed over the region of interest, in order to obtain a complete picture of the pseudospectra. It has also been recognized recently, that one get a fairly good impression of the pseudospectra as a sideproduct of Arnoldi iterations, as, for instance, carried out with ARPACK (LEHOUCQ, SORENSEN and YANG [1998]). We know that currently such tools are being used for the analysis of instability problems of large sets of ODE's, related to climate modelling, but results have not yet been published.

More discussion on pseudospectra, and an overview of state of the art techniques for their efficient computation, can be found in TREFETHEN [1999].

## 60 Homotopy methods

The subspace methods that we have discussed in previous chapters, are often applied in combination with shift and invert operations. That means that if one wants to have eigenvalues close to a value $\sigma$, then the methods are applied to the inverse $(A - \sigma I)^{-1}$ of the shifted matrix. As we have seen, the Jacobi-Davidson method can be interpreted as an inexact shift-invert method, since the invert step is usually approximated by a few steps of some convenient preconditioned inner iteration method.

Related to these inexact shift-invert approaches is the homotopy approach, that has received attention in the past five years. The idea is to compute some of the eigenvalues of a given matrix $A+E$, when eigenvalues of $A$ are known, or can be relatively easily computed. In order to this we use the homotopy $H(t) = A + tE$, $0 \leq t \leq 1$. If eigenpairs of $H(t_0)$ are known, then they are used as approximations for those of $H(t_0 + \Delta t)$. These approximations are improved by a convenient subspace iteration, for instance in Lui and Golub [1995] Rayleigh quotient iterations are used for symmetric $A$ and $E$ (see references in Lui and Golub [1995] for earlier work on homotopy for eigenproblems). For the Rayleigh quotient iteration one needs to solve systems like $(H(t_0 + \Delta t) - \lambda I)y = x$, where $(\lambda, x)$ represents the current approximation for an eigenpair of $H(t_0+\Delta t)$. In the context of large sparse matrices, it may be undesirable to do this with a direct solver, and in Lui and Golub [1995] the system is solved with SYMMLQ (Paige and Saunders [1975]). Of course, one could restrict oneself to only a few steps with SYMMLQ, and then try to accelerate the inexact Rayleigh quotient steps, as is done in the Jacobi-Davidson method. This indicates relations between these different approaches, but as far as we know, these relations have not yet been explored. There seem to be more relations. In Lui and Golub [1995] it is observed that SYMMLQ may find difficulty in converging for the nearly singular system $H(t_0 + \Delta t) - \lambda I)y = x$, and it is suggested to improve the situation by applying the Rayleigh quotient iteration to the approximately deflated matrix $H(t_0 + \Delta t) + xx^T$, where the term approximately deflated is used to indicate that $x$ is only an approximation to the desired eigenvector. Note that similar deflation procedures are incorporated in the Jacobi-Davidson process.

The whole procedure is repeated for successive increments $\Delta t$, until the final value $t = 1$ is reached. In Lui and Golub [1995] an elegant approach is followed for the selection of the step size $\Delta t$.

The homotopy approach lends itself quite naturally for situations where the matrix $A$ varies in time, or where it varies as a linearization of a nonlinear operator, as in bifurcation problems. Other situations that are obvious are for instance the Helmholtz eigenvalue problem (Lui and Golub [1995]):

$$-\Delta u + fu = \lambda u$$

in the unit square in two space dimensions with homogeneous Dirichlet boundary conditions. Here, $f$ is a function of the spatial variables. With the usual finite difference approximations on a uniform grid, this leads to the discrete Laplacian for $-\Delta u$, of which we know the eigensystem.

In Zhang, Law and Golub [1998], the homotopy approach is used for symmetric generalized eigenproblems, very much along the same lines as sketched above. The application for real unsymmetric eigenproblems is considered in Lui, Keller and Kwok [1998].

# 61 Implementation aspects

In the past ten years sophisticated software has been produced for the computation of eigenvalues and eigenvectors. We have mentioned already the Implicitly Restarted Arnoldi method, for which Lehoucq, Sorensen and Vu have written the package ARPACK (Lehoucq, Sorensen *et al* [1995]. We also mention the code SRRIT (Bai and Stewart [1992]) for the identification of a dominant invariant subspace of a nonsymmetric matrix. In the context of the Two-sided Lanczos method, software has been presented in Cullum, Kerner and Willoughby [1989], and by Freund and Nachtigal [1996]: QMRPACK. We also want to mention a recent approach to design robust software for the Two-sided Lanczos method, the so-called ABLE package (Bai, Day and Ye [1995]). In Bai, Demmel *et al* [1995] a project is announced for the production of software for relevant algorithm for large eigenproblems. This project is scheduled to appear in Bai *et al* [2000]. In this project, software is discussed for all sorts of methods for large scale eigenproblems.

In Lehoucq and Scott [1996] an overview of relevant software is given as well as numerical results for representative test problems.

Most of the iterative methods reduce the given large problem to a much smaller problem. The smaller problem can then be handled by standard software for dense or banded matrices. Excellent software is available in LAPACK (Anderson *et al* [1992]), the modern successor of the famous packages EISPACK and LINPACK.

Parallelism in the subspace methods is, except for the (approximate) shift-and-invert steps, usually no big problem. For some modern computers the required innerproducts may form a bottleneck with respect to scalable performance. For an overview of techniques to improve parallel behavior of algorithms for eigenproblems, see Demmel, Heath and van der Vorst

[1993]. Recently, it has been shown in Lui [1996] that domain decomposition techniques can be used for the computation of eigenvalues of partial differential operators. This is certainly a promising direction in view of parallel computation.

## 62 List of Notations

| | |
|---|---|
| $A, B, \ldots$ | matrices, 4.<br>Entries of $A$ are denoted by either $a_{i,j}$ or $(A)_{i,j}$ |
| $n$ | the order of the matrix, 4 |
| $x, y, \ldots$ | vectors. The elements of $x$ are denoted by $x_i$. 4 |
| $\lambda$ | an eigenvalue, 4 |
| $\theta$ | a Ritz value, 58 |
| $\alpha, \beta, \ldots$ | scalars |
| $A^T$ | the transpose of the matrix $A$: $(A^T)_{i,j} = (A)_{j,i}$ |
| $A^H$ | the conjugate transpose of a complex matrix $A$: $(A^H)_{i,j} = (\bar{A})_{j,i}$ |
| $A^*$ | the transpose if $A$ is real,<br>the conjugate transpose if $A$ is complex |
| $x^*y$ | the innerproduct between the vectors $x$ and $y$ |
| $\|x\|_2$ | the Euclidean norm of the vector $x$: $\|x\|_2 = \sqrt{x^*x}$, 23 |
| $\|A\|_2$ | the associated matrix norm: $\|A\|_2 = \sup_{x\neq 0} \|Ax\|_2/\|x\|_2$ |
| $A^{-1}$ | the inverse of $A$: $A^{-1}A = I$ |
| $I$ | the square identity matrix (dimension will be clear from the context) |
| $I_m$ | the identity matrix of dimension $m$<br>(if the dimension is not clear from the context), 56 |
| $I_{m,m-1}$ | the leading $m$ by $m-1$ part of the identity matrix, 59 |
| $H_{m,n}$ | an $m$ by $n$ upper Hessenberg matrix: $(H_{m,n})_{i,j} = 0$ for $i \geq j+2$, 56 |
| $T_{m,n}$ | an $m$ by $n$ tridiagonal matrix: $(T_{m,n})_{i,j} = 0$ for $\|i-j\| > 1$, 62 |
| $G_i$ | Givens rotation, 43 |
| $V_j$ | a matrix with $j$ columns: $v_1$, $v_2$, ..., $v_j$, 8 |
| $\mathcal{K}^m(A; x)$ | the Krylov subspace of dimension $m$ generated with $A$ and $x$, 7 |
| $J_i$ | Jordan matrix of dimension $i$, 19 |
| $A^{-H}$ | the inverse of $A^H$, 26 |
| $A^{\#}$ | the Drazin inverse of $A$, 26 |

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