Topological analysis of eigenvalues in engineering computations

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Abstract *The dynamics of coupling between spectrum and resolvent under ϵ-perturbations of operator and matrix spectra are studied both theoretically and numerically. The phenomenon of non-trivial pseudospectra encountered in these dynamics is treated by relating information in the complex plane to the behaviour of operators and matrices. On a number of numerical results we show how an intrinsic blend of theory with symbolic and numerical computations can be used effectively for the analysis of spectral problems arising from engineering applications.*

1. Introduction

The information on spectra of matrices and operators has primary importance in many branches of engineering sciences. In particular, this information is indispensable in analysing stability of mechanical systems, fluid flows, and electronic devices. It is at the heart of spectral-type (including pseudospectral) methods widely used for approximations of differential and integral operators arising from engineering applications (Fornberg, 1996; Quarteroni and Valli, 1997).

The study of eigenvalues has been revolutionised by the ready availability of computing power. Surprising results, however, are quick to appear in engineering practice and present well-known, yet non-trivial, difficulties. These difficulties often come from the following standard procedure applied to the stability analysis of many engineering problems (Baggett *et al.,* 1995):

- we linearise the mathematical model about a known solution (e.g. about the laminar flow for the Navier-Stokes equations);

- then we diagonalise the resulting operator (using the Schmidt factorisation); and

- finally, we use eigenvalues to analyse the stability of the system.

A variant of this procedure is often used in the solution of evolutionary non-linear partial differential equations by the method of lines (MOL) which leads typically to a non-linear ODE:

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}). \tag{1.1}$$

Then one can apply a linear analysis locally for a given, isolated solution $\mathbf{y}(t)$ of this equation, and consider trends of small perturbations. The analysis is then reduced to the investigation of the linear, variational equation (Ascher and Petzold, 1998):

$$\mathbf{z}' = A(t, \mathbf{y})\mathbf{z},$$

where

$$A = \frac{\partial \mathbf{f}}{\partial \mathbf{y}}. \tag{1.2}$$

It has been well-known for a long time that these local procedures may fail to predict correctly the evolution of the system, and the main reason for such a failure has been usually attributed to the linearisation procedure. However, recent results in fluid dynamics, magneto-hydrodynamics and other areas have clearly indicated that the increase of spectral instability (i. e. the departure of linearised operators or matrices from normality) gives another important reason for the discrepancy between theoretical and experimental predictions (Baggett and Trefothen, 1995; Reddy *et al.,* 1993; Reddy and Henningson, 1993; Trefethen *et al.,* 1993).

Although non-normal operators and matrices have been encountered in engineering practice for a long time and the effects of non-normality have been well-known to the mathematical community (see, for example, Henrici (1962), the number of engineering problems where this effect was of much concern was quite limited. Indeed, if the departure from normality remains bounded (which may occur in the presence of a nearby defective eigenvalue), the effect of non-normality on the spectrum remains local and a number of linear algebra packages such as LAPACK are able to treat efficiently the ill-conditioned eigenvalues as a clustered group of eigenvalues. However, the effect of non-normality on the spectrum of the operator/matrix may become non-local. In some applications, for example, it may happen, when the departure from normality is ruled by a physical parameter such as the Reynolds or Peclet number. Another area that brings problems that often requires dealing with operators and matrices on the edge of their spectral stability is coupled field theory where interconnection of physical fields of a different nature is essential in obtaining a plausible picture of the phenomenon under consideration (Melnik, 1998a). This class of problems is quite diverse and covers the range of applications from semiconductor device simulation to climate modelling (Melnik and Melnik, 1997; Melnik, 1998b); Kerner, 1989; Chatelin and Godet-Thobie, 1991).

To a great extent due to the ready availability of computer power (that made many large-scale problems in engineering tractable (Trefethen, 1999; Melnik, 1998b), the number of engineering problems where the spectral instability has to be seriously dealt with continues to grow. As the result, the computer

analysis of spectral behaviour of operators and matrices under data perturbations and the visualisation of the results of this analysis are obtaining a growing recognition in the engineering community.

From the mathematical point of view this analysis is especially important:

- in the presence of an eigenvalue of algebraic multiplicity k, $k \geq 2$ that admits less than k independent eigenvectors (called defective or clustered eigenvalue);
- in dealing with non-normal operators/matrices, for which separated eigenvalues in exact arithmetic tend to be coupled by the finite precision computation.

In such situations the definition of the ill-conditioning measure by the standard tools such as the condition number become problematic (Chaitin-Chatelin and Fraysse, 1996), and therefore the meaningfulness of a computed eigenvalue depends strongly on the information on its stability. This information can be provided by "topological" neighbourhoods of eigenvalues. Of course, in exact arithmetic an eigenvalue has a topological dimension $D_e = 0$, but in the finite precision arithmetic it has a positive fractal dimension $D_f = 1 - 1/l$, where $D_f \in (0,1)$ and l are the ascent of the defectiveness of this eigenvalue ($l > 1$) (Chaitin-Chatelin, 1996). This dimensionality of defective eigenvalues in the computer arithmetic leads to the possibility of displaying the spectral instability occurring in engineering problems. Using visualisation capabilities of modern computers, it is possible to study spectral instability (induced by the presence of defective eigenvalues) via measures that quantify the departure of linear operators or matrices from normality. This study, from both theoretical and numerical points of view, is the main focus of this paper.

We organised the rest of the paper as follows.

In Section 2 we provide the reader with necessary mathematical background, introduce ϵ-pseudosolutions of linear operator equations and explain the mathematical sources of non-normality.

In Section 3 we give examples of engineering problems where the non-normality of linear operators and/or matrices leads to spectral instability.

Absolute and relative measures of spectral instability are discussed in Section 4, where the effectiveness of spectral portraits in determining regions of potential instability is demonstrated by several examples.

The connection between the stability and the dichotomy of operator spectra and the Cayley transform technique is explored in Section 5. Our deliberations in this section are based on the Lyapunov method and the assumption of strong positivity of linear operators.

Section 6 is devoted to numerical procedures for the construction of spectral portraits.

Some computational results are presented in Section 7. Conclusions and future directions are also discussed in this section.

2. Mathematical foundations

The idea of coupling the property of the algorithm with the arithmetic of the computer is based on the notion of backward error and can be traced at least 40 years back (Hairer and Wanner, 1996). New engineering problems requiring reliable and robust computer methods for their solution have given a new impetus to further development of this idea within the theory of finite precision computations (Chaitin-Chatelin and Fraysee, 1996).

Many engineering problems can be written in the following generic form (Morozov, 1993):

$$Au = f, \tag{2.1}$$

where $A : U \to F$ is a given operator with domain of definition $\mathcal{D}_A \subseteq U$, U and F are given metric (Banach) spaces, $f \in F$ defines the set of input data, and $u \in \mathcal{D}_A$ is the unknown variable that defines the system output. Since operator A is typically given only approximately, element u is computed with error. Therefore, from the computational point of view this problem is tied to the problem of stable computation of values of (possibly discontinuous) operator L such that

$$g = Lu, \tag{2.2}$$

where $L : \mathcal{D}_L \subseteq U \to G$, G is the given metric (Banach) space, and $u \in \mathcal{D}_L$.

In the general case (the connection is obvious when A is a locally invertible operator) problems (2.1) and (2.2) are closely connected on the basis of the notion of pseudosolutions (Morozov, 1993)

$$U_f = \{u \in \mathcal{D} : \quad \|Au - f\|_F = \inf_{v \in \mathcal{D}} \|Av - f\|_F\} \neq \emptyset, \tag{2.3}$$

where $\mathcal{D} \subseteq \mathcal{D}_{AL} \equiv \mathcal{D}_A \cap \mathcal{D}_L \neq \emptyset$.

Another way of looking at this situation is that the computed solution to (2.1) can be viewed via the set of perturbed problems solved exactly by $\tilde{u}$ (Chaitin-Chatelin and Fraysse, 1996)

$$\tilde{u} = \tilde{P}(g), \tag{2.4}$$

where g is a point in the space G of perturbed data (parameter space) and $\tilde{P}$ is a perturbed operator $P : G \to U$ such that when A is locally invertible we can uniquely determine the value of u by the formula

$$u = A^{-1}(f) = P(g). \tag{2.5}$$

Provided that the norm on G and the class $\mathbb{C}_p$ of admissible data perturbations $\Delta g \in \mathbb{C}_p$ are specified, we can define the minimal distance (backward error) between the solution to the original problem (2.1) and the set of perturbed solutions defined by (2.4) as follows

$$B(\tilde{u}) = \inf\{\|\Delta g\| : \quad \Delta g \in \mathbb{C}_p, \quad P(g + \Delta g) = \tilde{u}\}. \tag{2.6}$$

Then, the set of ϵ-pseudosolutions to the original problem (2.1) can be defined naturally in terms of the backward error

$$\Sigma_\epsilon(u) = \{g : B(g) \le \epsilon\} \tag{2.7}$$

The notion of pseudosolution was first introduced by V. Morozov in the late 1960s (see Morozov (1993)) in order to reflect the sensitivity of computational schemes to perturbations (including, but not limited to, finite precision). Since then this notion and its various modifications have proved to be very useful in many branches of science and engineering. For example, in the context of dynamical systems an analogue of this notion (ϵ-trajectories) was used to characterise a computed trajectories system which can be viewed as ϵ-trajectories (see Chaitin-Chatelin and Fraysse (1996) and references therein). Another example arose from the solution of some spectral problems in linear algebra and engineering where computation of individual eigenvalues appeared to be problematic. This led in the late 1970s to the notion of ϵ-spectra or pseudospectra, formulated independently by several researchers (Godunov et al., 1992; Varah, 1979; Landau, 1977). It was shown that the invariant subspaces of non-normal operators, and even of moderate-size matrices, can be extremely ill-conditioned. We explain this situation below.

In many engineering applications we deal with matrices that have the diagonal Schur form. The spectral representation of such (normal) matrices is stable with respect to matrix perturbations, and all matrix eigenvalues and eigenvectors are well-conditioned. In the general case any matrix A (including defective) can be represented as

$$A = XJX^{-1}, \tag{2.8}$$

where J is the Jordan form and X is the Jordan basis of matrix A. Using the Schmidt factorisation for the Jordan basis $X = QR$ we can reduce (2.8) to

$$A = QSQ^*, \tag{2.9}$$

where $S = RJR^{-1}$ is the Schur form of A. If

$$J = D + \tilde{J}, \quad S = D + \tilde{S},$$

where

$$D = \text{diag}(A), \tag{2.10}$$

then the deviation matrices $\tilde{J}$ and $\tilde{N}$ can provide the key to some measures of matrix non-normality. Indeed, from (2.8) it follows that in principle there may exist matrix A for which $\text{cond}_2(X)$ can grow unboundedly (since $\|\tilde{J}\|_2 = 1$). Similarly, if $\text{cond}_2(Q)$ is normalised to 1, then from (2.9) it follows that $\|S\|$ can grow potentially without bound. In the next section we give examples of engineering problems where such situations arise.

3. Spectral instability phenomenon in engineering applications

During recent years much attention has been paid to the spectral instability in finite precision computations when dealing with non-normal operators. Since a necessary and sufficient condition of normality is the admission of an orthonormal basis, the problem stems from the fact that computed orthogonal bases may appear to be far from mutually orthogonal within machine precision. This leads to clusters of eigenvalues, the phenomenon well understood only when $\text{cond}_2(X)$ and the ascent l are bounded (or, alternatively, when $\|\tilde{S}\|$ is bounded).

In many engineering applications we have to deal with families of matrices that arise from the discretisation of differential and integral operators by finite-element, finite-difference or spectral (including pseudospectral) methods. These matrices depend often on one or several parameters such as the size of the matrix (n), the Reynolds number (Re) or the Peclet number (Pe). Whenever this family of matrices is such that the ascent l of at least one eigenvalue (the theoretical possibility of $l \to \infty$ exists only when $n \to \infty$) and the condition number of the Jordan basis are potentially unbounded (alternatively, $\|\tilde{S}\|$ is potentially unbounded) under the parameter variation, then such matrices are usually termed as highly non-normal (Trefethen, 1992).

A non-exhaustive list of engineering applications where such matrices are encountered include:

- convection-diffusion models where the predictions based on the exact spectrum depends on the model analogue of the Peclet number and could be misleading in the convection dominated region (Reddy and Trefethen, 1994; Gavrilyuk and Melnik, 1998);

- modelling of magneto-hydrodynamic (MHD) plasma with a coupled system (that combines the Navier-Stokes and Maxwell equations), where the linearised dissipative operator becomes highly non-normal with the decrease of plasma resistivity (Kerner, 1989);

- the study of dynamic responses and optimisation in structural engineering, for example, the modelling of self-induced vibrational motion initiated by a source of energy external to the structure (known as the the flutter phenomenon (Braconnier *et al.*, 1995)) with a coupled model for a torsional vibration and a bending motion of a wing in flight (a famous Tolosa matrix, available from the Harwell Boeing collection, arises in such applications (Chaitin-Chatelin and Fraysse, 1996));

- computational fluid dynamics, where linearised operators (for example, the Orr-Sommerfeld operator in the study of parallel shear flows as a mechanism of subcritical transition to turbulence) for the description of some flow configurations (such as Couette flow, plane and pipe Poiseulle flow) become highly non-normal with the increase of the Reynolds number (Reddy *et al.*, 1993; Reddy and Henningson, 1993; Baggett and Trefethen, 1995);

- coupled field theory (Melnik and Melnik, 1997; Melnik, 1998b), stochastic processes modelling (Jonsson and Trefethen, 1997), control theory (Hinrichsen and Kelb, 1993), optical and electronic engineering (Landau, 1977; Melnik and Melnik, 1997);

- aerospace industry (Chatelin and Godet-Thobie, 1991; Braconnier *et al.,* 1995) and other engineering applications.

In many of the above examples, spectral instability comes from the discontinuity of the spectrum with respect to a parameter which comes from physics, the numerical method or arithmetic. In some examples, in particular those from coupled field theory, this parameter appears naturally due to the coupling of two or more physical (chemical or biological) fields of different nature.

The common feature of all the above examples is that one has to deal with non-self-adjoint operators and/or non-normal matrices (i.e. with the situation when $A^*A \neq AA^*$). Since in such cases the use of eigenvalues may lead to an extreme distortion of the system state space, it may not be appropriate to analyse such engineering problems in terms of eigenvalues/eigenvectors (Trefethen, 1997). If short-time nature phenomena are well approximated by linear models (despite the fact that the long-time behaviour of the system under consideration may require more complex non-linear models), the eigenvalues may give the wrong tool to the engineer. Indeed, instead of determining the transient behaviour of the system, the spectral analysis will be directed to the long-time behaviour of a non-normal linear problem, which may be misleading in such cases (Trefethen, 1997).

4. Incompleteness of information on behaviour of matrices and linear operators from spectra or resolvents
As follows from a triangular Schur form $S = D + \tilde{S}$ (see (2.10)), the departure from normality of the original matrix A (i. e. the ill-conditioning of spectral decomposition) is determined by the strictly triangular part of this matrix $\tilde{S}$, whose Frobenius norm

$$(\|A\|_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2}),$$

$$\nu_1(A) = \|\tilde{S}\|_F, \tag{4.1}$$

can be taken as an absolute measure of non-normality. Since in some cases the value of $\nu_1(A)$ is not easily computable, it is much more common to use another absolute measure that follows directly from the definition of non-normality,

$$\nu_2(A) = \|AA^* - A^*A\|_F. \tag{4.2}$$

Since $\nu_2(A) \leq 2\|A\|_F^2$, the large $\nu_2(A)$ implies the large $\|A\|_F$.

A relative measure of non-normality is typically defined with the Henrici number

$$\text{He}(A) = \frac{\nu_2(A)}{\|A^2\|_F}, \tag{4.3}$$

which is easily computable and often thought of as the numerical analogue of the Reynolds number or the Peclet number in fluid dynamics. The choice of the norm in (4.1)-(4.3) becomes natural if we recall that the exact information about matrix behaviour cannot be inferred from the spectral norm of the resolvent ($\|A\|_2 = \sup\{\|Ax\| : \quad \|x\|_2 = 1\}$), and the equivalence

$$\|(zI - A)^{-1}\| = \|(zI - B)^{-1}\| \quad \Longleftrightarrow \quad \|p(A)\| = \|p(B)\| \quad \forall p \in \pi_n, \tag{4.4}$$

holds in the Frobenius, but not in the spectral, norm (see Trefethen (1999) and references therein). By π_n in (4.4) we denote the class of all polynomials degree not exceeding n.

In many applications the measures $\nu_2(A)$ and $\text{He}(A)$ together with $\text{cond}_2(A)$ and $\text{cond}_2(X)$ (see (2.8)) can provide a good insight into the problem of non-normality. Unfortunately, each of these measures separately may not be a reliable characteristic of non-normality, because their large values may simply indicate a presence nearby a multiple defective eigenvalue. The connection between these measures follows from their definitions and the Smith's inequality (Chaitin-Chatelin and Fraysse, 1996)

$$\text{cond}_2(X) \equiv \|X\|_2\|X^{-1}\|_2 \geq \left(1 + \frac{1}{2}\text{He}(A)\right)^{1/4} \equiv \text{He}_S(A), \tag{4.5}$$

where $\text{He}_S(A)$ is the Henrici-Smith number of the matrix A. However, for those engineering applications where the spectral instability test is required, the sensitivity analysis of the eigenvalues to the perturbations Δ on A in the spectral norm has to be included into the investigation (see Chaitin-Chatelin and Fraysse (1996) and references to the Harwell-Boeing collection given there). This analysis can be conducted efficiently by using one of the most reliable measures of spectral instability called pseudospectra.

Definition 4.1. Let A be a given matrix and $\epsilon > 0$. The ϵ-pseudospectrum of this matrix is called the set

$$\sigma_\epsilon(A) = \{z \in \mathbb{C}: \quad z \equiv \lambda_{A+\Delta}\}, \tag{4.6}$$

where $\|\Delta A\|_2 \leq \epsilon\|A\|_2$ and $\lambda_{A+\Delta}$ is an eigenvalue of matrix $A + \Delta$.

It can be shown (see Chaitin-Chaitlin and Fraysse, 1996) that

$$\sigma_\epsilon(A) = \left\{z \in \mathbb{C}: \quad \|(A - zI)^{-1}\|_2 \geq \frac{1}{\epsilon\|A\|_2}\right\}, \tag{4.7}$$

which in turn implies that the larger the set $\sigma_\epsilon(A)$, the more unstable the eigenvalues of matrix A. We take this result as the basis for the definition of pseudospectral sets for both matrices and linear operators.

Let A be a closed linear operator in a Banach space X. Then the union of all regular points $\lambda \in \mathbb{C}$ of the operator A (i.e. points for which the operator $\lambda I - A$ is continuously invertible) forms the resolvent set of the operator, $\rho(A)$, which is always open:

$$\rho(A) = \{\lambda \in \mathbb{C}: \quad (\lambda I - T)^{-1} \in \mathcal{L}(X)\}, \tag{4.8}$$

where $\mathcal{L}(X)$ is the space of all bounded linear operators A on X with the domain X. If $\lambda \in \rho(A)$, then the linear operator $R_\lambda(A) = (\lambda I - A)^{-1}$ is the resolvent of A.

Definition 4.2. For each $\epsilon > 0$ the ϵ-pseudospectrum of $A, \Sigma_\epsilon(A)$, is defined as the set of all $\lambda \in \mathbb{C}$ such that

$$\|A\|_2 \|(\lambda I - A)^{-1}\|_2 \geq \frac{1}{\epsilon}. \tag{4.9}$$

If, in addition to the assumptions made, the operator $A \in X$ is completely continuous, then its spectrum, $\Sigma(A)$, consists of an at most countable set of eigenvalues, for which the only limit point may be the point $\lambda = 0$.

Therefore, in principle the pseudospectra of linear operator A can be defined by either the closed set (Gallestey *et al.*, 1997)

$$\sigma_\epsilon(A) = \left\{ z \in \rho(A): \quad \|(zI - A)^{-1}\| \geq \frac{1}{\epsilon} \right\} \cup \Sigma(A). \tag{4.10}$$

or the open set (Davies, 1998).

Definition 4.3.

$$\omega_\epsilon(A) = \left\{ z \in \mathbb{C}: \quad \|(zI - A)^{-1}\| > \frac{1}{\epsilon} \right\} \cup \Sigma(A), \tag{4.11}$$

where the connection between these two sets is given by the following theorem (Chaitin-Chatelin and Harrabi, 1998).

Theorem 4.1. If A is a closed linear operator such that there is no open set in $\rho(A)$ on which the norm of the resolvent of A is constant, then

$$\overline{\omega_\epsilon(A)} = \sigma_\epsilon(A), \quad \epsilon > 0. \tag{4.12}$$

The ϵ-pseudospectrum of the operator A is continuous under the notion of uniform convergence (Harrabi, 1998a), and if $\|A_n - A\| \to 0$, where A and A_n, $n \in \mathbb{N}$ are bounded operators in X, then the spectrum of the operator family A_n, $n \in \mathbb{N}$ is equal to the spectrum of A.

The contour lines of sets defined by (4.9) give the borders of the ϵ-pseudospectra, called spectral portraits. Since the values of $\|(A - zI)^{-1}\|$ can be fairly large even when z is far away from eigenvalues, spectral portraits of matrices are defined by Godunov (1991).

Definition 4.4. The graphical display of the map

$$z \mapsto \Phi(z), \quad \text{where} \quad \Phi(z) = \log_{10} \|A\|_2 \times \|(A - zI)\|_2. \tag{4.13}$$

This map provides one of the most reliable tools for the analysis of spectral instability (Chaitin-Chatelin and Fraysse, 1996). Owing to the possibility of steep variations of values in uniform scales, the exponential (or logarithmic) scales, such as (4.13), are usually preferred in the definitions of spectral portraits. Since the eigenvalues of A are the poles of the resolvent $(A - zI)^{-1}$ for $z \in \mathbb{C}$, the dynamic behaviour of the norm $\|(A - zI)^{-1}\|_2$ as z moves away from eigenvalue is one of the major characteristics for the spectral instability test. Indeed, from the engineering point of view one may expect "pseudoresonance" for a non-normal system since $\|(zI - L)^{-1}\|$ may be large even if z is far away from an eigenvalue. That is why pseudospectra can be seen as a plot of contours of equal resonance magnitude, where the real axis corresponds to forcing at real frequencies (Trefethen *et al.,* 1993).

Two remarks about possible generalisations of the above notions follow.

Remark 4.1. In a more general setting we can define several different types of pseudospectra of matrices such as norm-wise and component-wise (see Fraysse and Toumazou (1998) and references therein). Since the borders of the latter are not easily computable (Chaitin-Chatelin and Fraysse, 1996), we consider only norm-wise ϵ-pseudospectra

$$\sigma_\epsilon^N(A) = \{z \in \mathbb{C} : \quad \|(A - zI)^{-1}\|_2 \geq (\epsilon\alpha)^{-1}\},$$

where

$$|\Delta A\| \leq \epsilon\alpha \tag{4.14}$$

with the choice of α given by the spectral norm of A, that is $\alpha = \|A\|_2$. This reduces our constructions to (4.9).

Remark 4.2. The above notions of ϵ-pseudospectrum and spectral portrait can be easily expended to matrix pencils (A,B) for generalised eigenvalue problems encountered in engineering applications (Fraysse and Toumazou, 1998).

The intrinsic connections between:

- the spectrum $\Sigma(A)$ (determined by the ϵ-pseudospectrum of A for $\epsilon \to 0^+$) and the asymptotic behaviour of A^n (as well as $\exp(tA)$) in the limit of $n \to \infty$ (respectively, $t \to \infty$);

· the numerical range of A (determined by the ϵ-pseudospectrum of A for $\epsilon \to \infty$) and the initial behaviour of A^n (as well as $\exp(tA)$) in the limit of $n \to \infty$ (respectively, $t \to \infty$)

are well elucidated in the literature (see, for example, references in Trefethen (1997)). It appears, however, that finite positive values of ϵ, n (and t), rather than their limiting values, present major interest for many engineering applications. A question of primary importance that arises in the context of such applications is how the above connections will be affected under spectrum perturbations characterised by the value of $\epsilon \in (0, +\infty)$, possibly very small. We explain the fundamental nature of this question with a simple, yet very demonstrable example.

Let us consider a simple homogeneous linear system

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x} \tag{4.15}$$

with a given matrix A. Assuming that that the initial conditions may be given precisely, the problem of dynamic stability for this model is equivalent to the investigation of ϵ-pseudospectrum of the matrix A. Indeed, we cannot extract complete information about matrix behaviour either from the spectral norm of the matrix or from the norm of its resolvent. However, it is reasonable to use an intrinsic connection between spectrum and resolvent of matrices under ϵ-perturbations. The main theoretical problem consists of the fact that without restrictions on ϵ, the absence of practical dichotomy of the matrix spectrum may be anticipated. This is a crucial point for many engineering applications. Indeed, for the linear dichotomy there might exist such $\epsilon = \epsilon(\delta)$ that the perturbed matrix $A_\epsilon = A + \Delta$ with $||\Delta|| \le \epsilon$ can have in the left-half plane a number of eigenvalues different from the number of points of the matrix A spectrum. If the matrices $A = (a_{ij})$ and $\Delta = (\delta_{ij})$ are defined as follows

$$a_{ij} = \begin{cases} -0.5, & j = i, \ i = 1, 2, \ldots, 24, \\ 10, & j = i+1, \ i = 1, 2, \ldots, 23, \\ 0, & \text{otherwise,} \end{cases} \quad \Delta = \begin{cases} \epsilon = 10^{-22}, & i = 24, j = 1, \\ 0, & \text{otherwise,} \end{cases}$$

then, though the matrix A has one negative eigenvalue, –0. 5, of multiplicity 24 (we will refer to this matrix as "Negative24"), the eigenvalues of the perturbed matrix A_ϵ (i.e. $\sqrt[24]{10} - 0.5$) are shifted to the right-half plane, indicating instability in the perturbed model:

$$\frac{d\mathbf{x}}{dt} = A_\epsilon\mathbf{x}. \tag{4.16}$$

This phenomenon is demonstrated by Figure 1 where we present the surface and pseudospectra plots of this matrix A (see the upper row). Any point from the "inside" region (or, equivalently, a "crater" region in the 3D plot) in effect can be considered as an eigenvalue of the matrix A with corresponding
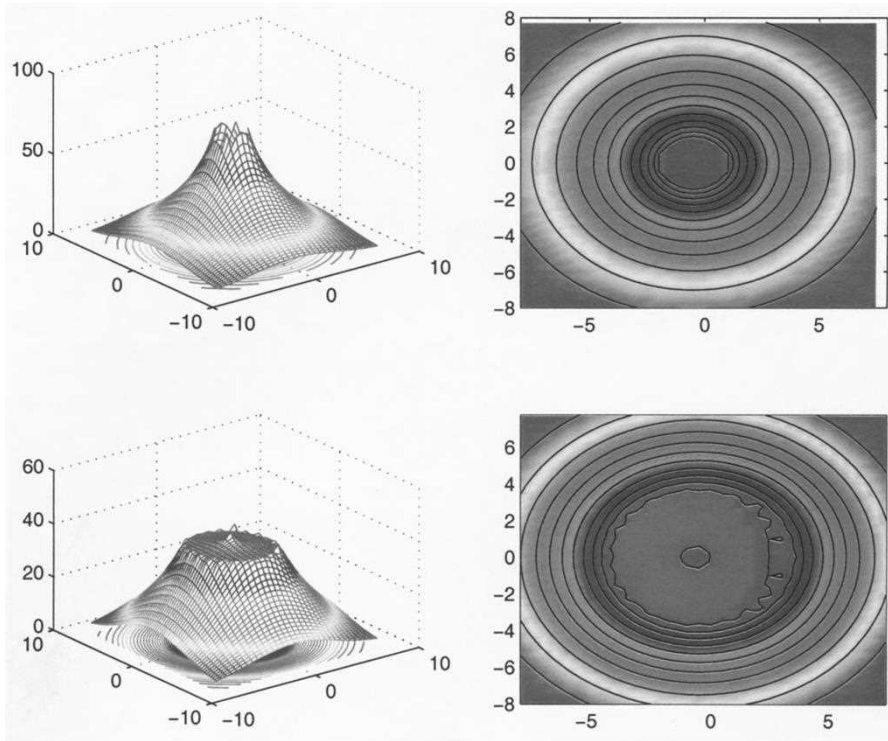
Figure 1.
Surface and
pseudospectral plots of
the original (Negative-
24) and perturbed
matrices appearing in
systems (4.15), (4.16)

Matrix	$\|A\|_1$	$\|A\|_2$	$\|A\|_\infty$	$\|A\|_F$	$\mathrm{Cond}_1(A)$	$\mathrm{Cond}_2(A)$	$\mathrm{He}_F(A)$
Negative24	10.5	10.4959	10.5	48.0208	1.8543e32	∞	0.2999
Godunov	6,825	4.322e3	6,825	6.57e3	4.5270e17	2.4777e16	2.8202
Polynomial	2,613	4.1788e3	8,999	4.1788e3	∞	∞	325.2822

Table I.
Matrix functions and
estimates as candidates
for non-normality
measures

accuracy. The surface plot and pseudospectra of a slightly perturbed matrix, defined by $\mathcal{A} = A + 1.e - 9 * \mathrm{rand}(\mathrm{size}(A, 2))$, are presented in the lower row of Figure 1. Essential topological changes of the "crater" region under matrix perturbations require further investigation of the instability phenomenon. Using standard Matlab commands, we computed some characteristic functions and estimates for this matrix. They are given in the first row of Table I. Note that the estimate of the 1-norm matrix condition number might result in the message that matrix is singular to working precision. It is seen that, unlike the Henrici number, neither $\mathrm{cond}_1(A)$ nor $\mathrm{cond}_2(A)$ can be reliable computational characteristics of matrix non-normality.

Similar examples can be constructed for any $\epsilon > 0$, no matter how small it is assumed to be. This implies that the use of computers (or the definition of matrices approximately) turns the problem of investigation of matrix spectra into the investigation of its pseudospectra under certain level of ϵ.

Of course, in many engineering applications the asymptotic stability of ordinary differential equations (ODEs), arising either from immediate applications or from the use of the MOL to partial differential equations, is extremely important. However, in the computational solution of engineering problems we often encounter transient phenomena that depend on how effects evolve over many finite time steps. In such cases, neither numerical stability nor stiffness of linear ODEs can properly be characterised in terms of the eigenvalues of the Jacobian, because these properties of the differential models are intrinsically transient (Higham and Trefethen, 1993; Trefethen *et al.,* 1993). In such situations the engineering problem at hand may be better described and controlled in terms of pseudospectra (or in some cases by pseudozeros of characteristic polynomials (see Chaitin-Chatelin and Fraysse (1996) for details) rather than a spectrum. Indeed, when the Godunov matrix (Godunov, 1991):

$$A_0 = \begin{bmatrix} 289 & 2,064 & 336 & 128 & 48,367 & 32 & 16 \\ 1,152 & 30 & 1,312 & 75,984,758 & 288 & 128 & 32 \\ -29 & -23,444,455 & 756 & 384 & 1,008 & 224 & 48 \\ 512 & 128 & 640 & 0 & 640 & 512 & 128 \\ 1,053 & 2,256 & -504 & -384 & -756 & 800 & 208 \\ -287 & -16 & 1,712 & -128 & 1,968 & -30 & 2,032 \\ -2,176 & -287 & -1,565 & -512 & -541 & -1,152 & -289 \end{bmatrix}$$

with distinct integer eigenvalues (namely, 0, ± 1, ± 2, ± 4) is used as input to MATLAB-5's *eig* function, one real and three complex conjugate pairs are returned as eigenvalues. Other numerical packages such as MAPLE, MATHEMATICA, APL, do not do any better (see also Godunov *et al.,* 1992; Godunov, 1991). Worse yet, similarity transforms of the matrix, which theoretically should leave the eigenvalues invariant, produce matrices with quite different eigenvalues. This example demonstrates convincingly that without some additional information on the matrix stability, engineering computations with standard software packages may result in completely misleading conclusions. This is demonstrated in Figure 2 where we present surface plot and pseudospectra of the Godunov matrix (see the upper row). As in our previous example, any point from the "crater" region (see the upper-left plot) can be considered as an eigenvalue of the Godunov matrix with given accuracy. Under perturbations the "inside" region grows and the eigenvalues move on the periphery of this region, far away from the eigenvalues of the original matrix. This is clearly demonstrated by the lower set of plots in Figure 2, where all seven eigenvalues are on the periphery of the "crater" region. Some candidates for measures of non-normality for the Godunov matrix are given in the second row of Table I. We conclude that, in cases such as this, condition numbers cannot provide reliable characteristics for the non-normality property. Instead, a good candidate for the reliable measure of non-normality in engineering practice could be the Henrici number. In Section 7 we will study the quality of estimates based on the Henrici number.

Examples of a similar nature become more common in engineering applications and include the Wilkinson matrices (Marques and Tomazou,
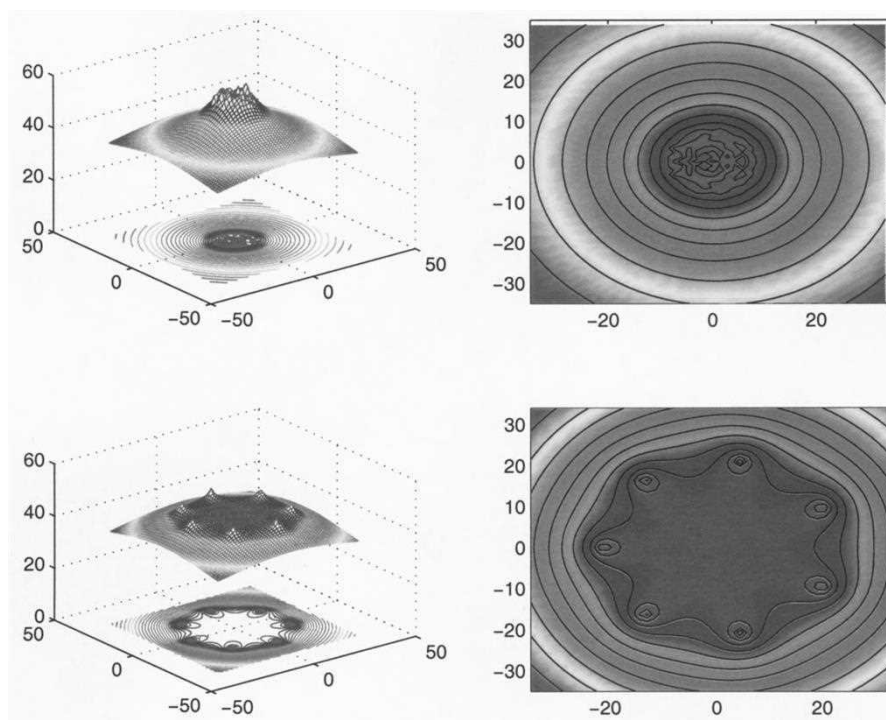
Figure 2.
Surface and
pseudospectral plots of
the Godunov matrix

1995), La Rose type matrices (Chaitin-Chatelin and Fraysse, 1996), Tolosa matrix (Braconnier *et al.,* 1995), Pores3 (Carpraux *et al.,* 1994), the "Kahan" matrix (Toh and Trefethen, 1996), Toeplitz matrices (Reichel and Trefethen, 1992) among others. Important examples exist in the study of hydrodynamic stability where the smooth flow may be amplified by factors of the order 10^5 by a linear mechanism even though all eigenmodes decay monotonically (Trefethen, 1997).

In the end, it is not a question of which software package does better, nor is it a choice between floating point or symbolic arithmetics that is of primary importance in the explanation of the phenomena, but rather a choice of what is feasible and appropriate to compute. Pseudospectra provide the engineer with a useful tool to make such a choice.

5. Spectrum dichotomy and the Lyapunov equation
Visualising capabilities of computational packages readily available to the engineer provides a convenient tool for analysing numerical localisation of operator spectra. For symmetric (or more generally Hermitian matrices) this analysis becomes more or less trivial due to the fact that ϵ-pseudospectra of corresponding matrices/operators form the union of ϵ-balls with centres in the points of their spectra. In the general non-Hermitian case the topology of pseudospectra may be quite complex with the possibility of becoming split into

several parts (grouped clusters of eigenvalues). Indeed, if an ϵ-pseudospectrum consists of p isolated parts ($p \geq 1$), and each of these parts contains several eigenvalues, eigenvalues belonging to the same part might not be separable by any finite-time numerical procedure. Therefore, in those engineering applications which involve non-Hermitian matrices and/or non-self-adjoint operators, it is often more reasonable to concentrate our efforts on topological aspects of spectral problems than on computation of individual eigenvalues. This situation is typical in the stability analysis of model (4.15) where the reasonable question to ask would be how ϵ-spectra are located with respect to the imaginary axis (linear dichotomy) or with respect to the unit circle (circular dichotomy) etc. Indeed, the dichotomy problem is closely connected with the investigation of matrix/operator stability, and this connection can be seen via model (4.15), the solution of which can be given in the matrix exponent form as

$$\mathbf{x}(t) = \exp(tA)\mathbf{x}(0). \tag{5.1}$$

If we assume that $\mathbf{x}(0)$ can be given with infinite precision, then the stability of the model will be defined by the behaviour of the matrix exponent itself, $\exp(tA)$. It is common for the engineer to think of the value

$$q = \min_{j=1,\ldots,n} |\Re e\, \lambda_j(A)| \tag{5.2}$$

as a condition number of the matrix A (λ_j are eigenvalues of the matrix A). However, in reality this characteristic is not appropriate for the description of $\exp(tA)$ when $t > 0$ is finite. Indeed, although the parameter (5.2) may be an adequate characteristic of matrix stability in the limit $t \to \infty$, many engineering applications require a conclusion about the stability of the model in the case when $0 < t < \infty$. This conclusion cannot be drawn solely on the information about the parameter q.

It is more appropriate, therefore, to confront the problem of matrix stability with an approach that combines information on spectra and resolvents. Such a combination is at the heart of the Lyapunov method that gives a criterion of matrix A-stability. In the case of real matrices the following result (see, for example, Godunov *et al.* (1992); Malyshev (1993) and references therein) is the key to further constructions.

Theorem 3.1. If the following matrix equation (the "continuous" Lyapunov equation)

$$A^T X + XA = -C \tag{5.3}$$

is satisfied for some symmetric positive definite matrices X and C, then the matrix A is stable. Conversely, if A is stable, then the solution of the equation (5.3) exists and is unique for any matrix C and may be represented by the following matrix integral

$$X = \int_0^\infty \exp(tA^T)C\exp(tA)dt. \tag{5.4}$$

From (5.4) it is clear that, if $C = C^T > 0$, then the solution of (5.3) is also positive/definite. In particular, if $C = I$ we have

$$X = H = \int_0^\infty \exp(tA^T) \exp(tA) dt. \tag{5.5}$$

We introduce the following measure of quality of matrix stability (all norms below are spectral):

$$\kappa(A) = 2||A||\,||H|| \tag{5.6}$$

sometimes referred to as the condition number of the problem on matrix stability (see Malyshev (1993) and references therein). The use of (5.6) as a characteristic of matrix stability allows us to derive the following upper bound on the matrix exponential in (5.1):

$$|| \exp(tA)|| \leq \kappa_t(A) = \sqrt{\kappa(A)} \exp[-t||A||/\kappa(A)]. \tag{5.7}$$

In turn the condition (5.7) is essential in proving the convergence of the matrix integral (5.4) (Godunov, 1991). Whereas the formula (5.7) couples the characteristics of quality of matrix stability with the time variable (the larger κ is the worse stability of A), the standard approach to the problem of stability largely ignores this coupling. In Section 4 we have demonstrated the importance of such a coupling, which has to be taken into account every time we deal with non-symmetric (or more generally non-Hermitian) matrices. Since in the general case perturbations of eigenvalues of such matrices may substantially exceed perturbations of matrix elements, the determination of all eigenvalues (as well as the eigenbasis) from the Jordan chains such as (2.8) may be inappropriate. The difficulty with such an approach in engineering computations consists of the fact that computational errors in the solution of the problem on spectral dichotomy are dependent not only on the norm of the matrix A but on the norm of matrix H as well. As follows from the above discussion, the information on H may be extracted from the solution of the Lyapunov equation.

Now, let us show how such difficulties may be obviated in the general non-Hermitian case under the assumption that the matrix A does not have eigenvalues on the imaginary axis. From the computational point of view we have to couple the accuracy of computation of the matrix H and the value of the condition number $\kappa(A)$ in the numerical procedure. Namely, if ϵ is the error of computation of H and $\mathcal{E}$ is the lower bound on the condition number such that

$$||H_\epsilon - H|| \leq \epsilon, \quad \kappa(A) \geq \mathcal{E}, \tag{5.8}$$

then the consistency between ϵ and $\mathcal{E}$ have to be chosen with respect to the digital arithmetic of the computer. In principle, ϵ may be arbitrarily small, yet it is always positive. As we have shown with the examples in Section 4, there might exist such $\delta = \delta(\mathcal{E})$ that the perturbed matrix A_ϵ with $||\Delta|| < \delta$ may have a different number of eigenvalues in the left-hand plane from the number

of spectrum points there. Since in such situations we cannot rely on computing individual eigenvalues, we will try to solve the dichotomy problem assuming the absence of eigenvalues on the imaginary axis (or on the unit circle for the circular dichotomy). This assumption is required for the following reason. It is well-known (see, for example, Godunov (1991); Godunov *et al.* (1992)), that the problem of linear dichotomy may be viewed as the problem of constructing projective operators P and $I - P$ on the invariant manifolds that correspond to the spectrum points on the left and on the right of the imaginary axis. The quality of the dichotomy can be defined from the inequalities (5.8), where H in the general case is defined as the Lyapunov integral

$$X = H_C = \frac{1}{2\pi} \int_{-\infty}^{\infty} (A^* + itI)^{-1} C (A - itI)^{-1} dt, \tag{5.9}$$

which provides the solution of the "continuous" Lyapunov equation

$$A^* H_C + H_C A = -C \tag{5.10}$$

when all the spectrum of A lies in the left-hand plane (i.e. $P = I$). Now, if A does not have purely imaginary eigenvalues, then there is an intrinsic connection between operator H_C and the solution of the differential equation

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x} + f(t) \tag{5.11}$$

provided that

$$\|f(t)\| < \infty \quad \text{when} \quad |t| < \infty. \tag{5.12}$$

Under the above conditions there exists a unique solution of the equation (5.11) defined as

$$\mathbf{x}(t) = \int_{-\infty}^{\infty} G(t - s) f(s) ds, \tag{5.13}$$

where G is the Green matrix. Then the solution of (5.10) may be represented as follows

$$H_C = \int_{-\infty}^{\infty} G^*(t) C G(t) dt. \tag{5.14}$$

The Green matrix function is bounded by the value of $\kappa_t(A)$ (see (5.7)), and is the solution of the equation:

$$\frac{dG(t)}{dt} = AG(t) + \delta(t)I, \tag{5.15}$$

where $G(+0) - G(-0) = I$. Furthermore, $P = G(+0)$ and for all $t, s > 0$ function $G(t)$ has the following semigroup property (Pazy, 1983)

$$G(t+s) = G(t)G(s). \tag{5.16}$$

Hence, computations of the projective operator P (as well as H_C) are reducible to the solution of a boundary value problem (5.15), and the accuracy of such computations will be defined by the value of $\kappa_t(A)$. One may control ϵ (see (5.8)) using an effective new method proposed recently in Gavrilyuk and Melnik (1998). The method is based on the Cayley transform technique (Gavrilyuk and Makarov, 1996; 1998; Gavrilyuk and Melnik, 1998)

$$T_\gamma = (\gamma I - A)(\gamma I + A)^{-1} \tag{5.17}$$

and does not require the normality condition. It has been proved that the solution of the Lyapunov equation (5.10) for stable matrices A may be represented in the following form:

$$H_C = -\frac{1}{2\gamma} \Big\{ C + S + 2T_\gamma(A^*)CT_\gamma(A) + T_\gamma(A^*)ST_\gamma(A) + \\ 2T_\gamma^2(A^*)CT_\gamma^2(A) + T_\gamma^2(A^*)ST_\gamma^2(A) + \ldots \Big\}, \tag{5.18}$$

where $S = -T_\gamma(A^*)C - CT_\gamma(A)$. Such a representation implies a natural approximation of H by H_ϵ^N with a finite number of terms $(N+1)$ in (5.18). Then (see details in Gavrilyuk and Makarov (1998)) the estimate

$$||H - H_\epsilon|| \leq 2||C|| \frac{\tilde{q}^{N+1}}{1 - \tilde{q}} \tag{5.19}$$

with $\tilde{q} = \max\{||T_\gamma(A^*)||, ||T_\gamma(A)||\} < 1$ provides an efficient way of controlling the accuracy of computation of matrix H. Other methods of spectral dichotomy have been recently discussed in Malyshev and Sadkane (1997).

An appropriate assumption for the applicability of the method described above is strong positiveness and densely definiteness of the operator A (Gavrilyuk and Makarov, 1996; 1998; Gavrilyuk and Melnik, 1998). For given positive numbers ϕ and γ ($\gamma_{\min} \leq \gamma \leq \gamma_{\max} \leq \infty$) in the complex plane $\mathbb{C}$ we define a closed path (see Figure 3):

$$\Gamma \equiv \Gamma(\phi, \gamma, A) = \mathcal{R}^\pm(\phi, \gamma) \cup \mathcal{W}(\phi, \gamma, A). \tag{5.20}$$

If A is an unbounded operator, then Γ consists of two rays

$$\mathcal{R}^\pm(\phi, \gamma, A) = \{\gamma \exp(\pm i\phi), \gamma_{\min} \leq \gamma \leq \gamma_{\max}\}, \tag{5.21}$$

and the circular arc

$$\mathcal{W} \equiv \mathcal{W}_{\min}(\phi, \gamma, A) = \{|z| = \gamma_{\min}, |\arg z| \leq \phi\}. \tag{5.22}$$

For a bounded operator A, $\mathcal{W}$ consists of 2 arcs $\mathcal{W}_{\min}$ and $\mathcal{W}_{\max}$ (the second arc is depicted in Figure 3 by a dashed line).
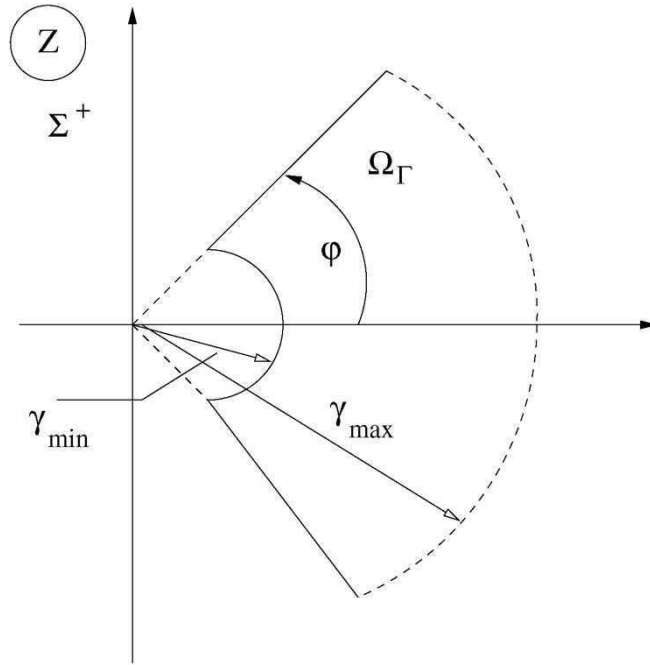
Figure 3.
Spectral angle and
positiveness of linear
operators

By (5.20) the complex plane is divided into two sets as shown in Figure 3, Σ^+ and Ω_Γ, where

$$\Sigma^+ = \{z \in \mathbb{C}: 0 < \phi \leq |\arg z| < \pi\} \cup \{z \in \mathbb{C}: |z| \leq \gamma\} \qquad (5.23)$$

(for certain γ and ϕ), such that the following connection between these sets, the resolvent set $\rho(A)$, and the spectral set $\Sigma^+(A)$:

$$\Sigma^+ \subset \rho(A), \ \Sigma(A) \subset \Omega_\Gamma \qquad (5.24)$$

hold. If we further assume that there exists a constant $M > 0$ such that

$$||(zI - A)^{-1}|| \leq \frac{M}{1 + |z|} \quad \forall z \in \Sigma^+, \qquad (5.25)$$

then the operator A is positive if there exists such $\phi, \gamma, M > 0$ that (5.23)-(5.25) are satisfied. The lower bound $\phi(A) \equiv \phi(A, E)$ of all ϕ for which A is positive is called the spectral angle of the operator A. Now we are in a position to formulate the main condition under which the technique described will work, i.e. the condition of strong positivity of operator A.

Definition 5.1. A positive operator A is called strongly positive if its spectral angle satisfies the inequality

$$\phi(A) < \frac{\pi}{2}. \qquad (5.26)$$

There is a natural competition in the inequalities (5.25) and (4.9) which stems from the connection between $\Sigma^+(A)$ and $\Sigma_\epsilon(A)$. Indeed, the closer $\lambda \in \Sigma_\epsilon$ approaches to an eigenvalue of the matrix A, the smaller the value ϵ and the larger the norm $||(\lambda I - A)^{-1}||$. Therefore, it may happen that, although the actual eigenvalues lie on the left of the curve Γ, such points λ occupy regions on the right of this curve. This leads naturally to the conclusion that in the general case

$$\Sigma_\epsilon^+ \equiv \Sigma_\epsilon(A) \cap \Sigma^+(A) \neq \emptyset. \tag{5.27}$$

Furthermore, we observe that, when $\epsilon \to 0^+$ and the set Σ_ϵ^+ contracts to a point, the spectral angle approaches to $\pi/2$,

$$\phi(A) \to \frac{\pi}{2}. \tag{5.28}$$

As a result of (5.28), $M \to \infty$ in (5.25) and, strictly speaking, one may use neither the assumption of strong positivity of A nor the assumption on the absence of purely imaginary eigenvalues. Although these difficulties have a fundamental theoretical nature, in practice they can be overcome by visualising topological neighbourhoods of eigenvalues.

6. Constructing spectral portraits

A number of algorithms are available in the literature for computing pseudospectra and the subsequent construction of spectral portraits. This includes (see Chaitin-Chatelin and Fraysse (1996); Marques and Toumazou (1995); Braconnier (1997); Braconnier et al. (1997); Braconnier and Higham (1996); Fraysse et al. (1996) and references therein):

- singular value decomposition;
- Lanczos algorithm on the augmented matrix;
- shift-and-invert algorithms.

The core of all such algorithms contains the following steps:

(1) determination of a region $\mathcal{R}$ of interest in $\mathbb{C}$;
(2) discretisation of this region (see below);
(3) computation of the value $||(A - zI)^{-1}||_2$ for each point $z \in \mathcal{R}$;
(4) display the computed values for $z \in \mathcal{R}$.

Below we briefly describe different options for these steps.

Step 1 for selecting the region which contains the values of interest for a spectral portrait can be completed using a number of available algorithms such as QR algorithm, the Gershgorin disk algorithm, matrix norm algorithm, field of values algorithm (Braconnier and Higham, 1996). The latter is often chosen as the most efficient in terms of the total computational cost (Braconnier et al., 1997). This algorithm consists of computing the field of values using the set of Rayleigh quotients as follows

$$F(A) = \left\{ \frac{z^*Az}{z^*z} : \quad z \in \mathbb{C}, \quad z \neq 0 \right\}. \tag{6.1}$$

Then the computation of boundary of F(A) can be done easily if we split the matrix into its Hermitian and skew-Hermitian parts:

$$z^*Az = z^*A_Hz + z^*A_Sz, \text{ where } A_H = (A + A^*)/2, \ A_S = (A - A^*)/2 \tag{6.2}$$

and notice that

$$\min(\max)\{Re(\omega) : \omega \in F(A)\} = \min(\max)_{z \neq 0} \frac{z^*A_Hz}{z^*z} = \lambda_{\min(\max)}(A_H). \tag{6.3}$$

We can apply the same procedure to any matrix $A_\theta = e^{i\theta}A$ (indeed, $F(e^{i\theta}A) = e^{i\theta}F(A)$). However, since $F(A)$ is a convex set, we have to apply the above procedure (i.e. to compute extremum eigenvalues for two Hermitian matrices) only twice, for $\theta = 0$ and $\theta = \pi/2$.

Step 2 involves dealing with the resolvent of a linear operator A for a regular point, $\lambda \in \mathbb{C}$, of the operator, i.e. $R_\lambda = (\lambda I - A)^{-1}$. We may expect that the points of ϵ-pseudospectrum fill some neighbourhoods of "exact" eigenvalues of A. Therefore in the complex plane (to be simulated by screen) we introduce a rectangular grid with a computer point with which (monitor pixel) we associate a small rectangle the size of which may be controlled. To each small rectangle we assign a colour number related to the value of λ at the centre in the complex plane. Further, for each of such λ we compute ϵ as follows

$$\epsilon = \frac{1}{||A|| ||R_\lambda(A)||} = \frac{1}{||A|| ||(\lambda I - A)^{-1}||} = \frac{\sigma_n(\lambda I - A)}{\sigma_1(A)}, \tag{6.4}$$

where $\sigma_{\max} = \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n = \sigma_{\min}$ are singular values of the corresponding $n \times n$ matrices. Depending on the value of the ratio (6.4) we define the colour that is used to fill-in the rectangle which corresponds to the specific value λ. For example, in computations presented in Sections 4 and 7 we defined L ($L = 30$) different intervals for ϵ using the following rule:

$$2 \times 2^{-3m} \leq \epsilon < 2 \times 2^{-3(m-1)}, m = 1, \ldots, 29, \tag{6.5}$$

$$0 \leq \epsilon \leq 2 \times 2^{-3(30-1)} = 2 \times 2^{-87} = 1.2925 \times 10^{-26}, m = 30. \tag{6.6}$$

Then we assign an integer number to each interval (6.5)-(6.6) according to the rule

$$m = [(1 - \log_2 \epsilon)/3]. \tag{6.7}$$

For example, for $m = 22$ we have

$$2 \times 2^{-66} \leq \epsilon < 2 \times 2^{-63}, \text{ i.e. } 2.7105 \times 10^{-20} \leq \epsilon < 2.1684 \times 10^{-19} \text{ etc.}$$

Step 3 is the most time-consuming part of the procedure and involves computation of $\|(A - zI)^{-1}\|_2$ for complex numbers z of a predefined region of interest $\mathcal{R} \subset \mathbb{C}$. One of the simplest algorithms, yet very reliable, is based on the use of the singular value decomposition (SVD), whose application is based on the following observation

$$\|(A - zI)^{-1}\|_2 = \sigma_{\min}^{-1}(A - zI), \tag{6.8}$$

where $\sigma_{\min}(A - zI)$ is the smallest singular value of $A - zI$. Recall that the singular value decomposition of A is

$$A = U\Sigma V^*, \quad \text{or} \quad Av_j = \sigma_j u_j, j = 1, \ldots, n, \tag{6.9}$$

where U (resp. V) is a unitary eigenbasis for AA^* (resp. A^*A). The singular value σ_j gives metric information about A. When A is non-normal, the SVD contains information about A which is more reliable and more robust to perturbations than the information provided by the spectral decomposition (Chaitin-Chatelin, 1996; Golub and van Loan, 1989; Trefethen, 1992). In the wide range of values of $\|(A - zI)^{-1}\|_2$ (say, $10^{-1} - 10^{12}$) this algorithm performs well. Its main drawback is relatively large computational time and the memory requirements (of order n^2). Therefore, for larger matrices Lanczos-type algorithms and the Arnoldi (Krylov subspace) iterations provide a useful alternative to the SVD decomposition (Braconnier and Higham, 1996; Carpraux *et al.*, 1994). Since their efficiency deteriorates when $\|(A - zI)^{-1}\|_2$ is small, a different techniques such as the shift and invert may provide further improvement (Braconnier, 1997). The review of such techniques can be found in Trefethen (1999).

The idea of spectral portraits comes naturally if together with the matrix A we consider a family $\mathcal{F}$ of perturbed matrices. This allows us to deal with the union of all spectra of $\mathcal{F}$-representatives. In this case the spectral norm of matrix A (invariant with respect to orthogonal transformations),

$$\|A\| = \sup\{\|Ax\| : \|x\| = 1\} = \sigma_{\max}(A), \tag{6.10}$$

is not sufficient to provide an appropriate characteristic on the behaviour of all representatives of the $\mathcal{F}$-family. One needs the information on the resolvent of A and such information should be coupled to the algorithm of computation. This is done in *Step 4* of the algorithm through ϵ which allows us to implement a hierarchy of different levels of perturbations. As a result of such implementation we obtain the visual representation of ϵ-pseudospectra of matrices or operators on the screen of the monitor. If for some matrices or operators the regions with sufficiently small ϵ become large, one should pay increasing attention to the geometry of such regional boundaries. They may become essentially irregular with patching patterns clearly visible on the screen of the monitor. In fact, one may expect that in the neighbouring pixels ϵ may take values from different intervals. These difficulties become increasingly noticeable when $\epsilon \to 0^+$.

7. Concluding examples and future directions

Important examples of instability in engineering computations are provided by matrices associated with polynomials. One of the classical examples is given by the La Rose matrix (see, for example, Chaitin-Chatelin and Fraysse (1996); Marques and Tamazou (1995)). In solving spectral problems associated with such matrices, it is important to take into account not only the information on the spectral norm of the matrix, but also the information on the norm of its resolvent. One of the reasons for this stems from the fact that condition numbers may not be appropriate characteristics of non-normality of such matrices.

Consider, for example, the following polynomial

$$P^0(x) = (x+4)^3 x^2 (x+1)^3 (x+2)^2 = \sum_{i=0}^{10} a_i x^i, \tag{7.1}$$

where

$$a_0 = a_1 = 0, \ a_2 = 256, \ a_3 = 1,216, \ a_4 = 2,416, \ a_5 = 2,612,$$
$$a_6 = 1,676, \ a_7 = 653, \ a_8 = 153, \ a_9 = 19,$$

and define the companion matrix $R = \{r_{i,j}\}_{i,j=1}^{10}$ of this polynomial by
$$r_{10,i} = -a_{i-1}, \ i = 1, \ldots, 10; \quad r_{i,j+1} = 1, \ j = 1, \ldots, 9. \tag{7.2}$$

Other elements of the matrix (7.2) are zero. This matrix, which is a typical example of non-normal matrices, does not have any single eigenvalue. All eigenvalues, –4, –2, –1, 0, are defective eigenvalues of multiplicity 3, 2, 3, 2, respectively. Some functions and estimates for this matrix are given in the last row of Table I. As expected in this case, the conditions number cannot provide an appropriate tool to characterise the non-normality property of this matrix.

Many polynomial matrices that arise from engineering applications depend on a parameter that may vary. In such cases it is very important to analyse pseudospectra for different values of the parameter, using reliable characteristics of matrix non-normality. Our next example explains this point in detail. We consider the following parametric polynomial:

$$P_\alpha(x, \alpha) = (x^2 + 2x + \alpha)^3 (x+2)(x+3)(x-6)^2 = \sum_{i=0}^{10} a_i x^i, \tag{7.3}$$

where α is a parameter,

$$a_0 = 216\alpha^3, \ a_1 = 1,296\alpha^2 + 108\alpha^3, \ a_2 = 2,592\alpha + 1,296\alpha^2 - 18\alpha^3,$$
$$a_3 = 1,728 + 3,888\alpha + 216\alpha^2 - 7\alpha^3, \ a_4 = 3,456 + +1,728\alpha - 96\alpha^2 + \alpha^3,$$
$$a_5 = 2,448 + 24\alpha - 15\alpha^2, \ a_6 = 592 - 126\alpha + 3\alpha^2, \ a_7 = -76 - 9\alpha,$$
$$a_8 = -48 + 3\alpha, \ a_9 = -1, \ a_{10} = 1.$$

Using the same procedure for (7.3) as for (7.1), we construct a parametric matrix (7.2) associated with (7.3). We start from $\alpha = -1$. The surface plot and the plot of pseudospectra for this case are presented in Figure 4 (see the set of plots in the upper row). Note that in addition to two single eigenvalues –2 and –3, and eigenvalue 6 of multiplicity 2, the constructed matrix has now also two distinct eigenvalues, $-1 \pm \sqrt{2}$. It might happen that, within the given accuracy, the region that corresponds to eigenvalues –2 and $-1 - \sqrt{2} \approx -2.4142$ almost merges with the region corresponding to eigenvalue –3. However, the surface plot helps to identify three distinct peaks that correspond to these eigenvalues. A very interesting behaviour exhibits the region that corresponds to eigenvalue $-1 + \sqrt{2} \approx 0.442$. The peak corresponding to this eigenvalue (presented in the surface plot) and the deepening of the region (from the right) in the pseudospectra plot show an approximate location of this eigenvalue.

The situation changes for $\alpha = 0.5$ (see the set of plots in the middle row in Figure 4). The increasing value of α leads to a re-orientation of the above regions. Indeed, now the region that corresponds to three eigenvalues, –3, –2 and $-1 - \sqrt{2}/2 \approx -1.7071$ splits into three sub-regions, while the deepening (from the left) of the central region indicates the presence of eigenvalue $-1 + \sqrt{2}/2 \approx -0.2929$.

A further increase in α leads to the "diffusion" of the central region to the left which, in turn, leads to the enlargement of distances between the above three
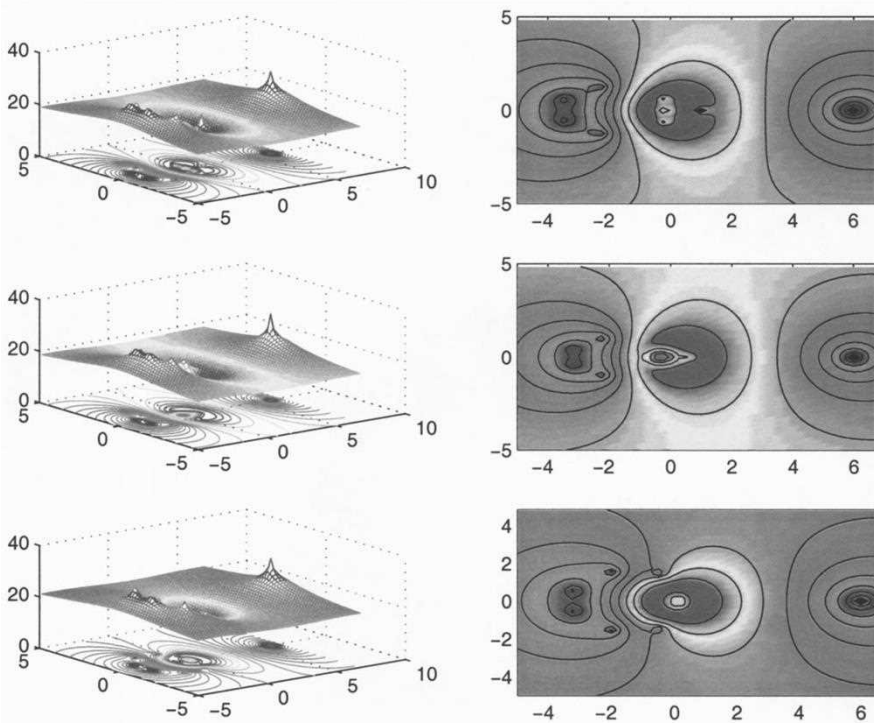

Figure 4.
Surface and
pseudospectral plots of
the parametric matrix
associated with (7.3) for
different values of
parameter α
($\alpha = -1$; 0.5; 1).

sub-regions (see the set of plots in the lower row in Figure 4 where the case $\alpha = 1$ is presented). Now, however, these three sub-regions correspond to two eigenvalues only, –3 and –2. The "diffused" central region corresponds to eigenvalue –1 of multiplicity 2 and hence, the corresponding peak in the surface plot moves to the left from the imaginary axis.

Since parameters may influence substantially on topological properties of pseudospectra, as demonstrated by the above example, we investigate this issue further. In particular, we compute the following four characteristics of non-normality of matrix A as functions of parameter α:

(1) $\nu_1(A)$, defined by formula (4.1);

(2) $\nu_2(A)$, defined by (4.2);

(3) $\mathrm{He}(A)$ defined by (4.3); and

(4) the low bound of the Smith inequality (see (4.5)), i.e. the Henrici-Smith number $\mathrm{He}_S(A)$.

The corresponding plots are presented in Figure 5 (from left to right and from top to bottom, respectively). These functions of α provide a qualitative description of the behaviour of the non-normal matrix associated with (7.3). It is seen that the scaling units of the Henrici-Smith number are the most appropriate for this description. After a local minimum at $\alpha \approx -0.5$, we observe the growth of non-normality of the parametric matrix associated with
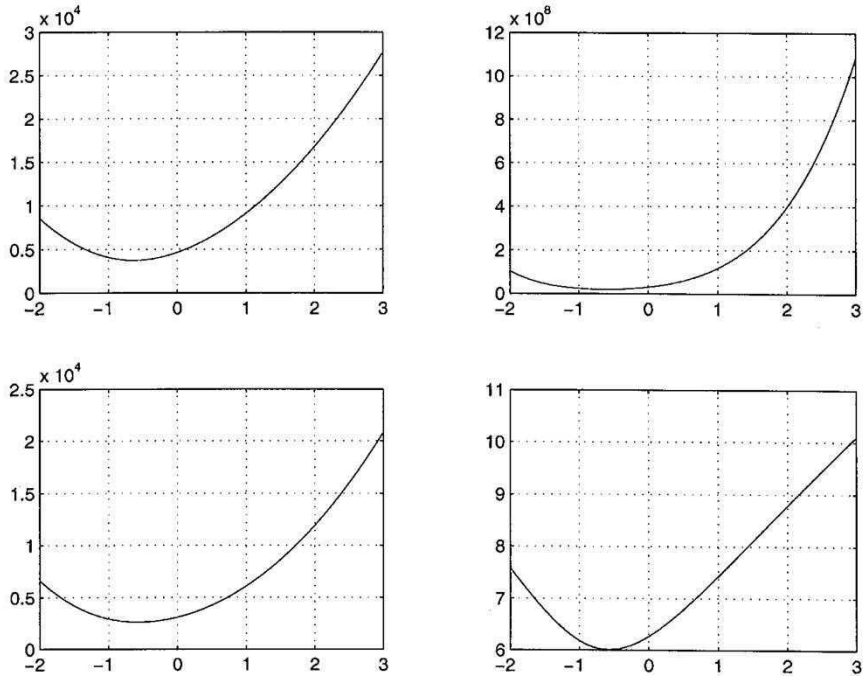

Figure 5.
Non-normality measures of the matrix associated with (7.3) (as functions of α)

(7.3). This behaviour suggests that sufficiently large values of α can provide a deeper insight into the effect of different perturbation patterns. We fix α at 100 and construct perturbed matrices according to the following principle

$$\mathcal{A} = A + 10^{-5} z \, \tilde{A}, \tag{7.4}$$

where

$$z = \cos(\theta_j) + i\sin(\theta_j), \ \ \theta_j = \frac{\pi}{4}(j - 1), \ \text{and} \ \tilde{A} = \text{rand}(\text{size}(A, 2)). \tag{7.5}$$

We note that in addition to single eigenvalues –2, –3 and eigenvalue 6 of multiplicity 2 which we have dealt with before, now we have two complex conjugate eigenvalues $-1 \pm \sqrt{99}$. We show that under perturbations of matrix A this leads to the break of the symmetry with respect to the real axis. By increasing j, we increase θ_j, moving its values along a unit circle $z = \exp(i\theta_j)$ clockwise. In Figure 6 we present contour plots for the original matrix A and for the perturbed matrices obtained from (7.5) for $j = 1$, $j = 3$, $j = 4$, $j = 5$, $j = 7$, respectively (from left to right and from top to bottom).

Regions of all eigenvalues (including complex) of the original matrix are clearly identifiable in Figure 6. Taking $\theta_j = 0$ (that is $j = 1$ and $z = 1$) will result in the splitting of regions that correspond to complex and multiple
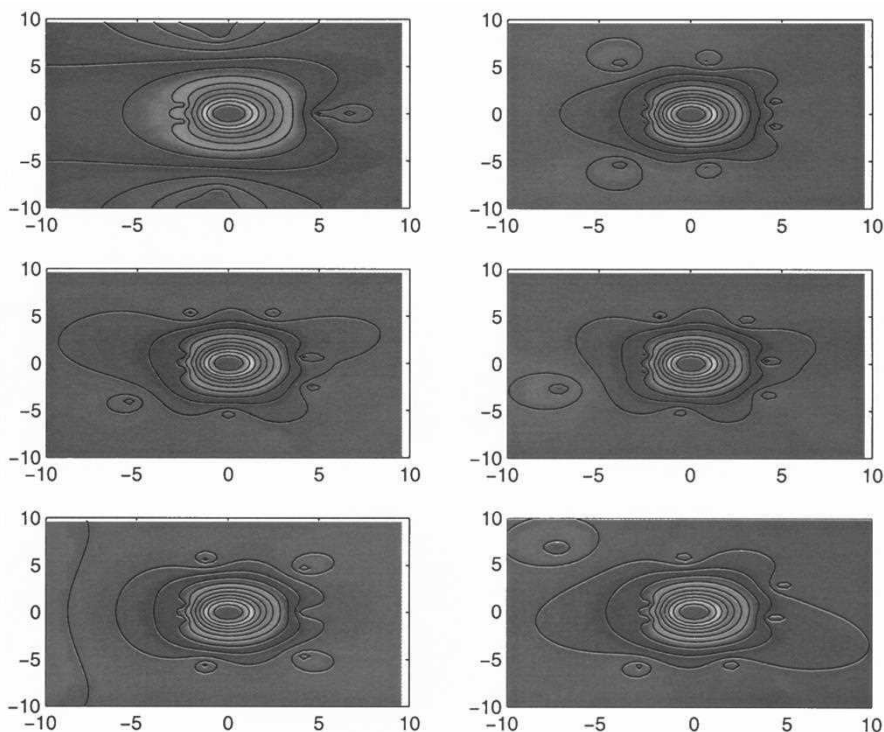

Figure 6.
Pseudospectral plots of
the parametric matrix
associated with (7.3)
under different
perturbation patterns
($\alpha = -0.5$)

eigenvalues. Moving along the unit circle about the angle $\theta_j = \pi/2$ (that is $j = 3$ and $z = i$) will break the symmetry. This is also demonstrated by the next plot presented for $\theta_j = 3\pi/4$ ($j = 4$ and $z = -\sqrt{2}/2 + i\sqrt{2}/2$). As expected, real values of z tend to restore the symmetry with respect to the real axis, as demonstrated by the next plot presented for $\theta_j = \pi$ ($j = 5$ and $z = -1$). The splitting of the region that corresponds to eigenvalue 6 of multiplicity 2, as well as the region that corresponds to the pair of complex eigenvalues are demonstrated by the next plot of Figure 6 presented for $\theta_j = 3\pi/2$ ($j = 7$, $z = -i$). This behaviour leads to the formation of patches which characterise the same eigenvalue with given accuracy.

In our last experiment the value of $\alpha = -0.5$ is chosen to give an approximation to local minima of functions $\nu_1(A), \nu_2(A), \text{He}(A), \text{He}_S(A)$ presented in Figure 5. In this experiment we analyse the main characteristics of non-normality, $\nu_1(A), \nu_2(A), \text{He}(A)$, and $\text{He}_s(A)$ as functions of j, and hence, according to (7.5), functions of θ_j. As functions of θ_j, good measures of non-normality have to exhibit a periodic behaviour when θ_j moves along the unit circle $z = \exp(i\theta_j)$. However, this periodicity is observed neither for $\nu_1(A)$ nor for $\nu_2(A)$. In fact, these functions exhibit a non-periodic oscillatory behaviour in a close vicinity of values 3.745×10^3 and 1.9839×10^7, respectively. At the same time, the Henrici number (the upper plot in Figure 7) and the Henrici-Smith number (the lower plot in Figure 7) provide good engineering measures of non-normality.

Our concluding remarks address three major issues:

(1) Any similarity transformation or other technique performed computationally on an operator or a matrix does perturb its spectrum. As a result, any computational package will provide only points of the spectra of perturbed rather than unperturbed operators/matrices. This means that the computed numbers, widely accepted as eigenvalues in a variety of applied engineering problems, are just a subset of the ϵ-pseudospectrum of the original operator/matrix. Of course, the "original" operators/matrices themselves might only be given approximately. Furthermore, no matter how small ϵ is, if it is fixed within certain bounds, there always exist operators/matrices with large regions of pseudospectra for any ϵ-bounds chosen a priori. In such cases a substantial error in computation of

Figure 7.
Non-normality measures of the matrix associated with (7.3) (as functions of j)
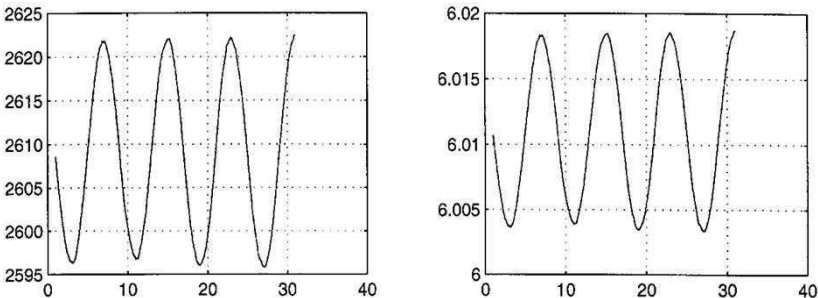
eigenvalues is inevitable. Having an algorithm for computing "pure" numbers does not necessarily lead to the correct conclusion on the behaviour operators/matrices. In order to draw adequate conclusions such numbers have to be supplemented by spectral portraits of the investigated operators/matrices (Trefethen, 1992; 1997; 1999).

(2) Since the classical convergence conditions such as that requiring the spectral radius to be less than 1 ($\rho(A) < 1$) may not be generic enough for finite precision computations (Chaitin-Chatelin and Gratton, 1996), an important development of the presented work is the analysis of convergence properties of numerical procedures in the discretisation of evolutionary partial differential equations. Indeed, it is often appropriate to formulate necessary and sufficient conditions of convergence of numerical methods in terms of pseudospectra (Reddy and Henningson, 1993; Trefethen, 1992), and the Kreiss matrix theorem technique has been proved to be a useful tool in the analysis of these methods (see Trefethen (1999) and Chaitin-Chatelin *et al.* (1999) and references therein). Using the idea of pseudospectra, convergence of convection-diffusion models was recently analysed in Harrabi (1998b) and a new numerical procedure for these models was recently proposed in Gavrilyuk and Melnik (1998).

(3) Since the stability analysis is relative to the choice of the class of perturbations, another important issue to be addressed in the future is the characterisation of the class of perturbations generated by the finite precision arithmetic. Indeed, due to natural limitations of numerical stability in finite precision computations, one has to couple the arithmetic precision with all computational parameters and input data (Chaitin-Chaletin and Fraysse, 1996). This idea leads to a fresh look at asymptotic methods applied in the theory of singular perturbations. Typically, an asymptotic expansion, say U_ϵ, may provide an approximation to the solution of the investigated problem under the assumption of $\epsilon \to 0^+$. In all practical problems ϵ may be small, yet it is always positive and fixed, providing the upper limit on perturbations. In such situations there always exist examples when U_ϵ may provide completely misleading results compared to the solution of the original problems (see also Melnik and Melnik (1997); Melnik (1997)). From the theoretical point of view, even if we formally consider a mathematical model as unperturbed, we have to investigate its stability to perturbation in a typically infinite dimensional space wider than the state space of the system. The natural choice for such a space is a non-reflexive space such as L^1 (rather than L^2 as it is commonly accepted). This idea has been recently developed from different directions in Borwein and Zhu (1997); Melnik (1997); Tveito and Winther (1995) where links to the recent advances in control theory as well as numerical procedures can also be found.

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