

ON THE ITERATIVE SOLUTION OF NONNORMAL PROBLEMS

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Abstract: *Iterative methods are widely used to solve systems of linear equations. The behavior of Krylov subspace methods is relatively well understood in the case of normal operators. Here we summarize the results of papers [I, II, III, IV, V, VI], in which tools to gain information on the convergence behavior of iterations for nonnormal operators are presented and tested in practice for a set of examples.*

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This thesis consists of this overview and the following papers.

Publications

- [I] S. Hyvönen, Convergence of the Arnoldi method when applied to the Picard-Lindelöf iteration operator, *Journal of computational and applied mathematics* **87** (1997), 303-320.
- [II] S. Hyvönen, Polynomial Acceleration of the Picard-Lindelöf Iteration, *IMA Journal of Numerical Analysis* **18**(4) (1998), 519-543.
- [III] S. Hyvönen, Numerical computation of the Nevanlinna characteristic function, *Institut Mittag-Leffler, Report 17, 1997/98*.
- [IV] S. Hyvönen, Case studies on growth properties of meromorphic resolvents, *Institut Mittag-Leffler, Report 18, 1997/98*.
- [V] S. Hyvönen, Growth of resolvents of certain infinite matrices, *Helsinki University of Technology, Institute of Mathematics, Research Reports A402 (1998)*.
- [VI] S. Hyvönen and O. Nevanlinna, Robust bounds for Krylov methods, *Helsinki University of Technology, Institute of Mathematics, Research Reports A403 (1998)*.

1 Introduction

In scientific computing one frequently encounters the problem of solving a linear system of the form

$$Ax = b.$$

When the dimension of the problem is small, it is natural to solve this problem using direct methods, such as Gaussian elimination. As the size of the problem grows, the computing time and the storage requirements may grow enough to make this approach unpractical. Now, the problems that arise in practice may be arbitrarily large. However, they often have special properties, such as sparseness, that can only partly be exploited by direct methods. An alternative approach to solve linear systems is to use iterative methods.

Some of the first iterative methods to solve large linear systems were relaxation-type methods, such as SOR [39], [40]. These methods modify the components of a given initial vector one (or a few) at a time according to some rule, until convergence is reached. One of the main difficulties here is choosing a good relaxation parameter in the general case. Today these methods are mainly used in some specific applications and in preconditioning [31].

Today most practical methods use matrix-vector multiplication, as this can be obtained relatively cheaply by taking advantage of sparseness (and other special properties of the system). Many such iterative methods have been introduced in the past years. The conjugate gradient method (CG), introduced by Hestens and Stiefel in 1952 [10] can be used to solve Hermitian positive definite linear systems. Though CG was introduced already in the 1950's, it was not properly appreciated until in the 1970's, when key developements were made in making preconditioned algorithms practical [29], [2]. For more information on the history of CG see [5].

A number of CG-type methods have been proposed for solving non-Hermitian systems, the most widely used one of which is the general minimal residual method (GMRES), due to Saad and Schultz [33]. GMRES generates the optimal solution in the sense, that it finds in the Krylov subspace generated from a given initial vector the approximation for which the 2-norm of the residual is minimal. However, the computing time and the storage requirements grow per iteration step, making this algorithm impractical in the long run. To avoid this problem we can restart the algorithm regularly, but this leads to slower convergence. Other non-Hermitian iterative methods have been introduced, such as BiCG, QMR, CGS, BiCGSTAB etc. These methods usually generate nearly optimal solutions and have (roughly) constant work and storage requirements per iteration step. However, they may fail. This problem can be avoided by look-ahead techniques, but then work and storage requirements are no longer constant per iteration step.

The behavior of iterative methods in the Hermitian case is relatively well understood via tools like spectral decomposition. This is not the case for non-Hermitian problems, especially in the case of nonnormal A . That is, as

long as A is normal, the decay of the error can be related to an approximation problem on the spectrum, but how to describe the decay of the error of the iteration per iteration step in terms of properties of A has been an open question. Understanding this would enable us to design better preconditioners, as we would know exactly what properties of A are desirable to guarantee fast convergence.

In practice the problems to be solved are always finite dimensional, and most literature dealing with solving linear systems assume A to be a matrix. However, the number of iteration steps we can afford to take is small compared to the dimension of the problem, which may be arbitrarily large. So though the iteration always terminates in a number of steps less or equal to the dimension of the problem, we do not witness this in practice, since we cannot afford take so many iteration steps (unless the problem is small enough to be efficiently solved e.g. using direct solvers). Therefore it is reasonable to discuss the more general case where A is a bounded linear operator in a Banach (or Hilbert) space. This way we get a better picture of the phenomena that occur during the iteration process. In particular we get a clear picture of the asymptotic behavior of the iteration error, as termination at the point where the iteration step equals the dimension of the problem does not occur.

In this discussion we assume exact arithmetic. For effects of finite precision arithmetic see e.g. [6] and references therein.

2 Convergence of Krylov methods

Assume A is a bounded linear operator in a Banach space B such that the spectrum of A has k distinct limit points $\lambda_1, \dots, \lambda_k \neq 0$. Consider the problem

$$Ax = b.$$

Define

$$p(\lambda) = \prod_{i=1}^k (\lambda - \lambda_i) = \lambda q(\lambda) + c,$$

where $c = (-1)^k \prod_{i=1}^k \lambda_i$ and $q(\lambda) = \frac{1}{\lambda}(p(\lambda) - c)$. Then

$$p(A)x = q(A)Ax + cx = q(A)b + cx,$$

from which we get the fixed point formulation

$$x = \frac{1}{c}(p(A)x - q(A)b) = \hat{A}x + \hat{b},$$

where $\hat{A} = \frac{1}{c}p(A)$ and $\hat{b} = -\frac{1}{c}q(A)b$. Note that the spectrum of \hat{A} has the origin as its only limit point. From now on we consider a fixed point problem of the form

$$x = Ax + b,$$

where the spectrum of A has the only limit point at the origin.

The simplest iterative scheme to solve this is the method of successive approximations

$$x^{n+1} = Ax^n + b, \quad n = 1, 2, \dots \quad (1)$$

Given a vector $x^n \in B$ we denote by d^n the associated residual

$$d^n := Ax^n - x^n + b.$$

In the method of successive approximations the residual satisfies $d^n = x^{n+1} - x^n$. The error $e^n := x - x^n$ and the residual are related:

$$(1 - A)e^n = d^n.$$

So (if $(1 - A)$ has a bounded inverse) controlling the residual controls the error up to an unknown constant $\|(1 - A)^{-1}\|$. It is easy to see that the error on the n^{th} iteration step is

$$e^n = x - x^n = A(x - x^{n-1}) = Ae^{n-1} = \dots = A^n e^0.$$

It is reasonable to ask whether one can find a better candidate for a solution in the affine space generated by the iterates x^n . This approach leads to *Krylov subspace methods*. Assume a given initial vector x^0 , compute the initial residual d^0 and from that the Krylov sequence $\{A^j d^0\}_{j=0}^{n-1}$. Now search a solution candidate from the affine space $x^0 + \text{span}\{A^j d^0\}_{j=0}^{n-1}$:

$$x^n = x^0 + \sum_{j=0}^{n-1} \gamma_{jn} A^j d^0.$$

Define the polynomials $q_{n-1}(\lambda) = \sum_{j=0}^{n-1} \gamma_{jn} \lambda^j$ and $p_n(\lambda) = 1 - (1 - \lambda)q_{n-1}(\lambda)$. Now

$$\begin{aligned} d^n &= p_n(A)d^0, \\ x^n &= p_n(A)x^0 + q_{n-1}(A)b, \\ e^n &= p_n(A)e^0. \end{aligned}$$

The method of successive approximations can be thought of as a special of the above, with $p_n(\lambda) = \lambda^n$.

The norm of the error satisfies

$$\|e^n\| = \|p_n(A)e^0\| \leq \|p_n(A)\| \|e^0\|,$$

so studying the convergence of Krylov methods leads to the following question: given a sequence of polynomials $\{p_n\}$, with $\deg p_n = n$ and $p_n(1) = 1$, how does $\|p_n(A)\|$ decay?

In particular, the GMRES algorithm minimizes the norm of the residual on each step. In other words, the residual d^n satisfies

$$\|d^n\| = \min_{p_n \in \mathcal{P}_n} \|p_n(A)d^0\|,$$

where \mathcal{P}_n is the set of all polynomials p_n such that $\deg p_n = n$ and $p_n(1) = 1$. The worst-case behavior of GMRES is given by

$$\|d^n\| = \max_{\|d^0\|=1} \min_{p_n \in \mathcal{P}_n} \|p_n(A)d^0\| \leq \min_{p_n \in \mathcal{P}_n} \|p_n(A)\|.$$

The problems of minimizing $\|p_n(A)d^0\|$ and minimizing $\|p_n(A)\|$ over \mathcal{P}_n have been studied e.g. in [9], [22]. For normal matrices these are equal and numerical experiments have shown that they are equal for a wide variety of matrices and values of n [6, p. 58]. Recently it has been shown that $\max_{\|d^0\|=1} \min_{p_n \in \mathcal{P}_n} \|p_n(A)d^0\|$ and $\min_{p_n \in \mathcal{P}_n} \|p_n(A)\|$ may differ [36], [3], so the bound given by $\min_{p_n \in \mathcal{P}_n} \|p_n(A)\|$ is not always sharp. In any case, knowing how $\min_{p_n \in \mathcal{P}_n} \|p_n(A)\|$ decays gives us an upper limit for the convergence of the residual (and therefore the error) of GMRES.

If $p_n(A)$ satisfies

$$\|p_{n+N}(A)\| \leq C \left(\frac{\tau e \omega}{n}\right)^{n/\omega}$$

for $n > 0$, we say that $p_n(A)$ admits a superlinear bound of order ω and type τ with delay N and constant C . If a Krylov method generates the polynomials p_n which admit a superlinear bound of order ω and type τ , we say that the error of the method decays with at most order ω and type τ .

The smaller the order and type with which the error decays are, the faster the iteration converges. Decreasing the order will lead to a more significant speedup than decreasing the type.

Normal operators. Let A be a bounded, normal operator in a Hilbert space H and let p_n be a polynomial. Then

$$\|p_n(A)\| = \sup_{\lambda \in \sigma(A)} |p_n(\lambda)|.$$

This follows from the Spectral theorem for normal operators, see e.g. [30, remark 12.24, pp. 309-310]. For matrices this follows easily from the fact that all normal matrices are unitarily similar to a diagonal matrix, the diagonal elements of which are the eigenvalues. Thus, for normal operators the convergence rate of GMRES is reduced to a problem in approximation theory, namely that of approximating zero on the spectrum with a polynomial. This problem is far from simple and no easy solutions to it exist. However, an intuitive idea on 'good' and 'bad' eigenvalue distributions still holds: eigenvalues clustered around a single point far from 1 are good, whereas eigenvalues scattered around 1 are bad, as by the maximum principle it is not possible to have a polynomial satisfying $p_n(1) = 1$ and $p_n(x) < 1$ for all x on some closed curve around 1 [6, pp. 51, 55]. For some results on the convergence

of GMRES for diagonalizable matrices see [31, pp. 194-197]. The convergence estimate given is valid not only for normal matrices, but as it involves the condition number of the transformation matrix, the bound is good only when this is of moderate size, which means that the matrix is not too far from being normal. Note that to get estimates for the convergence of GMRES for normal operators we need to know the spectrum. The problem of determining the spectrum is discussed shortly in Section 4.

Quasinilpotent operators. A class of operators very different from normal operators discussed above, the behavior of which nevertheless is also quite well understood, is provided by quasinilpotent operators, that is operators for which the spectral radius vanishes: $\rho(A) = 0$. For a quasinilpotent operator the resolvent $(1 - zA)^{-1}$ is always an entire function in z . If the maximum modulus of the resolvent

$$M_\infty(r, (1 - zA)^{-1}) := \sup_{z=r} \|(1 - zA)^{-1}\|$$

satisfies for some $0 < \omega < \infty$ and $0 < \tau < \infty$

$$M_\infty(r, (1 - zA)^{-1}) \leq Ce^{\tau r^\omega},$$

then [22] for $n \geq 1$

$$\min_{p_n \in \mathcal{P}_n} \|p_n(A)\| \leq \|A^n\| \leq C \left(\frac{\tau e \omega}{n}\right)^{\frac{n}{\omega}}. \quad (2)$$

This in fact gives a bound for the error of the method of successive approximations, and therefore one also for GMRES, though naturally this bound for the error of GMRES is not sharp. Just how large a gap is there between the decay of $\min_{p_n \in \mathcal{P}_n} \|p_n(A)\|$ and that of $\|A^n\|$ is investigated for the Picard-Lindelöf iteration operator (see Section 3) in [II] and for the integral operator and its powers (again see Section 3) in [IV].

Note that we frequently write the resolvent as $(1 - zA)^{-1}$ instead of $(\lambda - A)^{-1}$. We do this to avoid the inconvenience of having to deal with functions of $\frac{1}{\lambda}$ instead of z . Actually,

$$(\lambda - A)^{-1} = \frac{1}{\lambda} \left(1 - \frac{1}{\lambda} A\right)^{-1} = z(1 - zA)^{-1},$$

where $z = \frac{1}{\lambda}$. Here and later we use tools from function theory to analyze the growth of the resolvent. As entire (or later meromorphic) functions $z(1 - zA)^{-1}$ and $(1 - zA)^{-1}$ grow with the same speed, it suffices to look at the latter, which we call here the resolvent, though strictly speaking we are missing a z .

Thus, when A is normal or quasinilpotent, the behavior of GMRES is relatively well understood. But what about nonnormal operators in general? What is known is that the spectrum is not the answer in this case. It has been demonstrated [7] that any nonincreasing curve represents a plot of residual

norm versus iteration step for the GMRES method applied to some problem; moreover, the problem can be chosen to have any eigenvalues. One approach to estimating $\|p_n(A)\|$, suggested by Trefethen [34], [35], is using the *pseudospectrum*. Let γ be a curve enclosing the spectrum of A . Then

$$p_n(A) = \frac{1}{2\pi i} \int_{\gamma} p_n(\lambda)(\lambda - A)^{-1} d\lambda$$

so

$$\|p_n(A)\| \leq \frac{l(\gamma)}{2\pi} \sup_{\lambda \in \gamma} \|p_n(\lambda)(\lambda - A)^{-1}\|,$$

where $l(\gamma)$ is the length of the curve γ . Consider the curve γ_ε on which

$$\|(\lambda - A)^{-1}\| = \varepsilon^{-1}.$$

Then

$$\|p_n(A)\| \leq \frac{l(\gamma_\varepsilon)}{2\pi\varepsilon} \sup_{\lambda \in \gamma_\varepsilon} |p_n(\lambda)|. \quad (3)$$

This implies that the error of GMRES satisfies for any ε

$$\|e_k\| \leq \frac{l(\gamma_\varepsilon)}{2\pi\varepsilon} \inf_{p_n} \sup_{\lambda \in \gamma_\varepsilon} |p_n(\lambda)| \|e_0\|.$$

Here γ_ε is the boundary of the ε -pseudospectrum of A :

$$\Lambda_\varepsilon = \{\lambda \mid \|(\lambda - A)^{-1}\| \geq \frac{1}{\varepsilon}\}.$$

Note that the bound (3) is not sharp, for replacing $\|\int_{\gamma_\varepsilon} p_n(\lambda)(\lambda - A)^{-1} d\lambda\|$ by $l(\gamma_\varepsilon) \sup_{\lambda \in \gamma_\varepsilon} \|p_n(\lambda)(\lambda - A)^{-1}\|$ may lead to a significant overestimation. For some problems a careful choice of ε yields a good estimate of the actual error of GMRES, while for others no choice of ε leads to a realistic error estimate [8].

A different approach to estimating $\|p_n(A)\|$, which is also based on looking at the size of the resolvent, is provided by viewing the resolvent as a meromorphic function, and applying tools from function theory to measure the size of the resolvent. Remember, that an operator valued function $F(z)$ is called meromorphic for $|z| < R$, where $0 < R \leq \infty$ is fixed, if around each z_0 in $|z_0| < R$ it has a representation of the form

$$F(z) = \sum_{k=-h}^{\infty} F_k(z - z_0)^k. \quad (4)$$

Here F_k is a bounded linear operator in H and F_{-h} is nontrivial. If $-h < 0$, then F has a pole at z_0 of order h , otherwise F is analytic at z_0 . Here $F(z) = (1 - zA)^{-1}$, so the poles of F are the eigenvalues of A . Note that bounded linear operators with resolvents meromorphic for $|z| < \infty$ include, but are not restricted to, compact operators.

Rolf Nevanlinna [27], [28], introduced in 1925 a characteristic function $T(r, f)$ to measure the growth of meromorphic functions. This can be generalized to operator valued functions. The obvious way is to replace the absolute value by the norm of the operator valued function. This leads to a generalization denoted here by $T_\infty(r, F)$ [19], [20], [23], [VI], defined as follows:

Definition 1. Let $F(z)$ be a meromorphic operator valued function as above. Denote $h(z_0) := \max\{h, 0\}$ and define

$$n_\infty(r, F) := \sum_{|b| \leq r} h(b).$$

Thus n_∞ counts the poles in $\{z \mid |z| < r\}$ together with their orders. Furthermore define

$$N_\infty(r, F) := \int_0^r \frac{n_\infty(t, F) - n_\infty(0, F)}{t} dt + n_\infty(0, F) \log r$$

and

$$m_\infty(r, F) := \frac{1}{2\pi} \int_{-\pi}^{\pi} \log^+ \|F(re^{i\varphi})\| d\varphi.$$

Finally define

$$T_\infty(r, F) = m_\infty(r, F) + N_\infty(r, F).$$

We have the following result, which follows from Theorem 17 in [VI] with a suitable choice of constants. Let A be a bounded linear operator such that $(1 - zA)^{-1}$ is meromorphic in the whole complex plane and for all $r > 1$

$$T_\infty(r, (1 - zA)^{-1}) \leq \tau r^\omega. \quad (5)$$

Then there exists a sequence of polynomials $p_j \in \mathcal{P}_j$ such that for $j \geq \omega c(\omega)\tau$

$$\|p_j(A)\| \leq \frac{\|1 - A\|}{\prod_{k=1}^n |1 - \lambda_k|} \left(\frac{\tilde{\tau} e \omega}{j}\right)^{j/\omega}, \quad (6)$$

where λ_k are the eigenvalues of A ordered decreasingly,

$$\begin{aligned} n &= n_\infty(2, (1 - zA)^{-1}), \\ \tilde{\tau} &= 2c(\omega)\tau(1 + e^{\tau\omega}), \\ c(\omega) &= \frac{2(1 + \omega + \sqrt{1 + \omega^2})(1 + \sqrt{1 + \omega^2})^\omega}{(1 - \omega + \sqrt{1 + \omega^2})\omega^\omega}. \end{aligned} \quad (7)$$

Of course (6) also gives a bound for the decay of the error of GMRES. This bound is not sharp. First of all, for the sequence p_j for which the bound (6) holds, need not be the sequence of polynomials GMRES generates. Secondly, the choice of constants in Theorem 17 in [VI] which yields the bound (6) need not be optimal. Thirdly, though in general it is true for entire operators that for $\theta > 1$

$$T_\infty(r, F) \leq \log^+ M_\infty(r, F) \leq \frac{\theta + 1}{\theta - 1} T_\infty(\theta r, F), \quad (8)$$

for some entire operators in fact

$$T_\infty(r, F) = \log^+ M_\infty(r, F),$$

in which case if

$$M_\infty(r, F) \leq e^{\tau r^\omega}, \quad (9)$$

then

$$T_\infty(r, F) \leq \tau r^\omega. \quad (10)$$

(This is in fact true for F such that $F(z) = G(|z|)$ for some G , see Lemma 1 in [V].) An example of an operator for which (9) and (10) hold is provided by the resolvent of the weighted shift operator W discussed in [V]. From (2) we see that in this case

$$\min_{p_n \in \mathcal{P}_n} \|p_n(A)\| \leq C \left(\frac{\tau e^\omega}{n} \right)^{n/\omega},$$

while (6) gives a much worse estimate

$$\min_{p_n \in \mathcal{P}_n} \|p_n(A)\| \leq C \left(\frac{\tilde{\tau} e^\omega}{n} \right)^{n/\omega}, \quad \tilde{\tau} = 2c(\omega)\tau(1 + e^{\tau\omega}).$$

This overestimation is due to the fact that the upper limit in (8), which is used in the proof of Theorem 17 in [VI], is not necessarily sharp. A similar overestimation occurs whenever the types with which $M_\infty(r, (1 - zA)^{-1})$ and $T_\infty(r, (1 - zA)^{-1})$ grow are close.

Even though the bound given by (6) is not sharp, it does show that for meromorphic resolvents by looking at the growth of resolvent we obtain a bound for the rate of convergence of GMRES:

Theorem 1. *Let A be a bounded linear operator such that $(1 - zA)^{-1}$ is meromorphic in the whole complex plane and for all $r > 1$ (5) holds. Then the error of GMRES decays with at most order ω and with at most type $\tilde{\tau}$, where $\tilde{\tau}$ is as in (7).*

In practice $T_\infty(r, F)$ can be calculated analytically only for fairly simple problems. A numerical tool for computing $T_\infty(r, F)$ is introduced in [III].

3 Examples of nonnormal operators

The Picard-Lindelöf iteration operator. The Picard-Lindelöf iteration was originally known as a method for proving the existence and uniqueness of the solution of an initial value problem satisfying certain continuity assumptions. It was rediscovered in the early 1980s for the simulation of electrical networks [13]. Today the Picard-Lindelöf iteration is often referred to as the waveform relaxation method, and it is used to solve large, stiff systems of initial value problems. Let A be a $d \times d$ -matrix. We want to solve

$$\dot{x} + Ax = f(t), \quad t \in [0, T], \quad x(0) = x^0$$

using the iteration scheme based on the splitting $A = M - N$:

$$\dot{x}^n + Mx^n = Nx^{n-1} + f, \quad x^n(0) = x^0. \quad (11)$$

Introducing the linear convolution operator

$$\mathcal{K}x(t) = \int_0^t e^{-M(t-s)} Nx(s) ds$$

we can write the iteration (11) in the fixed point form

$$x^n = \mathcal{K}x^{n-1} + g, \quad (12)$$

where $g = e^{-Mt}x^0 + \int_0^t e^{-M(t-s)} f(s) ds$. For finite time intervals the iteration operator \mathcal{K} is quasinilpotent. For infinite time intervals \mathcal{K} has a nontrivial spectrum and is therefore no longer quasinilpotent, but it is still non-selfadjoint. So in both cases \mathcal{K} provides a good example of a highly nonnormal operator encountered in practice. The convergence of the iteration (12) on a finite time interval has been studied in e.g. [17], [18]. Convergence on an infinite time interval has been studied in [24], [16] with the motivation that this way we gain information on the rate of convergence which is relevant also on finite but relatively large time windows. See also [25].

The iteration (11) is in fact of the form (1), so from (2) we know that if

$$M_\infty(r, (1 - z\mathcal{K})^{-1}) \leq Ce^{\tau r^\omega}, \quad (13)$$

then

$$\|\mathcal{K}^n\| \leq C\left(\frac{\tau e^\omega}{n}\right)^{n/\omega},$$

which determines the rate of decay of the error of the iteration. In [18] it is shown that the smallest ω and τ for which (13) holds can be determined from the graph properties of the decomposition matrices M and N . The question of polynomial acceleration has been discussed in [II], where we show the following. Assume ω and τ are the smallest constants for which a bound of the form (13) holds. Furthermore assume that the decomposition matrices M and N commute. Then

$$\min_{p_n} \|p_n(\mathcal{K})\| \leq C\left(\frac{\hat{\tau} e^{\hat{\omega}}}{n}\right)^{n/\hat{\omega}},$$

where $\hat{\omega} = \omega$ and if $\omega > 0$ then

$$\frac{\tau}{4} \leq \hat{\tau} \leq \tau.$$

So the rates with which $\|\mathcal{K}^n\|$ and $\min_{p_n} \|p_n(\mathcal{K})\|$ decay do not differ greatly in this case. A more promising approach to speeding up the Picard-Lindelöf iteration is convolution based acceleration, see e.g. [14], [15], [38].

The Volterra operator V^2 and related operators. Another interesting example of the behavior of nonnormal operators is given by looking at the integration operator $Vx(t) = \int_0^t x(s)ds$ and related operators V^α ,

$$V^\alpha x(t) = \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} x(s)ds, \quad \alpha > 0,$$

on the interval $t \in [0, T]$. These are quasinilpotent operators. In [IV] we show that

$$M_\infty(r, (1 - zV^\alpha)^{-1}) \leq Ce^{\tau r^\omega}$$

where $\omega = \frac{1}{\alpha}$ and $\tau = T$, while

$$\min_{p_n} \|p_n(V^\alpha)\| \leq C \left(\frac{\hat{\tau}e^{\hat{\omega}}}{n}\right)^{n/\hat{\omega}},$$

where $\hat{\omega} = \omega$ and if $\hat{\tau} = \frac{1}{4^\omega}\tau$.

In particular V^2 is the iteration operator associated with the initial value problem

$$u'' = u + f, \quad t \in [0, T], \quad u(0) = a, \quad u'(0) = b.$$

Consider the related boundary value problem

$$u'' = u + f, \quad t \in [0, T], \quad u(0) = u(T) = 0.$$

The iteration operator H related to this problem is a self-adjoint Fredholm operator. Moreover, it is a rank-one modification of V^2 . The operator $A_\mu = \mu H + (1 - \mu)V^2$ varies thus from a quasinilpotent operator to a self-adjoint one as μ is varied. Interestingly enough the growth of the resolvent of A_μ as a meromorphic function is essentially independent of μ [IV].

Other examples of nonnormal operators in separable Hilbert spaces are discussed in [V].

4 Approximation of the spectrum

We shall now briefly address the question of approximating the spectrum of a bounded linear operator in a Hilbert space H . General methods for approximation the spectrum by looking at a sequence of finite dimensional matrix approximations have been recently considered in a number of papers, see e.g. [1], [26]. The approach suggested in [26] is based on producing a basis for a subspace of H by iterating with a fixed vector $b \in H$. More precisely, one uses the Arnoldi process to generate an orthonormal basis for the Krylov subspace

$$K(A, b) = \text{cl span}\{b, Ab, A^2b, \dots\}.$$

If the subdiagonal of the Hessenberg matrices created by the Arnoldi process has a subsequence which tends to zero, then the spectrum of the local

operator of A at b is obtained by looking at the resolvents of the Hessenberg matrices. The local operator of A at b is by definition the restriction of A to $K(A, b)$.

In [I] we have asked whether this approach could be used to find the spectrum of the Picard-Lindelöf iteration operator on an infinite time interval, see Section 3. From Theorem 1 in [16] we already know that the spectrum of \mathcal{K} is

$$\sigma(\mathcal{K}) = \text{cl} \cup_{\text{Re}z \geq 0} \sigma(K(z)),$$

where

$$K(z) := (z + M)^{-1}N.$$

So our goal is not to find the spectrum of the Picard-Lindelöf iteration operator, as this is already known. Instead, the Picard-Lindelöf iteration operator provides once again an interesting example of a non-selfadjoint operator which we use to examine the approach explained above. The result of [I] is negative: assumptions under which this approach is guaranteed to work in [26] do not hold.

For more information on numerical linear algebra techniques for spectral approximation see [11] and references therein. The question discussed here is of course related to eigenvalue problems for matrices. A nice review on this topic is given in [37]. See also e.g. [32].

5 Summary

The generalization $T_\infty(r, F)$ of the Nevanlinna characteristic function measures the growth of the operator valued meromorphic function F . In particular it can be used to measure the size of the resolvent operator of a bounded linear operator A provided that the resolvent is meromorphic. Knowing the rate of growth of the resolvent gives a bound for the decay of the error of GMRES as stated in Theorem 1, which follows directly from results given in [VI]. Examples discussed in [II] and [IV] show that though looking at the growth of the resolvent may lead to a bound which may be slightly pessimistic as far as the type with which the error decays is concerned, the order with which the error decays can in these examples be read from the growth of the resolvent. We remind the reader of the fact that the order with which the error decays tells more about the rate of convergence of the method than the type, and decreasing the order will lead to more significant speedup than decreasing the type.

Estimating the growth of the resolvent is therefore an interesting task. This has been done for a number of examples in [IV] and [V]. In practice computing $T_\infty(r, (1 - zA)^{-1})$ analytically is only possible for fairly simple A . A tool for the numerical computation of $T_\infty(r, (1 - zA)^{-1})$ is introduced in [III].

The examples discussed in [IV] and [V] show that even in the case of non-normal operators finding the spectrum is often of interest when determining

the growth of the resolvent. This problem is addressed in [I] for the Picard-Lindelöf iteration operator.

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Remarks and corrections to papers [I]–[VI]

Paper I

- p. 303, row 4 from the bottom: "by looking at those of" should read "by looking at the resolvents of"
- p. 307, row 8 from the bottom: "is obtained from those of" should read "is obtained by looking at the norms of the resolvents of"
- p. 307, row 6 from the bottom: "Arnoldi process a simple" should read "Arnoldi process in a simple"
- p. 309, row 3–5 should read: "at the resolvents of the Hessenberg matrices, as the assumptions of Theorem 4 do not hold. We have $\sigma(h_n) = \{-1\}$ while $\Sigma((h_n)_{n \in \mathbb{N}}) = \sigma(\mathcal{K}) = \{\lambda : |\lambda + 1| \leq 1\}$, as is demonstrated in the next section."
- p. 309, Proposition 2 : "the Laguerre functions are dense in L_1 " should read "the span of the Laguerre functions is dense in L_1 ".
- p. 310, row 12: "it is sufficient" should read "it was sufficient".
- p. 311, Prop. 4 : The assumptions in Proposition 4 should be $\nu \neq 0$, $\operatorname{Re} \mu > 0$.

Paper II

- p. 530, Lemma 9: this holds for h sufficiently small, e.g. $h \leq 1$.
- pp. 534–535, In fact the amount of work done by one step of the polynomially accelerated iteration grows with the iteration step, i.e. a grows with the iteration step. So we reach the point where $x > a$, i.e. using polynomial acceleration is no longer justified, even sooner.

Paper III

- p. 9, The upper right hand corner of the matrix H should be 0.

Paper IV

- p. 5, Lemma 3: $f(z) = g(|z|)$ should be $|f(z)| = g(|z|)$.
- p. 5, Section 3, first paragraph:
Here the resolvent of A is defined as $(I - zA)^{-1}$.
- p. 7, Lemma 4 should be omitted.

- p. 9–10, Lemma 6, from row 2 onwards: "Then there exists for every ε a constant C_ε such that for sufficiently large k

$$0 \leq |a_k| \leq C_\varepsilon \left(\frac{e(1+\varepsilon)}{\alpha k} \right)^{\alpha k}.$$

Moreover, there is a subsequence of $\{a_k\}$ which grows with the same order and type as the upper limit." In the proof, in formulas (15) and (16) the notation is slightly vague. For $0 < \alpha < 2$ see [6]. A relatively simple calculation shows that for $\alpha \geq 2$ and $R > 1$

$$M(E_\alpha \circ \Psi, R) = E_\alpha(R + 2\eta + \frac{\eta^2}{R}) < e^{(R+2\eta+\frac{\eta^2}{R})^{1/\alpha}} < C_\varepsilon e^{(1+\varepsilon)R^{1/\alpha}} \quad (*)$$

which yields the rest of the calculations on page 9, only C should be C_ε , $e^{R^{1/\alpha}}$ should be $e^{(1+\varepsilon)R^{1/\alpha}}$ and $e^{\alpha k}$ should be $e^{(1+\varepsilon)\alpha k} = ((1+\varepsilon)e)^{\alpha k}$. To finish the proof note that by (*) $M(E_\alpha \circ \Psi, r)$ grows with at most order $\omega = \frac{1}{\alpha}$ and type $\tau = 1$. But since $E_\alpha(r + 2\eta + \frac{\eta^2}{r}) > E_\alpha(r)$, which we know to grow with order $\omega = \frac{1}{\alpha}$ and type $\tau = 1$, we know that $M(E_\alpha \circ \Psi, r)$ grows with the same speed as $M(E_\alpha, r)$. Finally, Lemma 6 is used to prove Theorem 9, where also "Then for some constant C_2 " should read "Then there exists for every ε a constant C_ε such that" and in formulas (17) and (18) C_2 and C_3 should be C_ε and η should be $\eta(1+\varepsilon)$.

- p. 11, insert " $\sup_{|x|_\gamma=1}$ " in the beginning of the inequalities on rows 15 and 17.

- p. 11, In formula (21) the $x(t)$ in the middle expression should be omitted.

- p. 11, without Lemma 4 we have row 8 from the bottom onwards: Moreover

$$M(r, R(\lambda, V^\alpha)) \leq \sup_{|\lambda|=r} \left(\frac{1}{|\lambda|} + \frac{\Upsilon}{|\lambda|} E_\alpha \left(\frac{\Upsilon^\alpha}{|\lambda|} \right) \right) = \frac{1}{r} + \frac{\Upsilon}{r} M(r, E_\alpha \left(\frac{\Upsilon^\alpha}{\lambda} \right))$$

so we know that the growth parameters of the resolvent are bounded from above by those of $E_\alpha(\frac{\Upsilon^\alpha}{\lambda})$ (as $\omega_{mer} = \omega$ and $\tau_{mer} \leq \tau$ for entire functions).

- p. 13, row 8: "where he" should read "where the"

Paper V

- p. 12, row 9 from the bottom: $e^{-r \cos \phi (\tilde{\tau} \tilde{\omega})^{1/\tilde{\omega}}}$ should read $e^{-r \cos \phi (\tilde{\tau} \tilde{\omega})^{1/\tilde{\omega}}}$.

- p. 12, row 3 from the bottom: "denominator" should read "numerator" and "nominator" should read "denominator".

- p. 13, row 6 : "But this means that the norm of the resolvent of J is not bounded outside ..." should read "But this means that the resolvent of J is not a bounded operator outside ..."

- p. 14, rows 11 and 12: $r(1 + \frac{r}{e})$ should be $r(1 + \frac{1}{e})$

Paper VI

p. 22, formula (24): $\Pi(z)$ should be $\chi_A(z)$ and $n(t)$ should be $n_\infty(t, \chi_A)$.

p. 22, Example 4: $\lambda_n = \frac{1}{n}$ should be $\lambda_n = -\frac{1}{n}$.

p. 25, row 8 from the bottom: $\leq \frac{\tau(\beta\eta)^\omega}{\log \beta} \frac{\tau\beta^\omega}{\alpha^\omega \log \beta} j$ should be $\leq \frac{\tau(\beta\eta)^\omega}{\log \beta} = \frac{\tau\beta^\omega}{\alpha^\omega \log \beta} j$

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