University *of Ljubljana*
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Seminar I - 1st year, 2nd cycle

Pseudospectra

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Abstract

In systems described by non-normal matrices, dynamics often deviate from expectations based solely on eigenvalue predictions. While eigenvalues are essential for understanding system behavior, they fail to fully capture transient effects that influence stability and evolution. The concept of pseudospectra is introduced as a more comprehensive tool that provides deeper insight into the stability and dynamics of non-normal systems. By referring to applications in quantum mechanics, photonics, and general relativity, we highlight where pseudosectra is relevant in physics today.

Contents

1 Introduction

Eigenvalues of matrices are one of the most successful tools of analyzing and understanding physical systems. They form the foundation of quantum mechanics [1], give rise to Sturm–Liouville theory which plays a crucial role in solving partial differential equations [2] and are essential in characterizing the stability and dynamics of systems across various fields[3, chapter 5]. In physics, problems often involve unitary or hermitian operators, where determining the spectral decomposition is so fundamental that it often provides a complete solution to the problem.

However while looking at spectra one should always proceed with caution when a matrix or operator lacks an orthogonal basis of eigenvectors-that is, when $AA^* - A^*A \neq 0$. This class of operators are often called non-normal and tend to behave "not normally". Non-normal operators can exhibit transient growth, unexpected dynamics, extreme sensitivity to perturbations, and numerical challenges when computing spectra. These effects are not immediately apparent from eigenvalues alone, making standard spectral analysis insufficient.

Many methods have been proposed to characterize non-normality and examine its consequences. This seminar introduces pseudospectra, a method that extends the concept of spectra and helps in understanding the behavior of non-normal operators.

2 Introduction to pseudospectra

Before we define the pseudospectra let us first provide some motivation behind it. Consider very simple tridiagonal Toeplitz matrix and its symmetrized counterpart

$$A = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \frac{1}{4} & 0 & 1 & \cdots & 0 \\ 0 & \frac{1}{4} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & \frac{1}{4} & 0 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \cdots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 \\ 0 & \frac{1}{2} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \frac{1}{2} \\ 0 & \cdots & 0 & \frac{1}{2} & 0 \end{pmatrix}, \in \mathbb{C}^{N\times N}. \tag{1}$$

This are two examples of Toeplitz matrices. Toeplitz matrices are often found in physics [4]. More known examples can be associated with the nearest-neighbor tight-binding lattice systems, the Anderson model vortex pinning in type-II superconductors [5], biased random walks or coupled harmonic oscillators just to name the few. Matrix A and S defined here (1) are related by similarity transformation,

$$S = DAD^{-1}, \tag{2}$$

where $D = \text{diag}(2, 2^2, \ldots, 2^n)$. This transformation is useful because similarity transformations preserve the spectral structure while transforming the matrix A into a symmetric matrix S,

$$\lambda_k(A) = \lambda_k(S) = \cos(\frac{k\pi}{N+1}) \ , \ 1 \ \leq k \ \leq N. \tag{3}$$

Our interest lies in comparing the spectra of the perturbed matrices A and S.

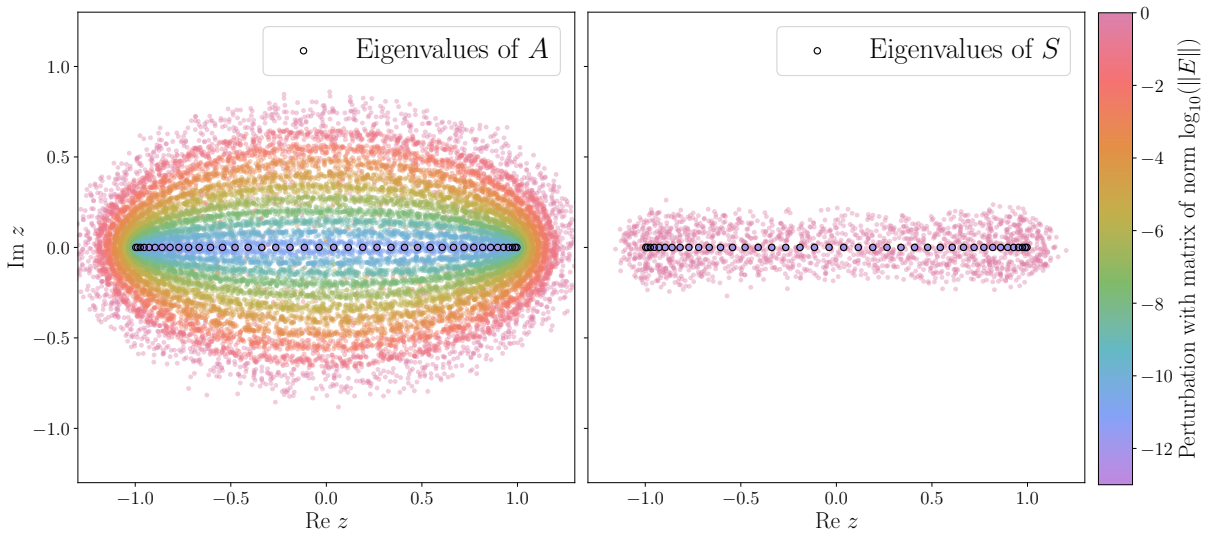

Figure 1: The spectra of the perturbed matrices $A + E \in \mathbb{C}^{40\times40}$ and $S + E \in \mathbb{C}^{40\times40}$, with E as the perturbation, are illustrated. Different colors represent varying magnitudes of the perturbation. While the spectra of matrices A and S are similar, the spectra of perturbed matrices are visually very different.

Figure 1 illustrates the differences between spectra of perturbed matrices $A + E \in \mathbb{C}^{40\times40}$ and $S + E \in \mathbb{C}^{40\times40}$, where E is a random perturbation. It shows that small perturbation of matrix A can lead to drastically different eigenvalues. What is the reason behind different sensitivity to perturbations and can this observation be quantified? As we will see, this unusual behavior is related to the non-normality of matrix A and can be understood using pseudospectra.

3 Pseudospectra

We define pseudospectra, which generalizes the notion of spectra in matrix theory. While the theory of pseudospectra is defined for operators, we will focus on matrices for simplicity.

Theorem 1 ([3]) *Let $A \in \mathbb{C}^{N\times N}$ act on Hilbert space $\mathbf{X}$ and $\varepsilon > 0$ be arbitrary. The ε-pseudospectrum $\sigma_\varepsilon(A)$ of A is the set of $z \in \mathbb{C}$ defined equivalently by any of the following conditions:*

(i) $\|(zI - A)^{-1}\| > \varepsilon^{-1}$,

(ii) $z \in \sigma(A + E)$ *for some* $E \in \mathbb{C}^{N\times N}$ *with* $\|E\| < \varepsilon$,

(iii) $z \in \sigma(A)$ *or* $\|(zI - A)u\| < \varepsilon$ *for some* $u \in \mathbf{X}$ *with* $\|u\| = 1$.

In the beginning we hinted that pseudospectra has something to do with eigenvalues of perturbed matrices. Statement *(ii)* in theorem (1) establishes the equivalence between the $\varepsilon-$*pseudospectra* and eigenvalues of ε-perturbed operator. We can informally state that $\varepsilon-$pseudospectra captures how large can eigenvalues get if we perturb matrix by another matrix of same shape with the norm ε. The equivalence between *(ii)* and (i) establishes a connection between the spectrum of a perturbed matrix and the norm of its resolvent, which is the origin of the term *pseudospectra*. Recall that the spectrum of a matrix $A \in \mathbb{C}^{N\times N}$ is the set of points $z \in \mathbb{C}$ for which $\det(zI - A) = 0$, or equivalently, where $(zI - A)$ is singular. Given a

norm $\|\cdot\|$, we can also characterize the spectrum as the set of points where the norm of the inverse satisfies $\|(zI - A)^{-1}\| = \infty$. The concept of pseudospectra arises from this perspective: the ε-pseudospectrum consists of all points z for which the norm of the resolvent satisfies $\|(zI - A)^{-1}\| > \varepsilon^{-1}$. Statement (*iii*) defines vectors u, which are referred to as ε-*pseudoeigenvectors*. These vectors are analogous to eigenvectors and can be viewed as exponentially good approximation of eigenvectors. As ε varies, the $\varepsilon - pseudospectra$ form a nested sequence of sets, and their intersection converges to the spectrum of the matrix:

$$\bigcap_{\varepsilon>0} \sigma_\varepsilon(A) = \sigma(A). \tag{4}$$

Pseudospectra depend on the choice of norm, which might seem problematic. However, in physics problems are often norm-dependent making the use of pseudospectra valid.

3.1 Perturbations

Given the definition of pseudospectra we can return to the example with matrices A and S. Calculating pseudospectra of matrices A and S requires choice of norm. When plotting figure 1 earlier we did not specify which norm were we using, this is because there is no "right" or "wrong" norm, however the resulting pseudosepctra will depend on the norm chosen. So what is the "right" norm? As mentioned earlier, most physical applications already specify the relevant norm. For example in signal processing the $\mathcal{L}^2$ norm is connected with the energy of the signal. In operator theory the norm is defined as

$$\|A\| = \sup_{\|x\|=1} \|Ax\|. \tag{5}$$

Since the matrices A and S are finite they can be regarded as a bounded operator, allowing us to use the operator norm (5). In the case of finite matrices this norm coincides with the largest singular value of matrix.

$$\|A\|_2 = \max_{z\in\sigma(AA^*)} \sqrt{\|z\|}. \tag{6}$$

Pseudospectra of A and S is calculated by evaluating $\|(zI - A)^{-1}\|_2$ for $z \in \mathbb{C}$. We again plot the spectra of perturbed matrices A and S and compare them with the curves given by $\|(zI - A)^{-1}\| = \varepsilon$ and $\|(zI - S^{-1}\| = \varepsilon$. The results shown on figure 2.

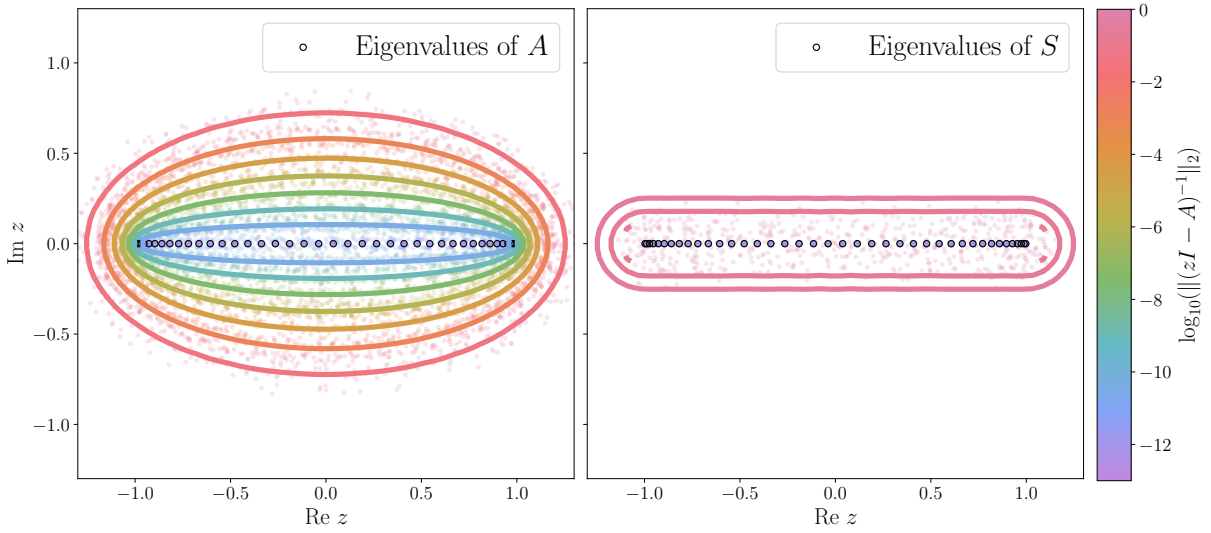

Figure 2: Comparison of pseudospectra computed via the resolvent norm (lines) and the spectra of the perturbed matrices A and S (dots). The solid curves represent the set of complex numbers z for which $\|(zI - A)^{-1}\| = \varepsilon$. By the equivalence of statements (i) and (ii) in Theorem 1, these curves mark the boundaries within which the furthest eigenvalues of A may move under any perturbation of norm ε.

Sensitivity to perturbation of A and S can be quantified by the Bauer–Fike theorem:

Theorem 2 (Bauer-fike [3]) *Let A be an $N \times N$ diagonalizable matrix such that $A = V\Lambda V^{-1}$, where Λ is diagonal. For any $\varepsilon > 0$, the ε-pseudospectra $\sigma_\varepsilon(A)$ satisfies:*

$$\{z \mid dist(\sigma(A), z) < \varepsilon\} \subseteq \sigma_\varepsilon(A) \subseteq \{z \mid dist(\sigma(A), z) < \kappa\varepsilon\}, \tag{7}$$

where $\kappa = \text{cond}(V) = \|V\|\|V^{-1}\|$ is the condition number of the eigenvector matrix V. Theorem 2 is central to understand the difference between perturbing normal and non-normal matrices. So far, we have not discussed much about non-normality, except to note that such operators lack an orthogonal basis of eigenvectors. Normal matrices are defined as matrices that commute with their adjoint:

$$AA^* - A^*A = 0. \tag{8}$$

This property implies that normal matrices have an orthogonal basis of eigenvectors and are therefore unitarily similar to diagonal matrices. Referring back to the Bauer-Fike theorem 2 this means that the condition number κ for such matrices is equal to $\kappa(V) = 1$ in the operator norm [3, chapter 1]. In contrast, for non-normal matrices that are diagonalizable the condition number $\kappa(V)$ can be much larger, $\kappa(V) \gg 1$. If matrices are not diagonalizable measuring non-normality becomes more complicated [3, chapter 10]. Knowing that for normal matrices $\kappa = 1$, theorem 2 states that perturbing a normal matrix by a matrix E with $\|E\|_2 < \varepsilon$ moves its eigenvalues by at most ε in distance. In contrast, for a non-normal matrix the same perturbation can displace eigenvalues by a maximum distance of $\kappa(V)\varepsilon$, where $\kappa(V) \gg 1$. For the numerical example with matrices A and S defined in (1) the condition number of A is given by $\kappa(D) = 2^{N-1}$. If we measure non-normality with condition number we see that it worsens with larger dimension, hinting at the results seen on figure 3. This result suggests that when working with large-dimensional matrices, calculating spectra can result in $\varepsilon - pseudospectra$ due to limitations in machine precision.

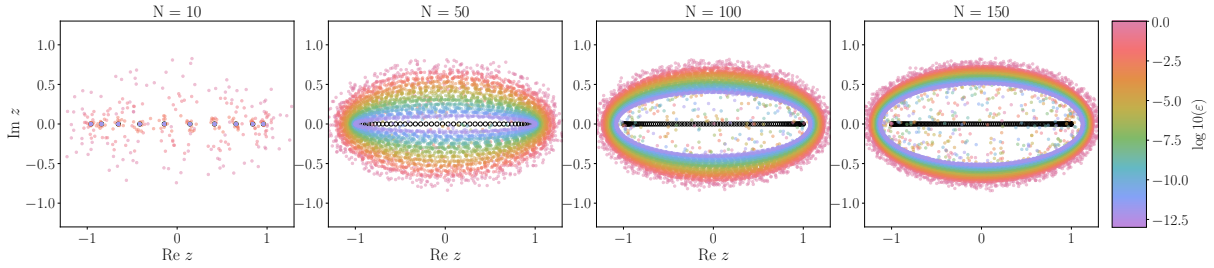

Figure 3: The impact of perturbations on the matrix A for different dimension N. As the dimension increases, the eigenvalues become increasingly sensitive to perturbations.

3.2 Connection to stability

Consideration of pseudospectra is important when analyzing stability of non-normal problems. Typically, stability is determined by calculating eigenvalues and verifying that they lie on the left half-plane. However, as highlighted by Trefethen [3, chapter 5], this criterion can be misleading for non-normal systems. Even if all eigenvalues lie in the left half-plane, small perturbations can be amplified leading to instability. An example of this is the stability of flow for operators derived from the linearized Navier-Stokes equation. These operators are strongly non-normal, with their non-normality increasing as the Reynolds number rises [6, 7]. At larger Reynolds numbers very small perturbations may get linearly amplified enough to trigger nonlinear effects that lead to transition to turbulence.

3.3 Transient dynamics

Referring back to the example (1) with the matrices A and S it was shown that despite having the same spectra, spectra of perturbed matrices were drastically different. To investigate further we examine whether they also differ in other aspects of their behavior. The key quantity of interest is the norm growth of a matrix, specifically $\|A^n\|$. Examples of where such quantity arises in physics go from Markov process to the evolution of purity in certain random quantum circuits [8]. Figure 4 shows the norms

of the matrices A and S raised to the power $n \in \mathbb{N}_0$. This behavior is surprising, especially given that absolute value of all eigenvalues (3), is less than one. What causes this transient effect in matrix A, how it changes with dimension, and why does knowledge of eigenvalues alone fail to predict such phenomena? Once again, we ask: can pseudospectra provide better insight into transient dynamics? The answer is "yes"—while pseudospectra rarely gives exact answers, it can effectively detect and quantify transient behavior that eigenvalues alone fail to capture [3, chapter 4].

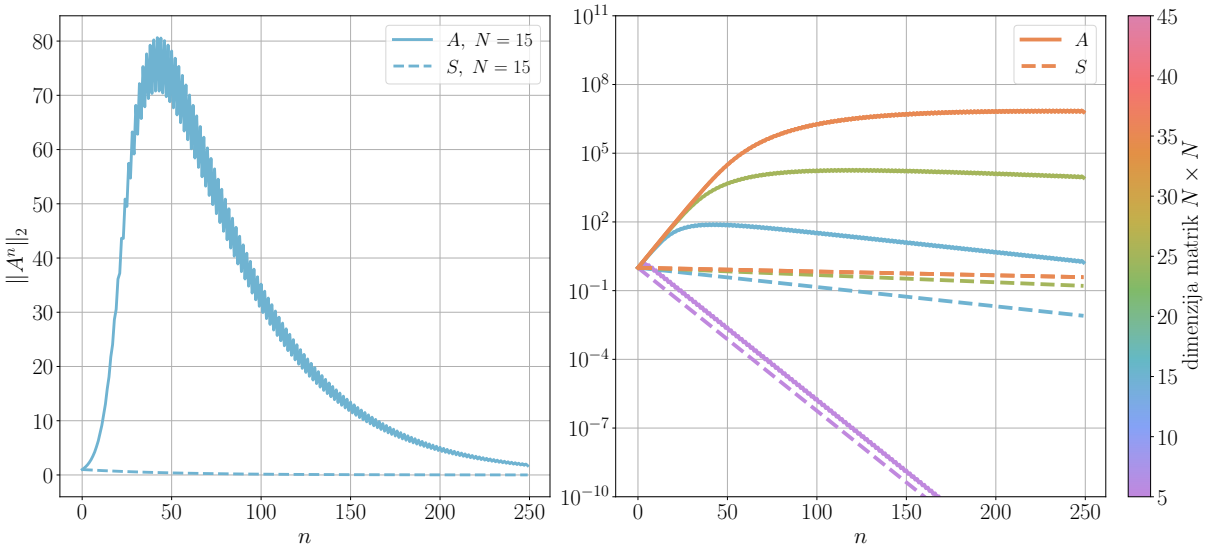

Figure 4: Here, we compare the norm growth of the matrices A and S from Example (1). The figure illustrates the transient growth of A, despite all its eigenvalues being less than one. Although A and S share the same eigenvalues, for larger-dimensions $\sup_{n\geq 0} \|A^n\|$ appears to increase while $\|S^n\|$ stays bounded.

We imagine a problem where we want to understand behavior of vector $\mathbf{u}_n$ obtained by iteration:

$$\mathbf{u}_{n+1} = A\mathbf{u}_n. \tag{9}$$

The equation (9) has a solution of the form $\mathbf{u}_n = A^n\mathbf{u}_0$, where A is a matrix or operator. We are interested in values of $\|A^n\|$ as a function of n, especially what can we tell about the initial growth, transient and decay. We already know if all eigenvalues of A satisfy $\|\lambda\| < 1$ then $\lim_{n\to\infty} \|A^n\| = 0$. However if A is not normal, solution can grow significantly before it eventually decays. To quantify this the following quantities will be important:

$$\rho(A) = \sup\{\|z\| \mid z \in \sigma(A)\}, \tag{10}$$
$$\rho_\varepsilon(A) = \sup\{\|z\| \mid z \in \sigma_\varepsilon(A)\} \tag{11}$$

$\rho(A)$ is called the spectral radius of A, $\rho_\varepsilon(A)$ is named pseudospectral radius. The value of $\rho(A)$ determines the long-time behavior. We state this results precisely.

Theorem 3 ([3]) *Let $A \in B(H)$ where $B(H)$ is denoting bounded operators. We have*

$$\rho(A) = \lim_{n\to\infty} \|A^n\|^{1/n}. \tag{12}$$

We also have

$$\|A^n\| \geq \rho(A)^n \quad \text{for all } n \geq 0. \tag{13}$$

Here we see that the norm of $\|A^n\|$ cannot decrease faster than $\rho(A)^n$, moreover in the limit of large n it behaves precisely that way.

Theorem 3 helps to determine asymptotic decay of iteration, however there is still an option that the value $\|A^n\|$ will grow large before decaying as predicted. This is where pseudospectra is useful.

Theorem 4 ([3]) *Suppose $A \in \mathcal{B}(H)$. Then, for every $\varepsilon > 0$, we have the inequality*

$$\sup_{n\geq 0} \|A^n\| \geq \frac{(\rho_\varepsilon(A) - 1)}{\varepsilon}. \tag{14}$$

These estimate show that if the pseudospectra protrude significantly outside the unit disk in the sense that $\rho_\varepsilon > 1 + \varepsilon$ for some ε, there must be transient growth. Equation (14) holds for all ε, therefore we can define the largest bound as the *Kreiss constant* of A with respect to unit disk by

$$\mathcal{K}(A) = \frac{(\rho_\varepsilon(A) - 1)}{\varepsilon} = \sup_{\|z\|\geq 1} (\|z\| - 1)\|(zI - A)^{-1}\|. \tag{15}$$

Moreover, an upper bound on $\|A^n\|$ is provided by the Kreiss matrix theorem,

Theorem 5 ([3]) *If A is an $N \times N$ matrix, then*

$$\mathcal{K}(A) \leq \sup_{n\geq 0} \|A^n\| \leq eN\mathcal{K}(A), \quad \text{for all } n \geq 0. \tag{16}$$

There are also bounds for finite n,

Theorem 6 ([3]) *Suppose $A \in \mathcal{B}(H)$ and for some z with $\|z\| = r > 1$, $\|(zI - A)^{-1}\| = \frac{K}{r-1}$. Then for any $\tau > 0$,*

$$\max_{0<n\leq\tau} \|A^n\| \geq r^\tau / \left(1 + \frac{r^\tau - 1}{rK - r + 1}\right). \tag{17}$$

Now if $r^\tau \ll rK$ there exist some n for which $\|A^n\|$ is approximately as big as r^τ, or bigger.

We now turn to continuous vesrion of the problem (9), where the solution to the equation

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = A\mathbf{u}, \tag{18}$$

is of form $\mathbf{u}(t) = \mathrm{e}^{At}\mathbf{u}(0)$. Again these are the relevant quantities,

$$\alpha(A) = \sup\{\mathrm{Re}\ z \mid z \in \sigma(A)\}, \tag{19}$$
$$\alpha_\varepsilon(A) = \sup\{\mathrm{Re}\ z \mid z \in \sigma_\varepsilon(A)\}, \tag{20}$$
$$\omega(A) = \sup\{\mathrm{Re}\ z \mid z \in W(A)\}. \tag{21}$$

Here $\alpha(A)$ is called the *spectral abscissa*, $\alpha_\varepsilon(A)$ *pseudospectral abscissa* and $\omega(A)$ is called the *numerical abscissa* of A. There exist analog results for initial grown and decay as in discrete example. We have the following result concerning the behavior for large t.

Theorem 7 ([3]) *Let $A \in B(H)$. Then we have*

$$\alpha(A) = \lim_{t\to\infty} \frac{1}{t} \log \|\mathrm{e}^{tA}\|. \tag{22}$$

Furthermore, we also have

$$\|\mathrm{e}^{tA}\| \geq \mathrm{e}^{t\alpha(A)} \quad \text{for all } t \geq 0. \tag{23}$$

The theorem ensures that the norm can never decay faster than $\mathrm{e}^{t\alpha(A)}$. Similarly as before the initial behavior is governed by the numerical absicssa.

Theorem 8 ([3]) *Let $A \in B(H)$. Then we have*

$$\omega(A) = \frac{d}{dt}\|\mathrm{e}^{tA}\|\Big|_{t=0} = \lim_{t\downarrow 0} \frac{1}{t} \log \|\mathrm{e}^{tA}\|. \tag{24}$$

We also have

$$\|\mathrm{e}^{tA}\| \leq \mathrm{e}^{t\omega(A)} \quad \text{for all } t \geq 0. \tag{25}$$

Meaning that the norm can never grow faster than $\mathrm{e}^{t\omega(A)}$, while the result tells us that initially the solution actually grows that fast. Again turning to pseudospectra for the bounds of maximal growth, we obtain the following theorem.

Theorem 9 ([3]) *For all $\varepsilon > 0$, we have*

$$\sup_{t\geq 0} \|\mathrm{e}^{tA}\| \geq \frac{\alpha_\varepsilon(A)}{\varepsilon}. \tag{26}$$

The estimate tells us that there will be values at some time $t > 0$ at least as large as $\frac{\alpha_\varepsilon(A)}{\varepsilon}$. We can define continuous Kreiss constant as $\mathcal{K}(A) = \sup_{\varepsilon>0} \frac{\alpha_\varepsilon(A)}{\varepsilon}$.

Theorem 10 ([3]) *If A is an $N \times N$ matrix, then it follows*

$$\mathcal{K}(A) \leq \sup_{t\geq 0} \|\mathrm{e}^{tA}\| \leq \mathrm{e}N\mathcal{K}(A). \tag{27}$$

It is also possible to get an estimate valid for a finite time interval, but the expressions are somewhat complicated. Several other estimates exist, but we will not state them here. For further details, see [3, chapter 4].
From here we see a distinction between normal and non-normal matrices when it comes to transient. Normal matrices can be orthogonally diagonalized and their Kress constant is equal to one, $\mathcal{K} = 1$, therefore the bounds for $\|A^n\|$ and $\|\mathrm{e}^{At}\|$ are determined by highest and lowest eigenvalues, wheres non-normal matrices are bounded above and below by pseudospectra. The purpose of this more technical part of seminar was to elaborate on the use value of pseudospectra, especially as these results are quantitative rather then just visual warning. Given numerical example 1 we calculate the upper and lower bounds for $\|A^n\|$. The results are shown in figure 5.

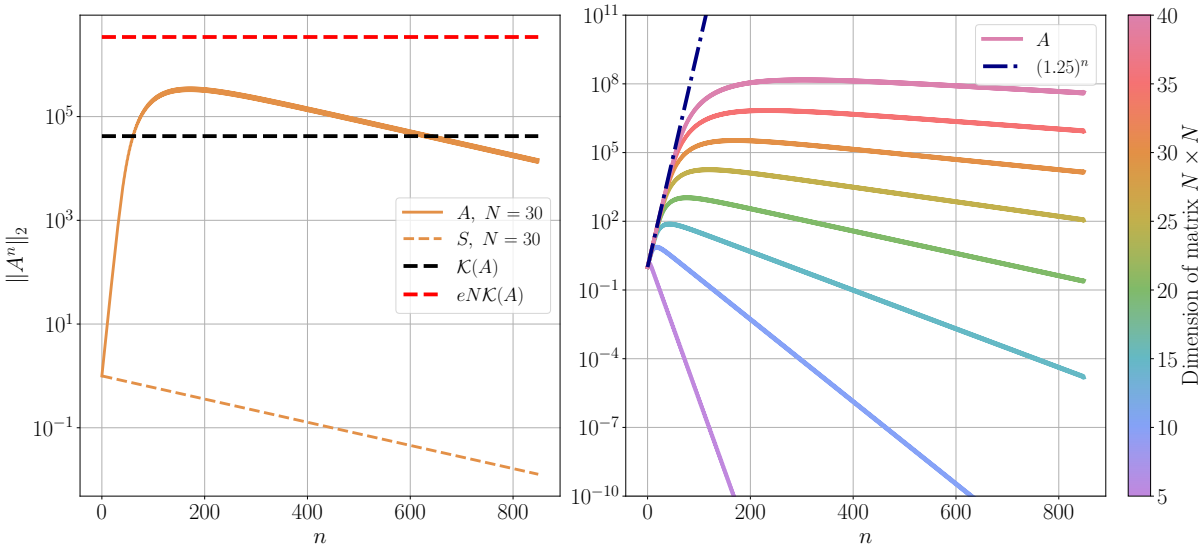

Figure 5: Figure shows lower and upper bounds determined by Kreiss matrix theorem (14) for the numerical example (1), the slope of $\|A^n\|$ for large n is the same as slope of $\|S^n\|$. The bound $(1.25)^n$ is inspired by theorem 6 where r is boundary of pseudospectrum of infinite operator $\lim_{N\to\infty} A_N$ for more details refer to [3, chapter 4, theorem (29.24)].

4 Pseudospectra in physics

As seen from the examples, pseudospectra become relevant when dealing with non-normal operators. In this section, we provide further details on where non-normality arises in various areas of physics and expand on where pseudospectra might be useful.
In physics non-normality can be viewed as the natural opposite of the hermiticity of the Hamiltonian. In quantum mechanics the key postulate is the hermiticity which ensures that that the norm in an isolated system is conserved. While norm conservation would also hold if the Hamiltonian were normal, since normal operators are isometries, we additionally require that measurements are real valued, which is true for Hermitian operators. However, when dealing with systems that do not conserve norm, the governing operators become non-normal. This happens when the system is open, meaning a presence of flows of energy, particles, and information to external degrees of freedom that are out of the Hilbert space of our interest [9]. This include parity-time-symmetric systems in non-hermitian quantum mechanics [10], open quantum systems [11]. Additionally non-Hermitian description has also been used in a variety of non conservative classical systems that include photonics, especially process where we gain or lose photons[12], stochastic processes that are nonreciprocal with respect to state transitions and perturbation of random matrices.
Pseudospectra can be applied to many of the examples mentioned above, to name just a few. In non-Hermitian $\mathcal{PT}$-symmetric quantum mechanics, pseudospectra is central to understanding behavior of these systems [13]. It can also be a way to view the non-Hermitian skin effect[14], as shown in recent works by Yoshida [15] and Okuna [16], pseudospectra could be measured experimentally in such systems. In general relativity, pseudospectra helps to study small perturbations in the gravitational field around black holes determening their stability [17]. In photonics, pseudospectra is used to analyze transient phenomena and quantify them[18].

5 Conclusions

In seminar, we introduced pseudospectra, a tool for understanding the unusual behavior of non-normal systems. We explored their applications in physics and discussed the origins of operator non-normality. Since their begining in the 1990s, a key question has been whether pseudospectra merely serve as a warning when dealing with non-normal systems or if they provide quantitative value. While we presented some quantitative results in the context of transient analysis, many gaps in our understanding remain. There is also many other concepts relevant to the study of non-normality. Some of these are Jordan normal form, singular value decomposition, exceptional points, biorthogonality of eigenstates, and pseudo-Hermiticity. Despite this, pseudospectra continue to be useful in connection with them.
Trefethen, who played a significant role in popularizing pseudospectra through his book [3], views value of pseudospectra today as following: "Anyone who plots eigenvalues of nonsymmetric/nonhermitian matrices operators in the complex plane should routinely include pseudospectra. This gives an instant check of whether the eigenvalues are likely to be meaningful. Some people do this. Most don't". [19].

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