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Volume 175

**Modern Aspects  
of Linear Algebra**

S. K. Godunov



**American Mathematical Society**

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# Modern Aspects of Linear Algebra

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Volume 175

**Modern Aspects  
of Linear Algebra**

S. K. Godunov



**American Mathematical Society**  
Providence, Rhode Island

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## СОВРЕМЕННЫЕ АСПЕКТЫ ЛИНЕЙНОЙ АЛГЕБРЫ

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ABSTRACT. Systematic exposition of the spectral theory of nonselfadjoint operators in finite-dimensional linear spaces is presented. Formulation of the computational problems related to the analysis of the spectrum and brief description of certain algorithms, including some non-standard ones, is given. Examples of operators approximating ordinary and partial differential operators are studied.

The book can be used by researchers and graduate students working in linear algebra, differential equations, applied mathematics, and computational physics.

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## Preface

This book, intended for specialists,<sup>1</sup> discusses fundamental ideas of linear algebra from the point of view the author had formed during more than 30 years of working with computational algorithms. Actually, only one chapter (Chapter 14) is devoted to algorithms per se (there are several additional examples in Chapters 2 and 3 where the theory of orthogonal and unitary transformations is discussed). However, even in Chapter 14 we consider not specific algorithms but rather basic principles of constructing such algorithms.

My goal in this book was not to give a detailed survey but to concentrate on some methods used by our research group. The main concepts presented in the book were elaborated in the analysis of algorithms described in Chapter 14.

There is a significant difference between the qualitative behavior of spectral problems for self-adjoint and for nonselfadjoint matrix operators. In particular, the spectra of two close operators are close if the operators are Hermitian, whereas this is far from being true if the operators are not Hermitian. This leads to some well-known paradoxes. For example, the computation of eigenvalues of an integer-valued matrix and of the transposed matrix, performed on the same computer using the same standard software can lead to different results (see §1.3). To understand the nature of such paradoxes, it is necessary to study the so-called  $\varepsilon$ -spectrum, i.e., the set of all eigenvalues of all matrices that are  $\varepsilon$ -close to the matrix under consideration.

It is clear that the  $\varepsilon$ -spectrum consists not of discrete points but of spots containing the exact eigenvalues. It turns out that the diameters of these spots are not necessarily small even for a very small  $\varepsilon$ . This led us (see [13, 16, 28]) and simultaneously Trefethen [32] to the introduction of spectral portraits, i.e., the graphic representation of  $\varepsilon$ -spectra (pseudospectra in the terminology used by Trefethen). Different domains of the complex plane are colored by different colors depending on the value  $\varepsilon$  for which points of these domains belong to the  $\varepsilon$ -spectrum of the matrix  $A$ . The boundaries of domains are level lines for the norm of the resolvent  $\|(\lambda I - A)^{-1}\|$ . Thus, studying the spectral portrait of a matrix  $A$ , we pay attention not only to the eigenvalues (poles of the resolvent) themselves, but to the behavior of the resolvent in a neighborhood of the poles.

The study of the resolvent is a usual tool in the study of operators in infinite-dimensional function spaces, e.g., in Hilbert spaces. However, many results obtained in the infinite-dimensional case are not represented in textbooks on linear algebra. In particular, we mention the estimate for the resolvent in terms of singular values of operators. As early as 1950s, Keldysh [20, 21] suggested to use some results in the theory of entire functions in the study of the location of spectral spots for

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<sup>1</sup>We recommend that the reader who is not familiar with the theory of nonselfadjoint operators start reading consecutively starting with Chapter 1.

matrix operators (other terminology was used at that time). This idea formed a basis for the study (see Chapters 12 and 13) of finite-dimensional models of elliptic differential operators. Such models are obtained by a widely used method known as the finite element method. In Chapters 12 and 13 we prove the completeness of eigenvectors and adjointed vectors. The proof is a simplified version of the proof suggested by Lidskii [25]. We note that Lidskii's work was significantly influenced by the discussions with Keldysh [21].

If we restrict ourselves (as in Chapter 13) to the study of spots corresponding only to the extremal (with the smallest module) points of the spectrum, then the conditions on the operator can be weakened and the proof can be simplified.

In the proof we use an estimate for the resolvent given in §8.6. The justification of this estimate follows the monograph by Gohberg and Krein [19], where the versions of the estimate obtained by Lidskii and Matsaev were improved.

Spectral portraits are particularly useful in theoretical studies, whereas the real construction of spectral portraits requires huge computational resources even for matrices of moderate size. It seems that a much more practical approach consists in using criteria for the absence of eigenvalues in certain parts of the complex plane. The study of such criteria occupies the central place in this book. In Chapters 8–10, 14 and §13.6 we study efficient division of the spectrum into disjoint parts. The division is realized by certain curves in such a way that the norm of the resolvent in each curve is not large. In fact, the search of an appropriate formulation of this problem was the main goal of our research. We tried to find a formulation that would be convenient in applications and simultaneously would admit a solution with guaranteed accuracy of the result. These investigations, started by the author as well as Sarybekov [31] and Bulgakov [4], were used in applications to differential equations. An analogy with the known ideas of Hermite and Lyapunov were useful in our research. Eigenvalues of a matrix  $A$  are often used in the study of the asymptotic behavior of solutions to differential equations of the form  $\dot{x} = Ax$  as  $t \rightarrow \infty$ . In particular, this is a subject of the stability theory which develops the Lyapunov approach.

As is known, for stability it is necessary that the spectrum lies in the left half-plane of the complex plane. However, this condition is not sufficient if we want to have a practical estimate for the rate of decrease of solutions. Furthermore, we must guarantee that the stability is preserved when coefficients vary in the limits determined by the given accuracy of computations or measurements. It is also necessary to require that the norm of the resolvent  $\|(\lambda I - A)^{-1}\|$  would be not too large on the imaginary axis. This condition is equivalent to the existence of the quadratic Lyapunov function  $(Hx, x)$ . The Lyapunov function is admissible if it is constant on the ellipsoid for which the ratio of the largest and the smallest semiaxes is small.

The matrix  $H$  corresponding to the quadratic form in the definition of the Lyapunov function can be represented as an integral along the imaginary axis  $\lambda = it$  of the product  $(-itI - A^*)^{-1}(itI - A)^{-1}$ . It is also represented as a solution to the classical matrix Lyapunov equation  $HA + A^*H + I = 0$ . The solution admits the integral representation

$$\int_0^{\infty} e^{tA^*} e^{tA} dt,$$

where the integrand is the product of the matrix exponential  $e^{tA}$  and the conjugate matrix  $e^{tA^*}$ . It is very important that for  $t > 0$  the norm of the matrix exponential satisfies the estimate

$$\|e^{tA}\| \leq \sqrt{\kappa(A)}e^{-t\|A\|/\kappa(A)},$$

where  $\kappa(A) = \|H\| \cdot 2\|A\|$ . With this estimate in mind, Bulgakov [4] suggested using  $\kappa(A)$  as a dimensionless parameter (the dichotomy quality) that characterizes how “deeply” the spectrum of the matrix  $A$  is located in the left half-plane.

Similar constructions can be used to study and describe the asymptotic behavior of the matrix powers  $A^n$  as  $n \rightarrow \infty$ . Some generalizations were also studied, e.g., to the cases where the spectrum is divided into parts lying in the right and left half-planes, or inside and outside a disk, or even inside and outside a domain bounded by a certain curve dividing the plane into two parts. Such problems are known as spectrum dichotomy problems. The use of quadratic forms in solving similar questions was suggested by Jacobi and Hermite back in the middle of the 19th century. This idea was described and developed in the small (45 page) monograph by M. G. Krein and M. A. Naimark, “The method of symmetric and Hermitian forms for separating roots of algebraic equations”. This book was published in Khar’kov in 1936 and is practically inaccessible at present.

We note that the quadratic Lyapunov function  $(Hx, x)$  can be regarded as a version of the Jacobi–Hermite form that is specifically adapted for formulation of the fact that the spectrum of a matrix  $A$  lies in one (left) half-plane.

For the numerical analysis of the spectrum dichotomy by the imaginary axis, it was suggested in [12] to use quadratic forms with matrices admitting the integral representation

$$H = \int_{-\infty}^{+\infty} G^*(t)G(t) dt,$$

where  $G(t)$  is the Green function for the boundary-value problem  $\dot{x} - Ax = f(x)$  on the real line.

It should be pointed out that to study the dichotomy of the spectrum by the imaginary axis, Daletskii and Krein suggested ([6], §7, Chapter 1, §7) using an indefinite quadratic form with the matrix  $W$  admitting the integral representation

$$W = - \int_{-\infty}^0 G^*(t)G(t) dt + \int_0^{\infty} G^*(t)G(t) dt,$$

which is similar to the integral form of  $H$ . I believe that the choice of a positive definite matrix  $H$  is more convenient in this case. However, indefinite forms play an important role in the study of the orthogonal-power algorithm (see Chapter 14).

Bulgakov [5] showed that if, together with a matrix  $H$  generalizing the Lyapunov matrix, we consider the (commuting with  $A$ ) projections  $P$  and  $I - P$  onto the invariant subspaces of  $A$  corresponding the points of the spectra lying in disjoint domains of the complex plane, then  $H$  and  $P$  satisfy a system of matrix equations that generalizes the classical Lyapunov equation and has similar properties. This allows us to develop algorithms for solving dichotomy problems with subsequent verification of accuracy.

It is interesting to note that the arguments of Bulgakov in the study of the matrices  $H$  and  $P$  were close to the analysis given in [6].

Actually, the suggestion developed in our group consists in using the dichotomy criteria rather than eigenvalues themselves in questions involving numerical solutions of spectral problems. This allows us to treat spectral problems for nonselfadjoint operators as problems admitting a solution with guaranteed accuracy. The dichotomy criteria and the corresponding matrix equations are considered in Chapters 9 and 10.

Introductory Chapters 1–4 present standard facts required in further considerations. These facts are illustrated by many important and not too trivial examples (see e.g., §1.3). Special orthogonal and unitary transformations are described. These transformations are used in the known computational algorithms (see §§2.1–2.3 and §§3.1–3.3). In the subsequent chapters we refer to the technique described in these introductory chapters. The detailed description of algorithms of orthogonal transformations and the use of these algorithms for solving symmetric spectral problem are given in [15]. In this book we concentrate mainly on nonselfadjoint problems. Self-adjoint problems (for example, variational principles in Chapter 7) are mentioned only when we want to make the exposition self-contained.

It should be noted that the introductory chapters of the monograph of Gohberg and Krein [19] significantly influenced the choice of the material. These chapters in [19] were often used in the special courses presented by the author. Once, a part in such a course was taught by A. N. Malyshev. In particular, he gave a lecture with a proof of the Horn theorem which is the converse of the Weyl theorem about the location of eigenvalues and singular values. His notes were used to plan topics of Chapters 5 and 6.<sup>2</sup>

The basic idea of the spectral theory is to use unitarily invariant characteristics of operators. As is known, such characteristics can be expressed in terms of singular values. Thus, in [25], where the infinite-dimensional case is considered, the author used Keldysh's assumption that the sum of certain powers of singular values converges. To formulate and prove the theorem about the annular spectrum dichotomy (see §13.5), the notion of the spectral condition numbers is introduced (see §7.8). These numbers give the quantitative criteria for an operator to belong to a certain Keldysh class. Chapter 12 deals with estimates for the spectral conditionality of operators used in the applications of finite element methods to the approximations of second order elliptic differential operators.

It is important to emphasize that we do not use the normal canonical Jordan form anywhere. We can avoid this because the whole space is decomposed into invariant subspaces corresponding to eigenvalues lying in disjoint spectral spots; moreover, in our approach the study of the detailed structure of the operator on the subspace corresponding to one of these spots can be avoided.

In Chapter 14, computational algorithms are discussed. The chapter begins with the quickly convergent Davison–Man method of solving the Lyapunov equation. Three sections are devoted to the orthogonal exhaustion method due to Malyshev [26]–[28] and to applications to spectrum dichotomy problems. Using

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<sup>2</sup>The representation of the geometry of Hausdorff sets in Chapter 11 was prepared by the author together with Gordienko and was based on the article S. K. Godunov and V. M. Gordienko, *The Hausdorff sets of matrices and estimates for the angle between invariant subspaces*, *Sibirsk. Mat. Zh.*, **26** (1995), no. 3, 531–533.

Malyshev's algorithm, we can solve some matrix equations generalizing the Lyapunov equation. Such equations are considered in Chapter 10. Malyshev's algorithm can be regarded as a modification of the matrix sign-function algorithm that was introduced by Roberts [30] (see also Abramov [1]) and has been widely used in recent years. However, the Malyshev modification has the advantage that it does not require the computation of the inverse matrix at each step of the iteration process.

The last three sections of Chapter 14 present the orthogonal-power method and its modification, the  $QR$ -algorithm. We apply this method to find a sequence of invariant subspaces with spectra separated by circles  $|\lambda| = \text{const}$  on which the norm of the resolvent is not too large. Such circles realize the circle dichotomy of the spectrum. The exposition is based on the article [18], where the stability of the process with respect to computation errors is proved using the ideas of the orthogonal sweep method of solving boundary-value problems. The appearance of a boundary-value problem in theory of iteration procedures is quite unexpected.

The orthogonal sweep method was developed in 1957 (and first published in 1961). Originally it was used in computing the critical parameters of nuclear reactors [2, 10].

We have already mentioned the book [15], which is devoted to the question of guaranteed accuracy for linear algebra problems. In [15] we focused on the algorithms for solving linear systems that are not too large and on the spectral problems for symmetric matrices. The study of these questions does not require significant changes in the point of view and modifications in the formulations of the problems. In fact, the only new aspect of [15] is the detailed exposition of the algorithm of two-sided Sturm sequences. This algorithm, suggested in [17], is used in the precision computation of eigenvectors of symmetric three-diagonal matrices.

Both this book and [15] complete the detailed exposition of ideas that appeared as a result of investigations of the seminar organized by the author in Novosibirsk. The main results of these works were included in the talk [11] at the 1986 International Congress of Mathematicians in Berkeley.

At present it is not clear how to formulate computational problems for large sparse matrices. However, I hope that Chapters 11–13 will be useful to specialists working in this area. It seems necessary to develop closer contacts between specialists in applications and specialists in functional analysis. I began to study aspects of linear algebra in connection with the study of sparse matrices. So far, I have no definite opinion about statements of problems in which such matrices appear. My reasoning is presented in Chapters 11–13. However, they cannot be taken as a final understanding of all ideas required in the analysis of the algorithms.

Work on this book started three years ago when T. N. Rozhkovskaya insisted that I allow her to edit the notes of my lectures. Later this material was repeatedly rewritten and supplemented. It formed a basis of the first ten chapters and a part of Chapter 14. Chapters 11–13 appeared later in the process of rewriting. In particular, I understood the role of the works of Keldysh and Lidskii in overcoming the difficulties connected with the necessity to use spots of the  $\varepsilon$ -spectrum but not a discrete sequence of eigenvalues. In many practical problems, such spots do not glue together, but fall into smaller spots containing spectral clusters of small multiplicity. I think that this fact will be useful in constructing algorithms of spectral analysis for nonselfadjoint operators appearing in a number of important applications.



For three years T. N. Rozhkovskaya arranged and edited numerous versions of my notes and then prepared the book for publication. I am deeply grateful to her. However, I should mention that it was not always easy to be the subject of her pressing. Of course, without this pressure the book would have never been written.

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