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Source: The American Mathematical Monthly, Feb., 2001, Vol. 108, No. 2 (Feb., 2001),

pp. 120-125

Published by: Taylor & Francis, Ltd. on behalf of the Mathematical Association of

America

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Around the Finite-Dimensional Spectral Theorem

Adam Korányi

To the memory of Béla Sz.-Nagy

The goal of this article is to describe an intuitive and natural approach to the spectral theorem and to the singular value decomposition of linear transformations. We are not proving anything new; we are only arranging definitions and proofs in an order that is meant to reveal clearly the relationships among the fundamental facts of the subject. Discussing the presentation of these facts is very much in order, especially in view of the ever-increasing number of students studying linear algebra.

We start with a direct geometric proof of the singular value decomposition. The proof uses nothing besides the notion of an orthogonal sum of subspaces and is essentially the same as the proof in [3, Thm. 2.3–1] or [7, Thm. 3.1.1]; see also [5], [6, Problem 10, Sec. 7.3] and, for the real case, [2]. The history of this proof is discussed

It is natural to start in this way since a linear transformation of one space into another is a more primitive notion than a transformation of a space into itself. Besides, the intrinsic importance of the singular value decomposition has been emphasized more and more in the last couple of decades; see [3], [6], [7], [8]. In our presentation we go even further, taking the singular value decomposition as the basis of the whole development. We use it to define the adjoint, and we derive from it the polar decomposition and the various standard forms of the spectral theorem. The idea of such an approach goes back at least to the work of L. Autonne in 1915 [1]. In [5] it is also used, although in a way rather different from ours.

Besides our claim of being intuitive and natural, we point out two advantages of our presentation:(i) the real and complex cases are treated together all the way up to the point where the actual results begin to differ, (ii) the arguments work without change for compact operators on Hilbert space.

As for the language of this article, we talk throughout in terms of abstract inner product spaces. We denote the inner product of two vectors by (x|y), the norm by ||x||. It is reasonable to use this language since we are talking about exactly that part of elementary linear algebra that makes use of the inner product. But it may create the impression that this is a highbrow approach, which is not so: Everything we say can be rewritten without change in terms of \mathbb{R}^n or \mathbb{C}^n and their natural inner product. In such a form our presentation may be appropriate for an introductory course.

Whichever way they are written down, it is of course essential to understand what the results mean in terms of normal forms or diagonalizations of matrices. This is briefly discussed in the last remark after Theorem 1.

1. THE SINGULAR VALUE DECOMPOSITION.

Theorem 1. Let H and K be (real or complex) finite dimensional inner product spaces and let $T: H \to K$ be a linear transformation. Then there exist unique orthogonal decompositions $H = H_1 \oplus \cdots \oplus H_r \oplus H_0$, $K = K_1 \oplus \cdots \oplus K_r \oplus K_0$ (with H_0 and/or K_0 possibly equal to $\{0\}$), numbers $\mu_1 > \cdots > \mu_r > 0$, and isometries $U_j: H_j \to K_j$ such that $T|_{H_j} = \mu_j U_j (1 \le j \le r)$ and $T|_{H_0} = 0$.

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Remark 1. The existence statement is equivalent to saying that there exist orthonormal bases $\{z_j\}_{j=1}^n$ in H and $\{\zeta_k\}_{k=1}^m$ in K, and numbers $\sigma_1 \ge \cdots \ge \sigma_k > 0$ such that $Tz_j = \sigma_j \zeta_j (1 \le j \le s)$, $Tz_j = 0 (s < j \le n)$.

The numbers $\sigma_1 \dots, \sigma_s$ are the *singular values* of T. The dimension of $H_1 \oplus \dots \oplus H_r$ and of $K_1 \oplus \dots \oplus K_r$ is s; it is the *rank* of T. Some authors write $\sigma_{s+1} = \dots \sigma_p = 0$, where $p = \min(m, n)$, and also call these zeros singular values of T.

Proof of Theorem 1. We prove uniqueness first. Any $x \in H$ has a decomposition of $x = x_1 + \cdots + x_r + x_0(x_j \in H_j)$ and we have $||x||^2 = \sum ||x_j||^2$, $||Tx||^2 = \sum |\mu_j^2||x_j||^2$. From this it is clear that

$$\mu_1 = \max_{\|x\|=1} \|Tx\| \tag{1.1}$$

and H_1 is the set $\{x \in H | ||Tx|| = \mu_1 ||x||\}$, μ_1 and H_1 are uniquely determined by T. Applying the same reasoning to the complements H_1^{\perp} and K_1^{\perp} we see inductively that everything is uniquely determined.

We prove existence in the form given in Remark 1. If T=0, the statement is trivial. Otherwise we set $\mu_1 = \max_{\|x\|=1} \|Tx\|$, we choose an element $z_1 = x$ where this maximum is realized, and we set $\zeta_1 = \mu_1^{-1} T z_1$.

All we have to show is that the orthogonal complement z_1^{\perp} is mapped by T into ζ_1^{\perp} ; the theorem then follows by induction. So, let y be a unit vector $y \perp z_1$. Multiplying y by a scalar of absolute value 1 we can arrange that $(Ty|Tz_1) \geq 0$. We must show that a = 0.

For all $\varepsilon > 0$ we have, by definition of μ_1 ,

$$||T(z_1 + \varepsilon y)||^2 \le \mu_1^2 ||z_1 + \varepsilon y||^2$$
.

Expanding the two sides gives

$$||Tz_1||^2 + 2a\varepsilon + ||Ty||^2\varepsilon^2 \le \mu_1^2(1+\varepsilon^2),$$

whence (using $||Tz_1||^2 = \mu_1^2$),

$$2a\varepsilon \leq \mu_1^2 \varepsilon^2$$
.

This can be true for all $\varepsilon > 0$ only if a = 0.

An amusing variant of the proof can be given (for purists who want to avoid Remark 1) by defining μ_1 as in (1.1) and then at once setting $H_1 = \{x \in H | ||Tx|| = \mu_1 ||x||\}$. To prove that H_1 is a subspace, we take $x, y \in H_1$ and observe that if $||T(x + y)|| < \mu_1 ||x + y||$, then two applications of the parallelogram law give

$$\begin{split} \mu_1^2(\|x+y\|^2 + \|x-y\|^2) &= 2\mu_1^2(\|x\|^2 + \|y\|^2) \\ &= 2(\|Tx\|^2 + \|Ty\|^2) = \|T(x+y)\|^2 + \|T(x-y)\|^2 \\ &< \mu_1^2(\|x+y\|^2 + \|x-y\|^2), \end{split}$$

a contradiction.

As a Corollary we get the minimax characterization of the singular values

$$\sigma_k = \min_{L \in S_{k-1}} \max_{\substack{x \in L \\ \|x\| = 1}} \|Tx\|, \tag{1.2}$$

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where S_{k-1} is the set of subspaces of H with codimension k-1. In fact, the span of z_1, \ldots, z_k being k-dimensional, every $L \in S_{k-1}$ contains some x with ||x|| = 1, $(x|z_{k+1}) = \cdots = (x|z_n) = 0$, so

$$||Tx||^2 = \sum_{j=1}^k |(x|z_j)|^2 = \sum_{j=1}^k \sigma_j^2 \ge \sigma_k^2.$$

Equality is realized when L is the span of z_{k+1}, \ldots, z_n and $x = z_k$.

For the matrix version of Theorem 1, suppose that T is a real m-by-n matrix. Writing the elements of \mathbb{R}^n and \mathbb{R}^m as column vectors, the matrix product Tx determines a linear transformation $\mathbb{R}^n \to \mathbb{R}^m$ that we still denote by T. Let e_1, \ldots, e_n be the standard unit basis of \mathbb{R}^n , and let $\varepsilon_1, \ldots, \varepsilon_m$ be the standard unit basis of \mathbb{R}^m . Let z_1, \ldots, z_n and ζ_1, \ldots, ζ_m be bases of \mathbb{R}^n and \mathbb{R}^m as in Remark 1. Let U be the orthogonal n-by-n matrix such that $Ue_j = z_j$ for all j (so U is just the matrix whose columns are z_1, \ldots, z_n) and let V be the orthogonal m-by-m matrix such that $V\varepsilon_j = \zeta_j$. Then $TUe_j = \sigma_j V\varepsilon_j$, or $V^{-1}TUe_j = \sigma_j \varepsilon_j$ for $1 \geq j \geq s$ and $V^{-1}TUe_j = 0$ for $s < j \leq n$. This can be rewritten as $V^{-1}TUe_j = \Sigma e_j (1 \leq j \leq n)$, where Σ denotes the m-by-n ("diagonal") matrix whose (j,j)-entry is σ_j for $1 \leq j \leq s$ and all other entries are 0. It follows that $V^{-1}TU = \Sigma$ and we have proved that there exist orthogonal matrices U and V such that $V^{-1}TU$ is diagonal. The same argument works for complex T, with unitary U and V.

2. ADJOINT, NORMALITY, POLAR DECOMPOSITION. Theorem 1 gives a unique way of writing the linear transformation $T: H \to K$ as

$$T = \mu_1 U_1 \oplus \dots \oplus \mu_r U_r \oplus 0 \tag{2.1}$$

(the 0 at the end may be absent). Taking this as our basic fact, we *define* the adjoint $T^*: K \to H$ by

$$T^* = \mu_1 U_1^{-1} \oplus \dots \oplus \mu_r U_r^{-1} \oplus 0.$$
 (2.2)

In particular, T is an isometry if and only if $T^* = T^{-1}$. The definition gives at once that $T^{**} = T$ and $||T^*|| = ||T||$.

For any $x = x_1 + \cdots + x_r + x_0$ in H and $\xi = \xi_1 + \cdots + \xi_r + \xi_0$ in K, we have

$$(x|T^*\xi) = \sum_{1}^{r} \mu_j(x_j|U_j^{-1}\xi_j) = \sum_{1}^{r} \mu_j(U_jx_j|\xi_j) = (Tx|\xi),$$

which shows that our definition of T^* agrees with the usual one.

It is clear that $H_0 = N(T)$ is the null-space of T and $H_1 \oplus \cdots \oplus H_r$ is the range $R(T^*)$ of T^* , so

$$H = N(T) \oplus R(T^*)$$

and similarly

$$K = N(T^*) \oplus R(T).$$

It is also clear that

$$\dim R(T) = \dim R(T^*)$$

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since H_j and K_j are isometric for $1 \le j \le r$. These crucial facts, together with the part of Theorem 1 asserting that T is diagonal with respect to the bases constructed there, amount to what is called in [2] the Fundamental Theorem of Linear Algebra.

Incidentally, the Moore-Penrose pseudoinverse $T^+: K \to H$ can immediately be defined with the help of (2.1) as

$$T^+ = \frac{1}{\mu_1} U_1^{-1} \oplus \cdots \oplus \frac{1}{\mu_r} U_r^{-1} \oplus 0.$$

One sees at once that $TT^+T = T$, $T^+TT^+ = T^+$, and that T^+T and TT^+ are orthogonal projections (onto $H_1 \oplus \cdots \oplus H_r$ and $K_1 \oplus \cdots \oplus K_r$). This shows that our definition is equivalent to the usual one.

Coming back to the main line of exposition, we consider the case where H = K. For $T: H \to K$, Theorem 1 now gives two decompositions of H. We say that T is *normal* if the two decompositions coincide, i.e., if $H_j = K_j (0 \le j \le r)$. By (2.1), isometries are particularly simple examples of normal linear transformations.

Since $T^*T = \mu_1^2 I_{H_1} \oplus \cdots \oplus \mu_r^2 I_{H_r} \oplus 0$ and $TT^* = \mu_1^2 I_{K_1} \oplus \cdots \oplus \mu_r^2 I_{K_r} \oplus 0$, our definition of normality coincides with the usual one, namely with the property $T^*T = TT^*$.

This expression for T^*T also shows that the singular values of T are the square roots of the eigenvalues of T^*T . Since $||Tx||^2 = (T^*Tx|x)$, it follows that (1.2) can also be derived from the minimax theorem for self-adjoint transformations.

Finally, we mention that for any $T: H \to K$, Theorem 1 immediately gives the polar decompositions $T = UP = \tilde{P}U$ where $P = \mu_1 I_{H_1} \oplus \cdots \oplus \mu_r I_{H_r} \oplus 0$ and $\tilde{P} = \mu_1 I_{K_1} \oplus \cdots \oplus \mu_r I_{K_r} \oplus 0$ are positive self-adjoint, and $U = U_1 \oplus \cdots \oplus U_r \oplus 0$ is a partial isometry. If H = K, it is now immediate that $P = \tilde{P}$, or equivalently, UP = PU, if and only if T is normal.

3. THE SPECTRAL THEOREM FOR SELF-ADJOINT TRANSFORMATIONS.

Theorem 2. If $A: H \to H$ is a linear transformation such that $A^* = A$, then there is a unique orthogonal decomposition $H = \tilde{H}_1 \oplus \cdots \oplus \tilde{H}_l$ and unique numbers $\lambda_1 > \cdots > \lambda_l$ such that $A|_{\tilde{H}_l} = \lambda_i I_{\tilde{H}_l} (1 \le i \le l)$.

Proof. In the decomposition given by Theorem 1, by (2.1) and (2.2) we now have $-U_j = U_j^{-1}$, i.e., $U_j^2 = I_{H_j}$ for all $1 \le j \le r$. It follows that each H_j splits as the orthogonal direct sum $H_j = H_j^+ \oplus H_j^-$ of the (+1) resp. (-1)-eigenspace of U_j . Indeed, every $x \in H_j$ can be written as $x = \frac{1}{2}(I + U_j)x + \frac{1}{2}(I - U_j)x$, and $((I + U_j)x|(I - U_j)y) = (x|y) - (U_jx|U_jy) + (U_jx|y) - (x|U_jy) = 0$. The values $\lambda_1, \ldots, \lambda_l$ are now those among the numbers $\pm \mu_j$ for which $H_j^{\pm} \ne \{0\}$, together with 0 in case $H_0 \ne \{0\}$. The space \tilde{H}_i is H_j^+ when $\lambda_i = \mu_j$, H_j^- when $\lambda_i = -\mu_j$, and H_0 when $\lambda_i = 0$.

Uniqueness follows from the uniqueness statement of Theorem 1, or more directly from the fact that the spaces \tilde{H}_i are characterized by the property of being eigenspaces of A.

4. THE SPECTRAL THEOREM FOR NORMAL AND ISOMETRIC TRANS-FORMATIONS. Any $T: H \to H$ can be written as T = A + B with A self-adjoint and B skew-adjoint (i.e., $B^* = -B$); we can take $A = \frac{1}{2}(T + T^*)$, $B = \frac{1}{2}(T - T^*)$. Clearly A and B commute if and only if T and T^* commute, i.e., if and only if T is normal.

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If A and B commute, B maps every eigenspace of A into itself. Indeed, if $Ax = \lambda x$, then $A(Bx) = BAx = \lambda Bx$.

From these remarks the spectral theorem for normal operators follows. Suppose T = A + B is normal. Applying Theorem 2 to A gives the eigenspaces \tilde{H}_j of A: now each one of these is mapped into itself by B.

If H is a complex space, notice that C=-iB is self-adjoint, and we can apply Theorem 2 to the restriction of C to each of the subspaces \tilde{H}_j . So finally H splits into an orthogonal direct sum of subspaces each of which is a joint eigenspace of A and of B=iC, hence an eigenspace of T. The special case where T is an isometry, i.e., $\|Tx\|=\|x\|$ for all $x\in H$, is distinguished by the property that every eigenvalue of T has absolute value 1.

If *H* is a real space, *B* can not be dealt with so easily. What is needed is really a structure theorem for skew-adjoint transformations, along the lines of Theorem 2:

Writing $B = \mu_1 U_1 \oplus \cdots \oplus \mu_r U_r \oplus 0$ and using (2.1) and (2.2), the condition $B^* = -B$ now gives $U_j^{-1} = U_j$, i.e., $U_j^2 = -I_{H_j}$ for each $1 \leq j \leq r$. Under such an U_j , the space of H_j does not uniquely split in two (its complexification does; the eigenvalues of U_j are i and -i, but we want to stay with real numbers). We can, however, construct a basis of H_j choosing an arbitrary $x_1 \in H_j$ with $||x_1|| = 1$, setting $x_2 = U_j x_1$, then choosing x_3 orthonormal to x_1 and x_2 , setting $x_4 = U_j x_3$, and continuing. Then $U_j x_{2k-1} = x_{2k}$, and hence also $U_j x_{2k} = -x_{2k-1}$. The matrix of U_j consists of 2-by-2 boxes of the form

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

arranged along the diagonal. The matrix of B consists of groups of such boxes with μ_i in place of 1, and possibly some zeroes along the diagonal, corresponding to H_0 .

For a normal operator T = A + B on a real space H we still have the splitting of H into the eigenspaces \tilde{H}_j of A, each of which is mapped into itself by B. We can now apply what we have observed to the restriction of B to each of the spaces \tilde{H}_j . We obtain a basis for H in which the matrix of T consists of a (real) diagonal part and a set of 2-by-2 blocks of the form

$$\begin{pmatrix} \lambda_i & -\mu_i \\ \mu_i & \lambda_i \end{pmatrix}$$

along the diagonal.

This is the spectral theorem for normal operators on a real space. T is an isometry if and only if the entries of the diagonal part are ± 1 and the numbers in the 2-by-2 blocks satisfy $\lambda_i^2 + \mu_i^2 = 1$.

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