Polar decomposition, singular-value decomposition, and Autonne-Takagi factorization

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This document provides an introduction to the polar decomposition, the singular-value decomposition, and Autonne-Takagi factorization of symmetric matrices, with an emphasis on how all of these are close to the same thing once one thinks about operators instead of their representations.

We begin by reviewing the polar decomposition and the singular-value decomposition, since Autonne-Takagi factorization is a special case of these.

Polar decomposition. Given a linear operator M, the polar decomposition starts with the positive operators $\sqrt{M^\dagger M}$ and $\sqrt{MM^\dagger}$. These two positive operators have the same (real, nonnegative) eigenvalues, denoted as λ_j. The eigenvalues of $M^\dagger M$ and $MM^\dagger$ are the squares, λ_j^2. If we let $|e_j\rangle$ and $|f_j\rangle$ be (orthonormal) eigenvectors of $\sqrt{M^\dagger M}$ and $\sqrt{MM^\dagger}$, respectively, with $|e_j\rangle$ and $|f_j\rangle$ having the same eigenvalue λ_j, we have

$$\sqrt{M^\dagger M} = \sum_j \lambda_j |e_j\rangle\langle e_j|\,, \tag{1}$$

$$\sqrt{MM^\dagger} = \sum_j \lambda_j |f_j\rangle\langle f_j|\,. \tag{2}$$

Now we notice that $MM^\dagger(M|e_j\rangle) = M(M^\dagger M|e_j\rangle) = \lambda_j^2 M|e_j\rangle$, so $M|e_j\rangle$ is an eigenvector of $MM^\dagger$ with eigenvalue λ_j^2. Thus, for eigenvectors $|e_j\rangle$ in the support of $M^\dagger M$, i.e., for which $\lambda_j \neq 0$, we *define* $|f_j\rangle \equiv M|e_j\rangle/\lambda_j$; this definition imposes a natural and unique way of pairing up eigenvectors $|e_j\rangle$ and $|f_j\rangle$ in degenerate subspaces and of phasing all the eigenvectors $|f_j\rangle$. For eigenvectors $|e_j\rangle$ in the null subspace of $M^\dagger M$, we can start with any orthonormal eigenvectors in the null subspace of $M^\dagger M$ and pair them up with any choice of orthonormal eigenvectors in the null subspace of $MM^\dagger$. With these choices, we can write

$$M|e_j\rangle = \lambda_j|f_j\rangle \qquad \Longleftrightarrow \qquad M = \sum_j \lambda_j |f_j\rangle\langle e_j|\,, \tag{3}$$

$$M^\dagger|f_j\rangle = \lambda_j|f_j\rangle \qquad \Longleftrightarrow \qquad M^\dagger = \sum_j \lambda_j |e_j\rangle\langle f_j|\,; \tag{4}$$

The eigenvalues λ_j are called the *singular values* of M, and the eigenvectors $|e_j\rangle$ and $|f_j\rangle$ are called the *right* and *left singular vectors*.

Letting U be the unitary operator that transforms between the two eigenbases, i.e.,

$$U|e_j\rangle = |f_j\rangle \qquad \Longleftrightarrow \qquad U = \sum_j |f_j\rangle\langle e_j|\,, \tag{5}$$

we have that U transforms between the two positive operators, i.e.,

$$U\sqrt{M^\dagger M}U^\dagger = \sqrt{MM^\dagger}\,. \tag{6}$$

This leads us to the *polar decomposition*,

$$M = U\sqrt{M^\dagger M} = \sqrt{MM^\dagger}U\,, \tag{7}$$

$$M^\dagger = \sqrt{M^\dagger M}U^\dagger = U^\dagger\sqrt{MM^\dagger}\,. \tag{8}$$

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The unitary operator U is unique if $M^\dagger M$ is invertible (i.e., all the eigenvalues λ_j^2 are nonzero). This is clear from the construction of the polar decomposition; moreover, when $M^\dagger M$ is invertible, we have $U = M(M^\dagger M)^{-1/2}$.

For a Hermitian operator H, with eigenvalues h_j and eigenvectors $|e_j\rangle$, we have $\sqrt{H^\dagger H} = \sqrt{H^2} = |H|$, i.e., $\lambda_j = |h_j|$; the only role of the unitary U in the polar decomposition is to insert a sign change for negative eigenvalues of H:

$$U = \sum_j \operatorname{sign}(h_j) |e_j\rangle\langle e_j| \,. \tag{9}$$

A unitary operator U is its own polar decomposition. A normal operator N, i.e., $N^\dagger N = NN^\dagger$, has an eigendecomposition $N = \sum_j \lambda_j e^{i\phi_j} |e_j\rangle\langle e_j|$, where the λ_js are nonnegative, so

$$\sqrt{N^\dagger N} = \sqrt{NN^\dagger} = \sum_j \lambda_j |e_j\rangle\langle e_j| \,; \tag{10}$$

the role of the unitary U in the polar decomposition is to put the phases back in:

$$U = \sum_j e^{i\phi_j} |e_j\rangle\langle e_j| \,. \tag{11}$$

What distinguishes normal operators is that the unitary U and the positive operator $\sqrt{N^\dagger N}$ in the polar decomposition commute.

Singular-value decomposition. The singular-value decomposition is really the same thing as the polar decomposition, the only difference being that there is a standard basis $|j\rangle$ in which we want the singular values to appear in diagonal form as

$$\Lambda = \sum_j \lambda_j |j\rangle\langle j| \,. \tag{12}$$

By introducing a unitary operator V that maps from the standard basis to the eigenbasis $|e_j\rangle$, i.e., $V|j\rangle = |e_j\rangle$, we can write

$$\sqrt{M^\dagger M} = \sum_j \lambda_j |e_j\rangle\langle e_j| = V\Lambda V^\dagger \tag{13}$$

and thus put the polar decomposition in the form

$$M = W\Lambda V^\dagger \,, \tag{14}$$

where $W = UV$, with $W|j\rangle = |f_j\rangle$. Equation (14) is the *singular-value decomposition.* It is important to reiterate that the only difference between the singular-value decomposition and the polar decomposition is that we want Λ to be diagonal in a basis $|j\rangle$ of our choosing, instead in the eigenbasis $|e_j\rangle$ of $\sqrt{M^\dagger M}$ or the eigenbasis $|f_j\rangle$ of $\sqrt{MM^\dagger}$; indeed, the only purpose of V is to do the map $|e_j\rangle = V|j\rangle$. Notice that in this construction, we have the freedom to rephase the right singular vectors $|e_j\rangle$ or, equivalently, to multiply V on the right by a unitary that is diagonal in the standard basis.

In the standard basis, the singular-value decomposition becomes

$$M_{jk} = \langle j|M|k\rangle = \sum_l \langle j|W|l\rangle \lambda_l \langle l|V^\dagger|k\rangle = \sum_l \langle j|f_l\rangle \lambda_l \langle e_l|k\rangle \,, \tag{15}$$

with $\langle j|W|l\rangle = \langle j|f_l\rangle$ and $\langle k|V|l\rangle = \langle k|e_l\rangle$ being the unitary matrices that transform from the standard basis to the singular vectors. The singular-value decomposition is usually stated directly in terms of matrices, i.e., the representations of operators in a standard basis, and this statement is that any matrix can be diagonalized by a pair of unitary matrices.

Autonne-Takagi factorization. Autonne-Takagi factorization is usually stated in terms of a complex symmetric matrix; if we wish to state it in terms of operators, we need a standard basis $|j\rangle$ relative to which transposition and complex conjugation are defined. Now let's state precisely what we want to prove:

If $M = M^T$ is a symmetric operator, relative to a standard basis $|j\rangle$, there exists a unitary operator V such that

$$V^T M V = \Lambda = \sum_j \lambda_j |j\rangle\langle j| \,, \tag{16}$$

where the diagonal elements are the (real, nonnegative) singular values of M.

Notice that

$$M = V^* \Lambda V^\dagger \,, \tag{17}$$

which means that this is a special case of the singular-value decomposition where the diagonalizing unitaries are complex conjugates of one another, i.e., $W = V^*$. Translated to the polar decomposition, the unitary operator in the polar decomposition becomes $U = WV^\dagger = V^* V^\dagger = (VV^T)^\dagger$.

Proof. Write $M^\dagger M$ in diagonal form,

$$M^\dagger M = \sum_j \lambda_j^2 |e_j\rangle\langle e_j| \,, \tag{18}$$

and let S be the unitary operator that maps between the eigenbasis and the standard basis relative to which we define transposition and complex conjugation, i.e.,

$$S|j\rangle = |e_j\rangle \,, \tag{19}$$

and relative to which M is by assumption symmetric. Now we have

$$S^\dagger M^\dagger M S = \Lambda^2 = \sum_j \lambda_j^2 |j\rangle\langle j| \,. \tag{20}$$

Consider the manifestly symmetric operator

$$L = S^T M S = L^T \,. \tag{21}$$

One has

$$L^\dagger L = S^\dagger M^\dagger S^* S^T M S = S^\dagger M^\dagger M S = \Lambda^2 \quad \text{and} \quad LL^\dagger = S^T M S S^\dagger M^\dagger S^* = S^T M M^\dagger S^* = (S^\dagger M^\dagger M S)^* = \Lambda^2 \,. \tag{22}$$

Since L is normal, it is diagonal in an orthonormal basis, and these equations show that the diagonalizing basis is the standard basis, so we have

$$L = \sum_j \lambda_j e^{i\phi_j} |j\rangle\langle j| = \bigg(\sum_j e^{i\phi_j} |j\rangle\langle j|\bigg)\Lambda = \bigg(\sum_j e^{i\phi_j/2} |j\rangle\langle j|\bigg)\Lambda\bigg(\sum_j e^{i\phi_j/2} |j\rangle\langle j|\bigg) \,. \tag{23}$$

The second form is the polar decomposition of the normal operator L. The last form is the one we now use by writing

$$\Lambda = \bigg(\sum_j e^{-i\phi_j/2} |j\rangle\langle j|\bigg) S^T M S \bigg(\sum_j e^{-i\phi_j/2} |j\rangle\langle j|\bigg) \,. \tag{24}$$

Defining

$$V = S\bigg(\sum_j e^{-i\phi_j/2} |j\rangle\langle j|\bigg) = \sum_j e^{-i\phi_j/2} |e_j\rangle\langle j| \tag{25}$$

completes the proof.

The unitaries S and V are nearly the same thing except for phasing. Indeed, if we rephase the right singular vectors,

$$|\tilde{e}_j\rangle = e^{-i\phi_j/2} |e_j\rangle \,, \tag{26}$$

which we always have the freedom to do, we have

$$V = \sum_j |\tilde{e}_j\rangle\langle j| \tag{27}$$

and

$$M = V^* \Lambda V^\dagger = \sum_j \lambda_j |\tilde{e}_j^*\rangle\langle\tilde{e}_j| \,. \tag{28}$$

Thus one may think of the content of Autonne-Takagi factorization as the fact that for symmetric matrices, the left and right singular vectors can be phased so that they are complex conjugates of one another, i.e., $|\tilde{f}_j\rangle = |\tilde{e}_j^*\rangle$.