

# What is the Polar Decomposition?

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A polar decomposition of  $A \in \mathbb{C}^{m \times n}$  with  $m \geq n$  is a factorization  $A = UH$ , where  $U \in \mathbb{C}^{m \times n}$  has orthonormal columns and  $H \in \mathbb{C}^{n \times n}$  is Hermitian positive semidefinite. This decomposition is a generalization of the polar representation  $z = re^{i\theta}$  of a complex number, where  $H$  corresponds to  $r \geq 0$  and  $U$  to  $e^{i\theta}$ . When  $A$  is real,  $H$  is symmetric positive semidefinite. When  $m = n$ ,  $U$  is a square unitary matrix (orthogonal for real  $A$ ).

We have  $A^*A = H^*U^*UH = H^2$ , so  $H = (A^*A)^{1/2}$ , which is the unique positive semidefinite square root of  $A^*A$ . When  $A$  has full rank,  $H$  is nonsingular and  $U = AH^{-1}$  is unique, and in this case  $U$  can be expressed as

$$U = \frac{2}{\pi} A \int_0^\infty (t^2 I + A^*A)^{-1} dt.$$

An example of a polar decomposition is

$$A = \begin{bmatrix} 4 & 0 \\ -5 & -3 \\ 2 & 6 \end{bmatrix} = \sqrt{2} \begin{bmatrix} \frac{1}{2} & -\frac{1}{6} \\ -\frac{1}{2} & -\frac{1}{6} \\ 0 & \frac{2}{3} \end{bmatrix} \cdot \sqrt{2} \begin{bmatrix} \frac{9}{2} & \frac{3}{2} \\ \frac{3}{2} & \frac{9}{2} \end{bmatrix} \equiv UH.$$

For an example with a rank-deficient matrix consider

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix},$$

for which  $A^*A = \text{diag}(0, 1, 1)$  and so  $H = \text{diag}(0, 1, 1)$ . The equation  $A = UH$  then implies that

$$U = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ \theta & 0 & 0 \end{bmatrix}, \quad |\theta| = 1,$$

so  $U$  is not unique.

The polar factor  $U$  has the important property that it is a closest matrix with orthonormal columns to  $A$  in any unitarily invariant norm. Hence the polar decomposition provides an optimal way to orthogonalize a matrix. This method of orthogonalization is used in various applications, including in quantum chemistry, where it is called Löwdin

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orthogonalization. Most often, though, orthogonalization is done through QR factorization, trading optimality for a faster computation.

An important application of the polar decomposition is to the orthogonal Procrustes problem<sup>1</sup>

$$\min\{\|A - BW\|_F : W \in \mathbb{C}^{n \times n}, W^*W = I\},$$

where  $A, B \in \mathbb{C}^{m \times n}$  and the norm is the Frobenius norm  $\|A\|_F^2 = \sum_{i,j} |a_{ij}|^2$ . This problem, which arises in factor analysis and in multidimensional scaling, asks how closely a unitary transformation of  $B$  can reproduce  $A$ . Any solution is a unitary polar factor of  $B^*A$ , and there is a unique solution if  $B^*A$  is nonsingular. Another application of the polar decomposition is in 3D graphics transformations. Here, the matrices are  $3 \times 3$  and the polar decomposition can be computed by exploiting a relationship with quaternions.

For a square nonsingular matrix  $A$ , the unitary polar factor  $U$  can be computed by a Newton iteration:

$$X_{k+1} = \frac{1}{2}(X_k + X_k^{-*}), \quad X_0 = A.$$

The iterates  $X_k$  converge quadratically to  $U$ . This is just one of many iterations for computing  $U$  and much work has been done on the efficient implementation of these iterations.

If  $A = P\Sigma Q^*$  is a singular value decomposition (SVD), where  $P \in \mathbb{C}^{m \times n}$  has orthonormal columns,  $Q \in \mathbb{C}^{n \times n}$  is unitary, and  $\Sigma$  is square and diagonal with nonnegative diagonal elements, then

$$A = PQ^* \cdot Q\Sigma Q^* \equiv UH,$$

where  $U$  has orthonormal columns and  $H$  is Hermitian positive semidefinite. So a polar decomposition can be constructed from an SVD. The converse is true: if  $A = UH$  is a polar decomposition and  $H = Q\Sigma Q^*$  is a spectral decomposition ( $Q$  unitary,  $D$  diagonal) then  $A = (UQ)\Sigma Q^* \equiv P\Sigma Q^*$  is an SVD. This latter relation is the basis of a method for computing the SVD that first computes the polar decomposition by a matrix iteration then computes the eigensystem of  $H$ , and which is extremely fast on distributed-memory manycore computers.

The nonuniqueness of the polar decomposition for rank deficient  $A$ , and the lack of a satisfactory definition of a polar decomposition for  $m < n$ , are overcome in the *canonical polar decomposition*, defined for any  $m$  and  $n$ . Here,  $A = UH$  with  $U$  a partial isometry,  $H$  is Hermitian positive semidefinite, and  $U^*U = HH^+$ . The superscript “+” denotes the Moore–Penrose pseudoinverse and a partial isometry can be characterized as a matrix  $U$  for which  $U^+ = U^*$ .

Generalizations of the (canonical) polar decomposition have been investigated in which the properties of  $U$  and  $H$  are defined with respect to a general, possibly indefinite, scalar product.

## References

This is a minimal set of references, which contain further useful references within.

- Nicholas J. Higham, *Functions of Matrices: Theory and Computation*, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2008. (Chapter 8.)

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<sup>1</sup>Procrustes: an ancient Greek robber who tied his victims to an iron bed, stretching their legs if too short for it, and lopping them if too long.

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- Nicholas J. Higham and Vanni Noferini, An algorithm to compute the polar decomposition of a  $3 \times 3$  matrix, *Numer. Algorithms* 73, 349–369, 2016.
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