Suppose that we are given an $m \times n$ real matrix A. Then $A^T A$ is a nonnegative matrix whose eigenvalues (i.e., the solutions of $\det(\lambda \mathbf{I}_n - A^T A) = 0$) are nonnegative real numbers. We let the eigenvalues be $\lambda_1, \lambda_2, \ldots, \lambda_n$ ($\lambda_1 \geqq \lambda_2 \geqq \cdots \geqq \lambda_n \geqq 0$). We also let

$$\sigma_i = \sqrt{\lambda_i}, \quad i = 1,2,\ldots,\min(m,n). \tag{A3.1}$$

Obviously we have $\sigma_1 \geqq \sigma_2 \geqq \cdots \geqq \sigma_{\min(m,n)} \geqq 0$. We can now express the matrix A as the product of three matrices:

$$A = U \Sigma V^T, \tag{A3.2}$$

where U is an $m \times m$ orthogonal matrix, V is an $n \times n$ orthogonal matrix, and Σ is an $m \times n$ matrix defined by

$$\Sigma = \begin{cases} \left[\begin{array}{ccc} \sigma_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \sigma_n \\ \hline & \mathbf{0} & \end{array}\right] & \text{if } m \geqq n \\[2ex] \left[\begin{array}{ccc|c} \sigma_1 & & \mathbf{0} & \\ & \ddots & & \mathbf{0} \\ \mathbf{0} & & \sigma_m & \end{array}\right] & \text{if } m < n. \end{cases} \tag{A3.3}$$

The right-hand side of equation A3.2 is called the *singular-value decomposition*, and σ_i ($i = 1,2,\ldots,\min(m,n)$) are called *singular values*. The number of nonzero singular values is

$$r = \operatorname{rank} A. \tag{A3.4}$$

Since U and V are orthogonal, they satisfy

$$UU^T = U^T U = \mathbf{I}_m, \quad VV^T = V^T V = \mathbf{I}_n. \tag{A3.5}$$

Let us consider the meaning of the singular-value decomposition of A in relation to the linear transformation $y = Ax$. Letting $y_U = U^T y$ and $x_V = V^T x$, from equation A3.2 we have

$$y_U = \Sigma x_V. \tag{A3.6}$$

This implies that the transformation from x to y can be decomposed into three consecutive transformations: the orthogonal transformation from x

to x_V by V^T, which does not change length; the one from x_V to y_U, in which the ith element of x_V is multiplied by σ_i and becomes the ith element of y_U without changing its direction; and the orthogonal transform from y_U to y by U, which does not change length. Therefore, the singular-value decomposition highlights a basic property of linear transformation.

A scheme to obtain the singular-value decomposition follows. First, we calculate the singular values by equation A3.1. We note that, since the numbers of nonzero eigenvalues for $A^T A$ and AA^T are the same, it is computationally more efficient to find the singular values using the eigenvalues of AA^T when $m < n$ and those of $A^T A$ when $m > n$.

Next we obtain U and V. We define a diagonal matrix Σ_r using r nonzero singular values by

$$\Sigma_r = \begin{bmatrix} \sigma_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \sigma_r \end{bmatrix}. \tag{A3.7}$$

This is the $r \times r$ principal minor of Σ. We let the ith row vectors of U and V be u_i and v_i, respectively, and let

$$U_r = [u_1, u_2, \ldots, u_r]$$

and

$$V_r = [v_1, v_2, \ldots, v_r].$$

Then, from equation A3.2,

$$A = U_r \Sigma_r V_r^T.$$

Also, from equation A3.5,

$$U_r^T U_r = \mathbf{I}_r$$

and

$$V_r^T V_r = \mathbf{I}_r.$$

Hence, we have

$$A^T A V_r = V_r \Sigma_r^2, \tag{A3.8}$$

$$U_r = A V_r \Sigma_r^{-1}. \tag{A3.9}$$

Since equation A3.8 can be decomposed into

$$A^T A v_i = v_i \sigma_i^2, \quad i = 1,2,\ldots,r \tag{A3.10}$$

we see that v_i is the eigenvector of unit length for eigenvalue λ_i of $A^T A$. Thus we can determine V_r from the eigenvectors of $A^T A$ for eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_r$. The part of V other than V_r, which consists of vectors v_{r+1}, $v_{r+2}, \ldots, v_n$, is arbitrary as long as it satisfies equation A3.5. From the obtained V we can determine U_r by equation A3.9 and the other part of U by equation A3.5. Instead of equations A3.8 and A3.9, we can also use

$$AA^T U_r = U_r \Sigma_r^2 \tag{A3.8$'$}$$

and

$$V_r = A^T U_r \Sigma_r^{-1}. \tag{A3.9$'$}$$

A numerical example will illustrate the above sheme. Suppose that

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

Then

$$A^T A = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 3 & -2 \\ -1 & -2 & 3 \end{bmatrix}.$$

Since

$$\det(\lambda \mathbf{I}_3 - A^T A) = \lambda(\lambda - 3)(\lambda - 5) = 0,$$

the eigenvalues of $A^T A$ are $\lambda_1 = 5$, $\lambda_2 = 3$, and $\lambda_3 = 0$, and the singular values of A are $\sigma_1 = \sqrt{5}$, $\sigma_2 = \sqrt{3}$, and $\sigma_3 = 0$. The eigenvectors v_i of $A^T A$ for λ_i $(i = 1, 2)$ are

$$v_1 = [0, 1/\sqrt{2}, -1/\sqrt{2}]^T$$

and

$$v_2 = [2/\sqrt{6}, -1/\sqrt{6}, -1/\sqrt{6}]^T.$$

Substituting $V_r = [v_1, v_2]$ into equation A3.9, we obtain

$$U_r = \begin{bmatrix} 2/\sqrt{10} & -1/\sqrt{10} & -1/\sqrt{10} & 2/\sqrt{10} \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} & 0 \end{bmatrix}^T.$$

Hence, a singular-value decomposition of A is given by

$$\Sigma = \begin{bmatrix} \sqrt{5} & 0 & 0 \\ 0 & \sqrt{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$U = \begin{bmatrix} 2/\sqrt{10} & 0 & 1/\sqrt{2} & 1/\sqrt{10} \\ -1/\sqrt{10} & -1/\sqrt{2} & 0 & 2/\sqrt{10} \\ -1/\sqrt{10} & 1/\sqrt{2} & 0 & 2/\sqrt{10} \\ 2/\sqrt{10} & 0 & -1/\sqrt{2} & 1/\sqrt{10} \end{bmatrix},$$

and

$$V = \begin{bmatrix} 0 & 2/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \end{bmatrix}.$$

The reader who wishes to learn more about singular-value decomposition is referred to the following:

V. C. Klema and A. J. Laub, "The Singular Value Decomposition: Its Computation and Some Applications," *IEEE Transactions on Automatic Control* 25, no. 2 (1980): 164–176.

G. E. Forsythe, M. A. Malcolm, and C. B. Moler, *Computer Methods for Mathematical Computations* (Prentice-Hall, 1977).