1. Positive definite matrices

From now on, we will stick with vectors and matrices that have real entries. As you might guess, everything done here can be generalized to the complex case, but we will not do that here. This means that we will only need to deal with transposes of vectors and matrices, rather than Hermitian transposes. Remember two important formulas:

- (Representing the dot product with matrix multiplication) $\vec{v} \cdot \vec{w} = \vec{v}^T \vec{w}$, where $\vec{v}$ and $\vec{w}$ are column vectors in $\mathbb{R}^n$.
- (Taking the transpose of a matrix product) $(AB)^T = B^T A^T$ for matrices $A, B$ for which the product $AB$ makes sense.

These two formulas give us the following useful equation:

(1) $\vec{v} \cdot (M\vec{w}) = \vec{v}^T M \vec{w} = (M^T \vec{v})^T \vec{w} = (M^T \vec{v}) \cdot \vec{w}$,

where $\vec{v}, \vec{w} \in \mathbb{R}^n$ and $M$ is an $n \times n$ matrix.

An $n \times n$ matrix $M$ is positive semidefinite if $\vec{v} \cdot (M\vec{v}) \geq 0$ for every column vector $\vec{v} \in \mathbb{R}^n$, and it is positive definite if $\vec{v} \cdot (M\vec{v}) > 0$ for every column vector $\vec{v} \in \mathbb{R}^n$. Positive semidefinite matrices are also called nonnegative definite.

Suppose $\vec{v}$ is an eigenvector of a matrix $M$, with eigenvalue $\lambda$. Then

$\vec{v} \cdot (M\vec{v}) = \vec{v} \cdot (\lambda \vec{v}) = \lambda (\vec{v} \cdot \vec{v}) = \lambda \|\vec{v}\|^2$.

If $M$ is positive definite, then this and the definition of positive definite imply that $\lambda > 0$. Similarly, if $M$ is positive semidefinite, then $\lambda \geq 0$. So all eigenvalues of positive definite matrices are positive, and all eigenvalues of positive semidefinite matrices are nonnegative.

Positive definite and semidefinite matrices arise frequently. Here is one reason why that is the case. Let $M$ be any $m \times n$ matrix (so $M$ is not necessarily square, and not necessarily positive definite or positive semidefinite). Now consider the matrix $M^T M$. This is an $n \times n$ matrix. Taking the transpose, we see that it is symmetric:

$$(M^T M)^T = M^T (M^T)^T = M^T M,$$

so we know it has real eigenvalues. But more is true: for any column vector $\vec{v} \in \mathbb{R}^n$,

$\vec{v} \cdot (M^T M \vec{v}) = \vec{v}^T (M^T M \vec{v}) = (\vec{v}^T M^T) (M \vec{v}) = (M \vec{v})^T (M \vec{v}) = (M \vec{v}) \cdot (M \vec{v}) = \|M \vec{v}\|^2 \geq 0,$
so $M^T M$ is always positive semidefinite. A similar argument shows that the $m \times m$ symmetric matrix $M M^T$ is also always positive semidefinite. This fact is the basis of many important applications of linear algebra.

2. Singular values

Throughout this section, $M$ will be an $m \times n$ matrix. A nonnegative real number $\sigma$ is called a singular value of $M$ if there exists a unit column vector $\mathbf{v} \in \mathbb{R}^n$ and a unit column vector $\mathbf{u} \in \mathbb{R}^m$ such that

$$M \mathbf{v} = \sigma \mathbf{u} \quad \text{and} \quad \mathbf{u}^T M = \sigma \mathbf{v}^T.$$ 

The vector $\mathbf{v}$ is called a right singular vector of $M$ and $\mathbf{u}$ is called a left singular vector of $M$.

Clearly, these definitions have something to do with the concepts of eigenvalues and eigenvectors, but please note the differences: (i) we are not necessarily dealing with square matrices; (ii) the singular values must be nonnegative; (iii) the vectors $\mathbf{v}$ and $\mathbf{w}$ both appear in both equations, and they must be unit vectors.

It may seem difficult to find singular values and singular vectors. But it is not so hard. We simply find eigenvalues and eigenvectors of the positive semidefinite matrices $M^T M$ and $M M^T$. For example, consider the symmetric, positive semidefinite $n \times n$ matrix $M^T M$. We know from the spectral theorem that there is an orthonormal basis $\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_n$ for $\mathbb{R}^n$ consisting of eigenvectors of $M^T M$, with corresponding eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Because $M^T M$ is positive semidefinite, we know these eigenvalues are nonnegative. Then it turns out that the quantities $\sqrt{\lambda_1}, \sqrt{\lambda_2}, \ldots, \sqrt{\lambda_n}$ are the singular values of $M$.

Let’s see why this is the case. Let’s assume that the eigenvalues are listed in decreasing order: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$. Choose $k$ between 1 and $n$ so that $\lambda_i > 0$ if $i \leq k$ and $\lambda_i = 0$ if $i > k$. Let $V_1$ be the $n \times k$ matrix whose columns are the eigenvectors $\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_k$, and let $V_2$ be the $n \times n - k$ matrix whose columns are the remaining eigenvectors. Then

$$(V_1 \ V_2)^T M^T M (V_1 \ V_2) = \begin{pmatrix} V_1^T M^T M V_1 & V_1^T M^T M V_2 \\ V_2^T M^T M V_1 & V_2^T M^T M V_2 \end{pmatrix} = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix},$$

where $D$ is the $k \times k$ diagonal matrix consisting of the positive eigenvalues of $M^T M$, and the 0s represent zero matrices of appropriate size, so that the matrix $\begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix}$ is a diagonal $n \times n$ matrix.

Now let

$$U_1 = M V_1 D^{-1/2},$$
where $D^{-1/2}$ is obtained by replacing the diagonal elements of $D$ by the reciprocals of their positive square roots. (You should check that these matrices are all compatible in size for the indicated matrix multiplications.) Then

$$U_1 D^{1/2} V_1^T = M V_1 D^{-1/2} D^{1/2} V_1^T = M V_1 V_1^T = M .$$

This gives us a decomposition of $M$ into the product of three matrices. It turns out that the matrix $U_1$ has $k$ orthogonal columns. How can we see this? Just calculate the product $U_1^T U_1$:

$$(MV_1 D^{-1/2})^T MV_1 D^{-1/2} = D^{-1/2} V_1^T M V_1 D^{-1/2} = D^{-1/2} DD^{-1/2} = I .$$

Thus, $U_1$ can be expanded to an orthogonal $n \times n$ matrix by appending a matrix $U_2$ with $n - k$ orthogonal columns (using Gram-Schmidt), so that

$$M = (U_1 U_2) \Sigma \begin{pmatrix} V_1^T & V_2^T \end{pmatrix},$$

where $\Sigma$ is of the form

$$\Sigma = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix}$$

with enough zeroes to make the matrix multiplication work out. Let $U$ be the $m \times m$ matrix $(U_1 U_2)$ and $V$ the $n \times n$ matrix $(V_1 V_2)$, and we have the following singular value decomposition of $M$:

$$M = U \Sigma V^T ,$$

where the matrices $U$ and $V$ are orthogonal. Multiply on the right by $V$ and we have

$$MV = U \Sigma ,$$

and multiply on the left by $U^T$ and we have

$$U^T M = \Sigma V^T ,$$

from which it follows that the diagonal elements of $\Sigma$ are the singular values of $M$, with right singular vectors being the columns of $V$ and left singular vectors being the columns of $U$.

### 3. What good is it?

Suppose we have obtained a singular value decomposition of $M$ as $M = U \Sigma V^T$. Recall that the nonzero diagonal elements of $\Sigma$ are listed in decreasing order. Also recall that we obtained all three matrices by expanding the matrices in the decomposition $M = U_1 D^{1/2} V_1^T$, in which all of the elements of $D$ are positive. Replace the lower right element of $D$ with 0. Remember that this is the smallest diagonal element of $D$. If this is small enough, it won’t make much of a difference. With
the 0 in that spot, we can ignore the rightmost columns of $U_1$ and $V_1$. If we eliminate them altogether and also eliminate the bottom row and rightmost column of $D$, we get a new matrix that is “very much like” $M$, but smaller! This is called dimension reduction, and it is the basis for principal component analysis.