Complement: Singular Value Decomposition

In this note we present a simple demonstration of the singular value decomposition of a complex $n \times n$ square matrix $A$, into the form

$$A = UDV^\dagger,$$

(1)

where $U$ and $V$ are unitary matrices and $D$ is a nonnegative diagonal matrix.

To begin with, we denote with $A = [a_{ij}]$ the square matrix $A$ of elements $a_{ij}$, $(i = 1, 2, \ldots, n, \ j = 1, 2, \ldots, n)$, where $a_{ij}$ are real or complex numbers. The adjoint of $A = [a_{ij}]$ is denoted $A^\dagger$ and is defined by $A^\dagger = [a_{ji}^*]$. We use boldface fonts to denote $n \times 1$ and $1 \times n$ matrices, as in

$$v = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}, \quad v^\dagger = \begin{bmatrix} v_1^* & v_2^* & \cdots & v_n^* \end{bmatrix}.$$

(2)

Given $A$, we can build the $2n \times 2n$ matrix $S$ defined as

$$S = \begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix},$$

(3)

where $0$ stands for a $n \times n$ matrix whose entries are all zero. By definition $S$ is self-adjoint, that is $S = S^\dagger$. Therefore, we can solve the eigenvalue equation

$$Sw = \lambda w,$$

(4)

where $\lambda$ is a real number and $w$ is a $2n \times 1$ matrix,

$$w = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_{2n} \end{bmatrix}.$$

(5)

There are $2n$ eigenvalues $\lambda$ and $2n$ eigenvectors $w$ that solve $Sw = \lambda w$. 

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If we rewrite the eigenvector $\mathbf{w}$ as

$$\mathbf{w} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix},$$  \hspace{1cm} (6)$$

where $\mathbf{u}$ and $\mathbf{v}$ are $n \times 1$ matrices, then Eq. (4) can be rewritten as

$$\begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix},$$ \hspace{1cm} (7)$$

which is equivalent to the pair of coupled equations

$$A \mathbf{v} = \lambda \mathbf{u},$$

$$A^\dagger \mathbf{u} = \lambda \mathbf{v}.$$ \hspace{1cm} (8)

Let $r$ be the rank of $S$, that it the number of its nonzero eigenvalues. It is easy to show that $r = 2k$, with $k \leq n$. In fact, if in (7) we replace $\lambda$ with $-\lambda$ and $\mathbf{u}$ with $-\mathbf{u}$, then equations (8) do not change. This means that both $(\lambda, \mathbf{w})$ and $(-\lambda, \bar{\mathbf{w}})$ are solutions of (4), where we have defined

$$\bar{\mathbf{w}} \equiv \begin{bmatrix} -\mathbf{u} \\ \mathbf{v} \end{bmatrix}. \hspace{1cm} (9)$$

Thus, all nonzero eigenvalues appears in $k$ pairs $(\lambda, -\lambda)$ and $r = 2k \leq 2n$. Since $\lambda$ is real, from now on we assume without loss of generality $\lambda \geq 0$.

How we determine $\mathbf{u}$ and $\mathbf{v}$? Let us multiply from left the first equation (8) by $A^\dagger$ and the second one by $A$. We obtain:

$$A^\dagger A \mathbf{v} = \lambda A^\dagger \mathbf{u} = \lambda^2 \mathbf{v},$$

$$AA^\dagger \mathbf{u} = \lambda A \mathbf{v} = \lambda^2 \mathbf{u}. \hspace{1cm} (10)$$

Therefore $\mathbf{u}$ and $\mathbf{v}$ are simply the eigenvectors of the self-adjoint matrices $AA^\dagger$ and $A^\dagger A$, respectively. From $\mathbf{u}$ and $\mathbf{v}$ we obtain two unitary square matrices, denoted $U$ and $V$, formed out of the $n$ eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$ and
\[ U = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix}, \]
\[ V = \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix}. \]  

(11)

Since by convention \( \lambda \geq 0 \), then the \( k \) nonzero pairs \((\lambda, -\lambda)\) can be written as \((+\sqrt{\lambda_i^2}, -\sqrt{\lambda_i^2})\), where \( \lambda_i^2 \) is the \( i \)th solution of either equations (10). Then, we can rewrite (8) as:

\[ A v_i = \sqrt{\lambda_i^2} u_i, \]
\[ A^\dagger u_i = \sqrt{\lambda_i^2} v_i, \]  

(12)

with \( i = 1, 2, \cdots, n \).

If we choose the following ordering for the eigenvalues,

\[ \lambda_1^2 \geq \lambda_2^2 \geq \cdots \geq \lambda_k^2 > 0, \quad \lambda_{k+1} = \cdots = \lambda_n = 0, \]  

(13)

then we can build the \( n \times n \) diagonal matrix

\[ D = \begin{bmatrix} \sqrt{\lambda_1^2} & & & \\ & \ddots & & \\ & & \sqrt{\lambda_k^2} & \\ & & & 0 \end{bmatrix}, \]  

(14)

and the first of equations (12) can be rewritten in matrix form as

\[ \begin{bmatrix} A v_1 & A v_2 & \cdots & A v_n \end{bmatrix} = \begin{bmatrix} \sqrt{\lambda_1^2} u_1 & \sqrt{\lambda_2^2} u_2 & \cdots & \sqrt{\lambda_k^2} u_k & 0 & \cdots & 0 \end{bmatrix}, \]  

(15)

or, more compactly,

\[ AV = UD. \]  

(16)
Finally, multiplying this equation from right by $V^\dagger$ and using $VV^\dagger = I_n$, where $I_n$ denotes the $n \times n$ identity matrix, we obtain the sought singular value decomposition:

$$A = UDV^\dagger.$$  \hspace{1cm} (17)