Chapter 9

Singular Value Decomposition

9.1 Diagonalization of Hermitian Matrices

Lemma 9.1.1 (Schur Decomposition). For any square matrix $A$, there exists a unitary matrix $U$ such that

$$ U^H AU = T $$

where $T$ is upper triangular. That is, every square matrix is similar to an upper-triangular matrix.

Proof. We prove this lemma by induction on the size $n$ of the matrix. Since it is clearly true for scalars (i.e., matrices of size $n = 1$), the base case is trivial. Now, suppose that the result holds for all $k = 1, 2, \ldots, n - 1$ and let $A \in \mathbb{C}^{n \times n}$. Since every matrix has at least one eigenvector, we let $u$ be an eigenvector of $A$ normalized so that $\|u\|_2 = 1$. Using the Gram-Schmidt procedure, it is possible to construct an orthonormal basis $B = x_1, \ldots, x_n$ for $\mathbb{C}^n$, with $x_1 = u$. Define the matrix $U_n$ by

$$ U_n = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}. $$

Since $B$ is a basis for $\mathbb{C}^n$, every column of the matrix $AU_n$ can be expressed as a linear combination of vectors in $B$, say,

$$ A x_i = \sum_{j=1}^{n} s_{ji} x_j \quad i = 1, \ldots, n. $$

Note that $A x_1 = \lambda_1 x_1$ for some $\lambda_1$ since $x_1 = u$, an eigenvector of $A$. We can then
write

\[
AU_n = \begin{bmatrix} A_{x_1} & \cdots & A_{x_n} \end{bmatrix} = U_n \begin{bmatrix} \lambda_1 & s_{1,2} & \cdots & s_{1,n} \\ 0 & s_{2,2} & \cdots & s_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & s_{n,2} & \cdots & s_{n,n} \end{bmatrix} = U_n \begin{bmatrix} \lambda_1 & s^T \\ 0 & A_{n-1} \end{bmatrix},
\]

where we have used the convenient notation

\[
A_{n-1} = \begin{bmatrix} s_{2,2} & \cdots & s_{2,n} \\ \vdots & \ddots & \vdots \\ s_{n,2} & \cdots & s_{n,n} \end{bmatrix}
\]

and \( s^T = (s_{1,2}, \ldots, s_{1,n}) \). By the inductive hypothesis, we can write \( A_{n-1} = U_{n-1} T_{n-1} U_{n-1}^H \) where \( T_{n-1} \) is upper triangular and \( U_{n-1} \) is unitary. It follows that

\[
AU_n = U_n \begin{bmatrix} \lambda_1 & s^T \\ 0 & A_{n-1} \end{bmatrix} = U_n \begin{bmatrix} \lambda_1 & s^T U_{n-1} \\ 0 & T_{n-1} \end{bmatrix} \begin{bmatrix} 1 & 0^T \\ 0 & U_{n-1}^H \end{bmatrix}.
\]

Let \( U \) be the matrix given by

\[
U = U_n \begin{bmatrix} 1 & 0^T \\ 0 & U_{n-1} \end{bmatrix},
\]

and note that \( U \) is unitary. It follows that

\[
U^H AU = \begin{bmatrix} \lambda_1 & s^T U_{n-1} \\ 0 & T_{n-1} \end{bmatrix}.
\]

That is, \( U \) is a unitary matrix such that \( U^H AU \) is upper-triangular. \( \Box \)

We use this lemma to prove the following theorem.

**Theorem 9.1.2.** Every Hermitian \( n \times n \) matrix \( A \) can be diagonalized by a unitary matrix,

\[
U^H AU = \Lambda,
\]

where \( U \) is unitary and \( \Lambda \) is a diagonal matrix.
Proof. Note that $A^H = A$ and $T = U^H AU$. Consider the matrix $T^H$ given by

$$T^H = (U^H AU)^H = U^H A^H U = U^H AU = T.$$ 

That is, $T$ is also Hermitian. Since $T$ is upper triangular, this implies that $T$ is a diagonal matrix. We must conclude that every Hermitian matrix is diagonalized by a unitary matrix.

This proves every Hermitian matrix has a complete set of orthonormal eigenvectors.

9.2 Singular Value Decomposition

The singular value decomposition (SVD) provides a matrix factorization related to the eigenvalue decomposition that works for all matrices. In general, any matrix $A \in \mathbb{C}^{m \times n}$ can be factored into a product of unitary matrices and a diagonal matrix, as explained below.

**Theorem 9.2.1.** Let $A$ be a matrix in $\mathbb{C}^{m \times n}$. Then $A$ can be factored as

$$A = U \Sigma V^H$$

where $U \in \mathbb{C}^{m \times m}$ is unitary, $V \in \mathbb{C}^{n \times n}$ is unitary, and $\Sigma \in \mathbb{R}^{m \times n}$ has the form

$$\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_p),$$

where $p = \min(m, n)$.

The diagonal elements of $\Sigma$ are called the **singular values** of $A$ and are typically ordered so that

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0.$$

**Proof.** Let

$$A^H AV = V \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$$

be the spectral decomposition of $A^H A$, where the columns of $V$ are orthonormal eigenvectors

$$V = \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix},$$
with \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > 0 = \lambda_{r+1} = \cdots = \lambda_n \) and \( r \leq p \). For \( i \leq r \), let
\[
\mathbf{u}_i = \frac{A \mathbf{v}_i}{\sqrt{\lambda_i}},
\]
and observe that
\[
\langle \mathbf{u}_i | \mathbf{u}_j \rangle = \frac{v_i^H A^H A \mathbf{v}_j}{\sqrt{\lambda_i \lambda_j}} = \frac{v_i^H \mathbf{v}_j \lambda_i}{\sqrt{\lambda_i \lambda_j}} = \delta_{ij}.
\]
Also note that \( \{ \mathbf{u}_i \} \) are eigenvectors of \( A A^H \) since
\[
A A^H \mathbf{u}_i = A A^H A \mathbf{v}_i \sqrt{\lambda_i} = \sqrt{\lambda_i} A \mathbf{v}_i = \lambda_i \mathbf{u}_i.
\]
The set \( \{ \mathbf{u}_i : i = 1, \ldots, r \} \) can be extended using the Gram-Schmidt procedure to form an orthonormal basis for \( \mathbb{C}^m \). Let
\[
U = \begin{bmatrix} \mathbf{u}_1 & \cdots & \mathbf{u}_m \end{bmatrix}.
\]
For the zero eigenvalues, the eigenvectors must come from the nullspace of \( A A^H \) since the eigenvectors with zero eigenvalues are, by construction, orthogonal to the eigenvectors with nonzero eigenvalues that are in the range of \( A A^H \).

For \( \mathbf{u}_i \) where \( i \leq r \), we get
\[
\mathbf{u}_i^H A V = \frac{1}{\sqrt{\lambda_i}} \mathbf{v}_i^H A^H A V = \sqrt{\lambda_i} \mathbf{v}_i^H.
\]
On the other hand, if \( i > r \) then \( \mathbf{u}_i^H A V = 0 \). Hence,
\[
U^H A V = \text{diag} \left( \sqrt{\lambda_1}, \ldots, \sqrt{\lambda_n} \right) = \Sigma,
\]
as desired.

This proof gives a recipe for computing the SVD of an arbitrary matrix. Consider the matrix
\[
A = \begin{bmatrix} 1 & 1 \\ 5 & -1 \\ -1 & 5 \end{bmatrix}.
\]
The eigenvalue decomposition of \( A^H A \) is given by
\[
A^H A = \begin{bmatrix} 27 & -9 \\ -9 & 27 \end{bmatrix} = V \Lambda V^H = \left( \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \right) \begin{bmatrix} 36 & 0 \\ 0 & 18 \end{bmatrix} \left( \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \right).
\]
This implies that $\Sigma_1 = \Lambda^{1/2}$ and $V_1 = V$. Therefore, we can compute $U_1 = AV_1\Sigma_1^{-1}$ with

$$ U_1 = \begin{bmatrix} 1 & 1 \\ 5 & -1 \\ -1 & 5 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{36}} & 0 \\ 0 & \frac{1}{\sqrt{18}} \end{bmatrix} = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix}. $$

Putting this all together, we have the compact SVD

$$ A = U_1\Sigma_1V_1^H = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{3}{2} \end{bmatrix} \begin{bmatrix} \sqrt{36} & 0 \\ 0 & \sqrt{18} \end{bmatrix} \begin{bmatrix} 1 \sqrt{2} \\ -1 \sqrt{2} \end{bmatrix}. $$

### 9.3 Properties of the SVD

Many of the important properties of the SVD can be understood better by separating the non-zero singular values from the zero singular values. To do this, we note that every rank $r$ matrix $A \in \mathbb{C}^{m \times n}$ has a singular value decomposition

$$ A = U\Sigma V^H = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1^H \\ V_2^H \end{bmatrix} = U_1\Sigma_1V_1^H, $$

where $U \in \mathbb{C}^{m \times m}$ and $V \in \mathbb{C}^{n \times n}$ are unitary and $U_1 \in \mathbb{C}^{m \times r}$, $U_2 \in \mathbb{C}^{m \times m-r}$, $V_1 \in \mathbb{C}^{n \times r}$, and $V_2 \in \mathbb{C}^{n \times n-r}$ have orthonormal columns. The diagonal matrix $\Sigma_1 \in \mathbb{R}^{r \times r}$ contains the non-zero singular values

$$ \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0. $$

The factorization $A = U\Sigma V^H$ is called the **full SVD** of the matrix $A$ while the factorization $A = U_1\Sigma_1V_1$ is called the **compact SVD** of $A$. The compact SVD of a rank-$r$ matrix retains only the $r$ columns of $U, V$ associated with non-zero singular values.

Let $X, Y$ be inner product spaces and let $A$ define a mapping from $X$ to $Y$. Then, the columns of $V_1$ form an orthonormal basis for the vectors in $X$ that are mapped to non-zero vectors (i.e., $N(A)^\perp$) while the columns of $V_2$ form an orthonormal basis of $N(A)$. Likewise, the columns of $U_1$ form an orthonormal basis for the vectors in $Y$ that lie in the range of $A$ while the vectors in $U_2$ form orthonormal basis for $R(A)^\perp$. It follows that the full SVD computes orthonormal bases for
all of the four fundamental subspaces of the matrix $A$. For example, it is easy to show that

\[
\mathcal{R}(A) = \text{span}(U_1) \\
\mathcal{R}(A^H) = \text{span}(V_1) \\
\mathcal{N}(A) = \text{span}(V_2) \\
\mathcal{N}(A^H) = \text{span}(U_2)
\]

To see this, notice that $A \sum_{i=1}^r c_i u_i = \sum_{i=1}^r c_i \sigma_i u_i$.

From this, we can compute easily any projection onto a fundamental subspace. First, we point out that the projection onto the column space of any matrix $W \in \mathbb{C}^{m \times n}$ with orthonormal columns (i.e., $W^H W = I$) is given by

\[
P_W = W (W^H W)^{-1} W^H = WW^H.
\]

Therefore, the projection matrices for the fundamental subspaces are given by

\[
P_{\mathcal{R}(A)} = U_1 U_1^H \\
P_{\mathcal{R}(A^H)} = V_1 V_1^H \\
P_{\mathcal{N}(A)} = V_2 V_2^H = I - V_1 V_1^H \\
P_{\mathcal{N}(A^H)} = U_2 U_2^H = I - U_1 U_1^H.
\]

This decomposition also provides a rank revealing decomposition of a rank-$r$ matrix

\[
A = \sum_{i=1}^r \sigma_i u_i v_i^H,
\]

where $u_i$ is the $i$th column of $U$ and $v_i$ is the $i$th column of $V$. This shows $A$ as the sum of $r$ rank-1 matrices. It also allows one to compute

\[
\|A\|_F = \sum_{i=1}^r \sigma_i^2 \\
\|A\|_2 = \sigma_1
\]

The pseudoinverse of $A$ is also very easy to compute from the SVD. In particular, one finds that

\[
A^\dagger = V \Sigma^\dagger U^H = V_1 \Sigma_1^{-1} U_1^H.
\]

One can verify this by computing $A^\dagger A$ and $AA^\dagger$. It also follows from the fact that the pseudoinverse of a scalar $\sigma$ is $\sigma^{-1}$ if $\sigma \neq 0$ and zero otherwise.