Singular Value Decomposition

For m by n (complex) matrix A there is a unitary m by m matrix U and a unitary n by n matrix V with

$$A = USV^*$$

where $S = \begin{bmatrix} D & O \\ O & O \end{bmatrix}$, and $D = \mathrm{diag}(\mu_1, \ldots, \mu_r)$ with $\mu_1 \geq \cdots \geq \mu_r > 0$.

Proof:

Since A^*A is Hermitian, it has an orthonormal basis of eigenvectors $\mathbf{v}_1, \cdots, \mathbf{v}_n$ and the eigenvalues are real; arrange the basis so that the eigenvalues λ_i are in descending order.

$$A^*A\mathbf{v}_i = \lambda_i \mathbf{v}_i.$$

The eigenvalues λ_i are non-negative because $\lambda_i \langle \mathbf{v}_i, \mathbf{v}_i \rangle = \langle \mathbf{v}_i, \lambda_i \mathbf{v}_i \rangle = \langle \mathbf{v}_i, A^*A\mathbf{v}_i \rangle = \langle A\mathbf{v}_i, A\mathbf{v}_i \rangle \geq 0$ and $\langle \mathbf{v}_i, \mathbf{v}_i \rangle > 0$ as $\mathbf{v}_i \neq \mathbf{0}$ for eigenvectors. If $\lambda_i = 0$ this also shows $\langle A\mathbf{v}_i, A\mathbf{v}_i \rangle = 0$ so $A\mathbf{v}_i = 0$.

For those i with $\lambda_i \neq 0$, say r in number, set $\mu_i = \sqrt{\lambda_i}$ and define

$$\mathbf{u}_i = \frac{1}{\mu_i} A\mathbf{v}_i.$$

These are orthonormal since

$$\begin{aligned} \langle \mathbf{u}_i, \mathbf{u}_j \rangle &= \frac{1}{\mu_i \mu_j} \langle A\mathbf{v}_i, A\mathbf{v}_j \rangle \\ &= \frac{1}{\mu_i \mu_j} \langle \mathbf{v}_i, A^*A\mathbf{v}_j \rangle \\ &= \frac{\lambda_j}{\mu_i \mu_j} \langle \mathbf{v}_i, \mathbf{v}_j \rangle \end{aligned}$$

which is 0 if $i \neq j$ and 1 if $i = j$.

Extend the $\mathbf{u}_i$'s to an orthonormal basis of $\mathbb{C}^m$. Let $U = (\mathbf{u}_1 | \ldots | \mathbf{u}_m)$ and $V = (\mathbf{v}_1 | \ldots | \mathbf{v}_n)$.

Then $AV = US$ since

$$AV\mathbf{e}_i = A\mathbf{v}_i = \begin{cases} \mu_i \mathbf{u}_i & \text{if } i \leq r \\ \mathbf{0} & \text{if } i > r \end{cases} = \begin{bmatrix} \mu_1 & 0 & \ldots \\ 0 & \ddots & \ldots \\ \vdots & \vdots & \vdots \end{bmatrix} \mathbf{e}_i = US\mathbf{e}_i.$$

As an aside, note that AA^* has an orthonormal basis of eigenvectors the $\mathbf{u}_1, \cdots, \mathbf{u}_n$ with eigenvectors μ_j (on defining $\mu_j = 0$ for $j > r$).

The decomposition of A is often written as $A = \mu_1 \mathbf{u}_1 \mathbf{v}_1^* + \cdots + \mu_r \mathbf{u}_r \mathbf{v}_r^*$ and the vectors $\mathbf{u}_i$ and $\mathbf{v}_i$ are called the left and right singular vectors respectively.