Generalised Inverse from the Singular Value Decomposition

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Let $\boldsymbol{A} \in \mathbb{C}^{m \times n}$ be a general matrix. The Singular Value Decomposition (SVD) says that $\boldsymbol{A}$ may be written as the product of three special matrices:

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^H \tag{1}$$

where $\boldsymbol{U} \in \mathbb{C}^{m \times m}$ and is unitary, $\boldsymbol{S} \in \mathbb{R}^{m \times n}$ and is diagonal and $\boldsymbol{V} \in \mathbb{C}^{n \times n}$ is also unitary. Provided that $\boldsymbol{A}$ is of full-rank, then we can obtain the *generalised inverse* of $\boldsymbol{A}$ by inverting the right hand side, that is:

$$\boldsymbol{A}^+ = V\boldsymbol{S}^{-1}\boldsymbol{U}^H \tag{2}$$

this is equivalent to the least-squares inverse of $\boldsymbol{A}$, i.e. $\boldsymbol{A}^+ = (\boldsymbol{A}^H\boldsymbol{A})^{-1}\boldsymbol{A}^H$. However, it is often better to compute the generalised inverse using the SVD for reasons of numerical stability; particularly when $\boldsymbol{A}$ is, or is nearly, rank-deficient. When $\boldsymbol{A}$ is rank deficient, some of the singular values along the diagonal of $\boldsymbol{S}$ will be zero, and as such they are not inverted when computing $\boldsymbol{S}^{-1}$.

A computational consideration of (2) is that the matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ do not need to be computed fully when the dimensions of $\boldsymbol{A}$ are not equal, since some of their columns will be multiplied by zero when constructing $\boldsymbol{A}^+$. The two cases are as follows, for $m > n$

$$\boldsymbol{U} \in \mathbb{C}^{m \times n} \tag{3}$$
$$\boldsymbol{S} \in \mathbb{R}^{n \times n} \tag{4}$$
$$\boldsymbol{V} \in \mathbb{C}^{n \times n} \tag{5}$$

and for $n > m$

$$\boldsymbol{U} \in \mathbb{C}^{m \times m} \tag{6}$$
$$\boldsymbol{S} \in \mathbb{R}^{m \times m} \tag{7}$$
$$\boldsymbol{V} \in \mathbb{C}^{n \times m} \tag{8}$$

LAPACK provides the “economy decomposition” SVD, using the routine `??GESVD`, computing only the required columns. This provides a big computational saving and makes the inverting of large, non-sparse matrices possible.