Further Mathematical Methods (Linear Algebra) 2002

Lecture 20: Singular Values Decomposition

Recall that the spectral decomposition of a matrix A is only possible if the matrix is normal, that is, if it is such that $\mathsf{AA}^\dagger = \mathsf{A}^\dagger\mathsf{A}$. But, if A is an $m \times n$ matrix with $m \neq n$ (i.e. A is *not* square), then A cannot be a normal matrix as:

- $\mathsf{AA}^\dagger$ is an $m \times m$ matrix.
- $\mathsf{A}^\dagger\mathsf{A}$ is an $n \times n$ matrix.

and so, since these matrices are of different sizes, they cannot be equal. However, we can find something, called the *singular values decomposition*, which is the non-square matrix *analogue* of the spectral decomposition. To see this, we first note that:

Theorem 20.1 *Let A be an $m \times n$ matrix. The matrices $\mathsf{AA}^\dagger$ and $\mathsf{A}^\dagger\mathsf{A}$ are both Hermitian and they have the same positive eigenvalues. Further, the orthonormal sets of eigenvectors $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$ and $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k\}$ corresponding to the positive eigenvalues of $\mathsf{AA}^\dagger$ and $\mathsf{A}^\dagger\mathsf{A}$ can be chosen so that*

$$\mathbf{x}_i = \frac{1}{\sqrt{\lambda_i}}\mathsf{A}\mathbf{y}_i \quad \text{and} \quad \mathbf{y}_j = \frac{1}{\sqrt{\lambda_j}}\mathsf{A}^\dagger\mathbf{x}_j.$$

Proof: To start with, since $(\mathsf{AA}^\dagger)^\dagger = \mathsf{AA}^\dagger$ and $(\mathsf{A}^\dagger\mathsf{A})^\dagger = \mathsf{A}^\dagger\mathsf{A}$, the matrices $\mathsf{AA}^\dagger$ and $\mathsf{A}^\dagger\mathsf{A}$ are both Hermitian. As such, we know from the lecture on complex matrices that they will have real eigenvalues. We further note that:

- For any eigenvalue λ of $\mathsf{AA}^\dagger$, we have $\mathsf{AA}^\dagger\mathbf{x} = \lambda\mathbf{x}$ with $\mathbf{x} \neq \mathbf{0}$. Thus, since

  $$\mathbf{x}^\dagger\mathsf{AA}^\dagger\mathbf{x} = (\mathsf{A}^\dagger\mathbf{x})^\dagger\mathsf{A}^\dagger\mathbf{x} = \|\mathsf{A}^\dagger\mathbf{x}\|^2 \geq 0,$$

  and

  $$\mathbf{x}^\dagger\mathsf{AA}^\dagger\mathbf{x} = \lambda\mathbf{x}^\dagger\mathbf{x} = \lambda\|\mathbf{x}\|^2,$$

  we have $\lambda \geq 0$ since $\|\mathbf{x}\|^2 \geq 0$. Consequently, any eigenvalue of $\mathsf{AA}^\dagger$ is non-negative.

- For any eigenvalue λ of $\mathsf{A}^\dagger\mathsf{A}$, we have $\mathsf{A}^\dagger\mathsf{A}\mathbf{x} = \lambda\mathbf{x}$ with $\mathbf{x} \neq \mathbf{0}$. Thus, since

  $$\mathbf{x}^\dagger\mathsf{A}^\dagger\mathsf{A}\mathbf{x} = (\mathsf{A}\mathbf{x})^\dagger\mathsf{A}\mathbf{x} = \|\mathsf{A}\mathbf{x}\|^2 \geq 0,$$

  and

  $$\mathbf{x}^\dagger\mathsf{A}^\dagger\mathsf{A}\mathbf{x} = \lambda\mathbf{x}^\dagger\mathbf{x} = \lambda\|\mathbf{x}\|^2,$$

  we have $\lambda \geq 0$ since $\|\mathbf{x}\|^2 \geq 0$. Consequently, any eigenvalue of $\mathsf{A}^\dagger\mathsf{A}$ is non-negative.

Now, we also have to show that the matrices $\mathsf{AA}^\dagger$ and $\mathsf{A}^\dagger\mathsf{A}$ have the *same* non-zero eigenvalues and to do this, we note that:

- For any eigenvalue λ of $\mathsf{AA}^\dagger$, we have $\mathsf{AA}^\dagger\mathbf{x} = \lambda\mathbf{x}$ with $\mathbf{x} \neq \mathbf{0}$. That is, multiplying through by $\mathsf{A}^\dagger$, we have

  $$\mathsf{A}^\dagger(\mathsf{AA}^\dagger)\mathbf{x} = \lambda\mathsf{A}^\dagger\mathbf{x} \implies (\mathsf{A}^\dagger\mathsf{A})(\mathsf{A}^\dagger\mathbf{x}) = \lambda(\mathsf{A}^\dagger\mathbf{x}) \implies \mathsf{A}^\dagger\mathsf{A}\mathbf{y} = \lambda\mathbf{y},$$

  where we have set $\mathbf{y} = \mathsf{A}^\dagger\mathbf{x}$. Thus, provided that $\mathbf{y} \neq \mathbf{0}$, any eigenvalue of $\mathsf{AA}^\dagger$ is also an eigenvalue of $\mathsf{A}^\dagger\mathsf{A}$. However, if $\mathbf{y} = \mathbf{0}$, then

  $$\lambda\mathbf{x} = \mathsf{AA}^\dagger\mathbf{x} = \mathsf{A}\mathbf{y} = \mathsf{A}\mathbf{0} = \mathbf{0},$$

  i.e. since $\mathbf{x} \neq \mathbf{0}$, we have $\lambda = 0$. Consequently, this analysis only holds if we are considering the non-zero eigenvalues of $\mathsf{AA}^\dagger$.

- For any eigenvalue λ of $\mathsf{A}^\dagger\mathsf{A}$, we have $\mathsf{A}^\dagger\mathsf{A}\mathbf{x} = \lambda\mathbf{x}$ with $\mathbf{x} \neq \mathbf{0}$. That is, multiplying through by A, we have
$$\mathsf{A}(\mathsf{A}^\dagger\mathsf{A})\mathbf{x} = \lambda\mathsf{A}\mathbf{x} \implies (\mathsf{A}\mathsf{A}^\dagger)(\mathsf{A}\mathbf{x}) = \lambda(\mathsf{A}\mathbf{x}) \implies \mathsf{A}\mathsf{A}^\dagger\mathbf{y} = \lambda\mathbf{y},$$
where we have set $\mathbf{y} = \mathsf{A}\mathbf{x}$. Thus, provided that $\mathbf{y} \neq \mathbf{0}$, any eigenvalue of $\mathsf{A}^\dagger\mathsf{A}$ is also an eigenvalue of $\mathsf{A}\mathsf{A}^\dagger$. However, if $\mathbf{y} = \mathbf{0}$, then
$$\lambda\mathbf{x} = \mathsf{A}^\dagger\mathsf{A}\mathbf{x} = \mathsf{A}^\dagger\mathbf{y} = \mathsf{A}^\dagger\mathbf{0} = \mathbf{0},$$
i.e. since $\mathbf{x} \neq \mathbf{0}$, we have $\lambda = 0$. Consequently, this analysis only holds if we are considering the non-zero eigenvalues of $\mathsf{A}^\dagger\mathsf{A}$.

Thus, the matrices $\mathsf{A}\mathsf{A}^\dagger$ and $\mathsf{A}^\dagger\mathsf{A}$ have the *same* positive eigenvalues (as required).

Further, we have to prove that the orthonormal sets of eigenvectors $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$ and $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k\}$ corresponding to the positive eigenvalues of $\mathsf{A}\mathsf{A}^\dagger$ and $\mathsf{A}^\dagger\mathsf{A}$ can be chosen so that
$$\mathbf{x}_i = \frac{1}{\sqrt{\lambda_i}}\mathsf{A}\mathbf{y}_i \quad \text{and} \quad \mathbf{y}_j = \frac{1}{\sqrt{\lambda_j}}\mathsf{A}^\dagger\mathbf{x}_j.$$

Now, from the lecture on complex matrices, we know that such sets of orthonormal eigenvectors can be found since the matrices $\mathsf{A}\mathsf{A}^\dagger$ and $\mathsf{A}^\dagger\mathsf{A}$ are Hermitian, and hence normal. So, given such orthonormal sets of eigenvectors, we note that:

- $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k\}$ is an orthonormal set of eigenvectors corresponding to the non-zero eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of $\mathsf{A}^\dagger\mathsf{A}$ and from above, we know that $\{\mathsf{A}\mathbf{y}_1, \mathsf{A}\mathbf{y}_2, \ldots, \mathsf{A}\mathbf{y}_k\}$ are eigenvectors for the non-zero eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of $\mathsf{A}\mathsf{A}^\dagger$. So, since
$$\langle\mathsf{A}\mathbf{y}_i, \mathsf{A}\mathbf{y}_j\rangle = (\mathsf{A}\mathbf{y}_i)^\dagger\mathsf{A}\mathbf{y}_j = \mathbf{y}_i^\dagger\mathsf{A}^\dagger\mathsf{A}\mathbf{y}_j = \lambda_i\mathbf{y}_i^\dagger\mathbf{y}_j = \begin{cases}\lambda_i & \text{if } i = j\\ 0 & \text{if } i \neq j\end{cases},$$
we can see that the set of vectors $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$ where
$$\mathbf{x}_i = \frac{1}{\sqrt{\lambda_i}}\mathsf{A}\mathbf{y}_i,$$
is an orthonormal set of eigenvectors corresponding to the non-zero eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of $\mathsf{A}\mathsf{A}^\dagger$.

- $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$ is an orthonormal set of eigenvectors corresponding to the non-zero eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of $\mathsf{A}\mathsf{A}^\dagger$ and from above, we know that $\{\mathsf{A}^\dagger\mathbf{x}_1, \mathsf{A}^\dagger\mathbf{x}_2, \ldots, \mathsf{A}^\dagger\mathbf{x}_k\}$ are eigenvectors for the non-zero eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of $\mathsf{A}^\dagger\mathsf{A}$. So, since
$$\langle\mathsf{A}^\dagger\mathbf{x}_i, \mathsf{A}^\dagger\mathbf{x}_j\rangle = (\mathsf{A}^\dagger\mathbf{x}_i)^\dagger\mathsf{A}^\dagger\mathbf{x}_j = \mathbf{x}_i^\dagger\mathsf{A}\mathsf{A}^\dagger\mathbf{x}_j = \lambda_j\mathbf{x}_i^\dagger\mathbf{x}_j = \begin{cases}\lambda_j & \text{if } i = j\\ 0 & \text{if } i \neq j\end{cases},$$
we can see that the set of vectors $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k\}$ where
$$\mathbf{y}_j = \frac{1}{\sqrt{\lambda_j}}\mathsf{A}^\dagger\mathbf{x}_j,$$
is an orthonormal set of eigenvectors corresponding to the non-zero eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ of $\mathsf{A}^\dagger\mathsf{A}$.

Thus, we have established the required result. ♠

Now, using this Theorem, it is possible to derive the analogue of the spectral decomposition that we spoke of earlier. That is:

Theorem 20.2 *Let* A *be an* $m\times n$ *matrix where the matrices* $\mathsf{AA}^\dagger$ *and* $\mathsf{A}^\dagger\mathsf{A}$ *have positive eigenvalues* $\lambda_1, \lambda_2, \ldots, \lambda_k$ *and orthonormal sets of eigenvectors given by* $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$ *and* $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k\}$ *corresponding to these eigenvalues such that*

$$\mathbf{x}_i = \frac{1}{\sqrt{\lambda_i}}\mathsf{A}\mathbf{y}_i \quad \text{and} \quad \mathbf{y}_j = \frac{1}{\sqrt{\lambda_j}}\mathsf{A}^\dagger\mathbf{x}_j.$$

In this case, we can write

$$\mathsf{A} = \sum_{i=1}^{k} \sqrt{\lambda_i}\mathbf{x}_i\mathbf{y}_i^\dagger,$$

and this is called the singular values decomposition of A *and the scalars* $\sqrt{\lambda_1}, \sqrt{\lambda_2}, \ldots, \sqrt{\lambda_k}$ *are called the singular values of this matrix.*

Proof: Clearly, by Theorem 19.4, we know that this Theorem will hold for any $m \times n$ matrix with $m \neq n$. So, to establish this result, we note that we can extend the orthonormal set of eigenvectors $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k\}$ corresponding to the positive eigenvalues of the matrix $\mathsf{A}^\dagger\mathsf{A}$, to an orthonormal set of eigenvectors $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k, \mathbf{y}_{k+1}, \ldots, \mathbf{y}_n\}$ for the non-negative eigenvalues of the $n \times n$ matrix $\mathsf{A}^\dagger\mathsf{A}$.[1] Now, we recall from the lecture on complex matrices that the spectral decomposition of the identity matrix can be written in terms of this extended orthonormal set of eigenvectors, i.e.

$$\mathsf{I} = \sum_{i=1}^{n} \mathbf{y}_i\mathbf{y}_i^\dagger,$$

and multiplying this through by the matrix A we get

$$\mathsf{A} = \sum_{i=1}^{n} \mathsf{A}\mathbf{y}_i\mathbf{y}_i^\dagger.$$

However, for $k+1 \leq i \leq n$, we have zero eigenvalues which means that $\mathbf{y}_i^\dagger\mathsf{A}^\dagger\mathsf{A}\mathbf{y}_i = \lambda_i\|\mathbf{y}_i\|^2 = 0$ and so,

$$\mathbf{y}_i^\dagger\mathsf{A}^\dagger\mathsf{A}\mathbf{y}_i = (\mathsf{A}\mathbf{y}_i)^\dagger\mathsf{A}\mathbf{y}_i = \|\mathsf{A}\mathbf{y}_i\| = 0 \implies \mathsf{A}\mathbf{y}_i = \mathbf{0},$$

that is, the last $n-k$ terms in our summation are zero. Thus, we have

$$\mathsf{A} = \sum_{i=1}^{k} \mathsf{A}\mathbf{y}_i\mathbf{y}_i^\dagger.$$

and since,

$$\mathbf{x}_i = \frac{1}{\sqrt{\lambda_i}}\mathsf{A}\mathbf{y}_i,$$

this means that we can write

$$\mathsf{A} = \sum_{i=1}^{k} \sqrt{\lambda_i}\mathbf{x}_i\mathbf{y}_i^\dagger,$$

as required. ♠

You may wonder why we have bothered to do this. However, the singular values decomposition of a matrix gives us a nice way of calculating its strong generalised inverse, namely:

Theorem 20.3 *If* A *is an* $m \times n$ *matrix whose singular values decomposition is given by*

$$\mathsf{A} = \sum_{i=1}^{k} \sqrt{\lambda_i}\mathbf{x}_i\mathbf{y}_i^\dagger,$$

then the strong generalised inverse of A *is given by*

$$\mathsf{A}^G = \sum_{i=1}^{k} \frac{1}{\sqrt{\lambda_i}}\mathbf{y}_i\mathbf{x}_i^\dagger.$$

[1] That is, the vectors $\mathbf{y}_{k+1}, \mathbf{y}_{k+2}, \ldots, \mathbf{y}_n$ are eigenvectors corresponding to the eigenvalue $\lambda = 0$ of $\mathsf{A}^\dagger\mathsf{A}$ (which has multiplicity $n-k$).

Proof: See Question 7 of Problem Sheet 10. ♠

For example: For an example of calculating the singular values decomposition of a matrix and then using this to find its strong generalised inverse, see Question 6 of Problem Sheet 10. ♣