Numerical Linear Algebra

Lecture Notes 4:Singular Value Decomposition

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1 Motivation

Square matrix has eigenvalues, but rectangular matrix has not. Here is why singular value decomposition (SVD) comes. Consider $\mathbf{A} \in \mathbb{R}^{m \times n} (m \ge n)$, rank $(\mathbf{A}) = k(k \le n)$.

$$\mathbf{A}\mathbf{A}^T\mathbf{Y} = \mathbf{Y}\mathbf{\Lambda},$$

where $\Lambda = \operatorname{diag}(\lambda_1, ..., \lambda_k)$.

Let $\mathbf{Z} \triangleq \mathbf{A}^T \mathbf{Y} \mathbf{\Sigma}^{-1/2}$, then $\mathbf{Z}^T \mathbf{Z} = \mathbf{I}_k$. From the definition of \mathbf{Z} , we can get $\operatorname{span}(\mathbf{Z}) \subset \operatorname{span}(\mathbf{A}^T)$. $\mathbf{A}\mathbf{Z} = \mathbf{Y}\mathbf{\Lambda}^{1/2}$. Since $\operatorname{rank}(\mathbf{Z}) = \operatorname{rank}(\mathbf{A})$, $\operatorname{span}(\mathbf{Z}) = \operatorname{span}(\mathbf{A}^T)$. Let \mathbf{Z}_0 in \mathbf{Z} 's complementary space, $\hat{\mathbf{Z}} = (\mathbf{Z} \quad \mathbf{Z}_0)$ and $\hat{\mathbf{Z}}^T \hat{\mathbf{Z}} = \hat{\mathbf{Z}}\hat{\mathbf{Z}}^T = \mathbf{I}_n$.

$$\mathbf{A}\hat{\mathbf{Z}} = (\mathbf{A}\mathbf{Z} \quad \mathbf{A}\mathbf{Z}_0) \qquad \mathbf{A}\mathbf{Z}_0 = \mathbf{0}$$

$$\mathbf{A} = \mathbf{A}\hat{\mathbf{Z}}\hat{\mathbf{Z}}^T = \mathbf{Y}\mathbf{\Lambda}^{1/2}\mathbf{Z}^T$$

 ${\bf Y}$ is a column-orthogonal matrix, ${\bf Z}$ is a column-orthogonal matrix and ${\bf \Lambda}^{1/2}$ is a diagonal matrix.

2 SVD theorem

Theorem 2.1 (SVD Theorem). Let $\mathbf{A} \in \mathbb{R}^{m \times n} (m \ge n)$ be a nonzero matrix, then there exist orthogonal matrices $\mathbf{U} = [\mathbf{u}_1, ..., \mathbf{u}_m] \in \mathbb{R}^{m \times n}$ and $\mathbf{V} = [\mathbf{v}_1, ..., \mathbf{v}_n] \in \mathbb{R}^{n \times n}$, such that

$$\mathbf{U}^T \mathbf{A} \mathbf{V} = \mathbf{\Sigma} = diag(\sigma_1, ..., \sigma_p) \in \mathbb{R}^{m \times n},$$

where $p = \min\{m, n\}$ when $\sigma_1 \ge \sigma_2 \ge ... \ge \sigma_p \ge 0$.

Proof via induction.

- 1. When n = 1, it is surely correct.
- 2. Suppose the theorem holds when $\mathbf{A} \in \mathbb{R}^{(m-1)\times (n-1)}$. Now consider $\mathbf{A} \in \mathbb{R}^{m\times n}$. If $\mathbf{A} = 0$, then it is correct. If $\mathbf{A} \neq 0$, then $\sigma_1 = |||\mathbf{A}|||_2 = \max_{||\mathbf{v}||_2=1} ||\mathbf{A}\mathbf{v}||_2 \neq 0$. Let $\mathbf{v}_1 = \arg\max_{||\mathbf{v}||_2=1} ||\mathbf{A}\mathbf{v}||_2 + ||\mathbf{A}\mathbf{v}||_2$. Construct

$$\hat{\mathbf{V}} = \begin{bmatrix} \mathbf{v}_1, \mathbf{V}_1 \end{bmatrix}$$
 and $\hat{\mathbf{U}} = \begin{bmatrix} \mathbf{u}_1, \mathbf{U}_1 \end{bmatrix}$,

where $\mathbf{U}_1\mathbf{U}_1^T = \mathbf{U}_1^T\mathbf{U}_1 = \mathbf{I}_m$ and $\mathbf{V}_1\mathbf{V}_1^T = \mathbf{V}_1^T\mathbf{V}_1 = \mathbf{I}_n$. Then we have

$$\hat{\mathbf{U}}^T \mathbf{A} \hat{\mathbf{V}} = \begin{bmatrix} \mathbf{u}_1^T \mathbf{A} \mathbf{v}_1 & \mathbf{u}_1^T \mathbf{A} \mathbf{V}_1 \\ \mathbf{U}_1^T \mathbf{A} \mathbf{v}_1 & \mathbf{U}_1^T \mathbf{A} \mathbf{V}_1 \end{bmatrix}.$$

It is easy to note that $\mathbf{U}_1^T \mathbf{A} \mathbf{v}_1 = \sigma_1 \mathbf{U}_1^T \mathbf{u}_1 = 0$. Let $\mathbf{a} = \mathbf{u}_1^T \mathbf{A} \mathbf{V}_1$, $\mathbf{z} = (\sigma_1 \ \mathbf{a}^T)$, $\mathbf{Y} = \hat{\mathbf{U}}^T \mathbf{A} \hat{\mathbf{V}}$. Then we have

$$\sigma_1 \sqrt{\sigma_1^2 + \mathbf{a}^T \mathbf{a}} \ge ||\mathbf{Y}||_2 ||\mathbf{z}||_2 \ge ||\mathbf{Y}\mathbf{z}||_2 = ||(\sigma_1^2 + ||\mathbf{a}_1||_2^2 \quad \mathbf{a}^T \mathbf{V}_1^T \mathbf{A}^T \mathbf{U}_1^T)^T||_2 \ge \sigma_1^2 + \mathbf{a}^T \mathbf{a}$$

Therefore, $\sigma_1 \sqrt{\sigma_1^2 + \mathbf{a}^T \mathbf{a}} \ge \sigma_1^2 + \mathbf{a}^T \mathbf{a}$, we can get $\mathbf{a}^T \mathbf{a} = 0$, i.e. $\mathbf{a} = 0$. So

$$\hat{\mathbf{U}}^T \mathbf{A} \hat{\mathbf{V}} = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \mathbf{U}_1^T \mathbf{A} \mathbf{V}_1 \end{bmatrix}$$

. Since $\mathbf{U}_1^T \mathbf{A} \mathbf{V}_1 \in \mathbb{R}^{(m-1) \times (n-1)}$, there exist orthogonal $\hat{\mathbf{U}}_1$, $\hat{\mathbf{V}}_1$ and diagonal $\hat{\Sigma}_1$, such that $\mathbf{U}_1^T \mathbf{A} \mathbf{V}_1 = \hat{\mathbf{U}}_1 \hat{\Sigma}_1 \hat{\mathbf{V}}_1$. Then one has

$$\mathbf{A} = \hat{\mathbf{U}} \begin{bmatrix} 1 & 0 \\ 0 & \hat{\mathbf{U}}_1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \hat{\mathbf{\Sigma}}_1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \hat{\mathbf{V}}_1 \end{bmatrix} \hat{\mathbf{V}}^T.$$

Both $\hat{\mathbf{U}} \begin{bmatrix} 1 & 0 \\ 0 & \hat{\mathbf{U}}_1 \end{bmatrix}$ and $\begin{bmatrix} 1 & 0 \\ 0 & \hat{\mathbf{V}}_1 \end{bmatrix} \hat{\mathbf{V}}^T$ are orthogonal matrices, so the theorem is correct.

Proposition 2.1 (Unique problem). If $\sigma_1 > \sigma_2 > ... > \sigma_p$, then there exists an unique SVD for $\mathbf{A} \in \mathbb{R}^{m \times n}$. Otherwise, suppose $\sigma_1 = \sigma_2 = ... \sigma_{i_1} > \sigma_{i_1+1}... > \sigma_p > 0$, i.e. the number of σ_{i_1} is i_1 , the number of σ_{i_2} is i_2 , ..., the number of σ_{i_k} is i_k . Then we have

$$egin{aligned} \mathbf{A} &= \mathbf{U} egin{bmatrix} \sigma_{i_1} \mathbf{I}_{i_1} & & & & \\ & & \ddots & & \\ & & & \mathbf{Q}_k \end{bmatrix} \mathbf{V}^T \ &= \mathbf{U} egin{bmatrix} \mathbf{Q}_1 & & & & \\ & & \ddots & & \\ & & & \mathbf{Q}_k \end{bmatrix} egin{bmatrix} \sigma_{i_1} \mathbf{I}_{i_1} & & & \\ & & \ddots & & \\ & & & \sigma_{i_k} \mathbf{I}_{i_k} \end{bmatrix} egin{bmatrix} \mathbf{Q}_1^T & & & \\ & & \ddots & & \\ & & & \mathbf{Q}_k^T \end{bmatrix} \mathbf{V}^T, \end{aligned}$$

where Q_j is an orthogonal matrix in $\mathbb{R}^{i_j \times i_j}$.

Since $\mathbf{U}\begin{bmatrix} \mathbf{Q}_1 & & & \\ & \ddots & & \\ & & \mathbf{Q}_k \end{bmatrix}$ and $\begin{bmatrix} \mathbf{Q}_1^T & & & \\ & \ddots & & \\ & & \mathbf{Q}_k^T \end{bmatrix} \mathbf{V}^T$ are still orthogonal matrices, the

SVD for A is not unique.