SINGULAR VALUE DECOMPOSITION (SVD)

Motivation:

Recall from ALAFF, SVD is used in understanding the underlying structure of a sparse matrix.

SVD:

Given matrix A, it can be decompose as:

$$A = USV^T$$

What is the relationship between SVD and PCA?

They are closely related, both are common techniques used for dimensions reduction, but have different primary applications:

- PCA: used for dimensionality reduction for visualization or noise reduction, also useful when dealing with data covariance
- SVD: used for matrix approximation, recommendation systems, or analyze latent factors in dataset.

Let X be a dataset size $m \times d$

C be covariance matrix

We know that:

$$\begin{aligned} C &= \frac{1}{m} X^T X \\ &= \frac{1}{m} (USV^T)^T (USV^T) && \langle \text{SVD} \rangle \\ &= \frac{1}{m} V S U^T U S V^T \\ &= \frac{1}{m} V S^2 V^T \\ &\approx Q D Q^T && \langle \text{PCA} \rangle \end{aligned}$$

We can say that:

- vectors of V are the eigenvectors of covariance matrix, or principle components of dataset matrix X
- the singular values in S are related to the eigenvalues of covariance matrix. $\lambda = \frac{\sigma^2}{m}$

PCA is computationally expensive, do it through SVD.

On large dataset, a more common approach to find the principle components is to apply SVD directly on the dataset. The principle components is determined by: $X_{proj} = X \cdot V$, where $X = USV^T$

SVD Example:

Given dataset matrix $X = \begin{bmatrix} 126 & 78 \\ 128 & 80 \\ 128 & 82 \\ 130 & 82 \\ 130 & 84 \\ 132 & 86 \end{bmatrix}$, assume both features use same measurements

Find the principle components through SVD

Step 1: Standardize the data

- Since both features use the same measurements, we only need to center the dataset:

$$X := \begin{bmatrix} 126-129 & 78-82 \\ 128-129 & 80-82 \\ 128-129 & 82-82 \\ 130-129 & 82-82 \\ 130-129 & 84-82 \\ 132-129 & 86-82 \end{bmatrix} = \begin{bmatrix} -3 & -4 \\ -1 & -2 \\ -1 & 0 \\ 1 & 0 \\ 1 & 2 \\ 3 & 4 \end{bmatrix}$$

Step 2: Form X^TX

$$X^TX = \begin{bmatrix} 22 & 28 \\ 28 & 40 \end{bmatrix}$$

Step 3: Calculate eigenvalues $\Rightarrow$ singular values, form matrix S

$$\det(X^TX - \lambda I) = 0$$

$$\Leftrightarrow \det\left(\begin{bmatrix} 22-\lambda & 28 \\ 28 & 40-\lambda \end{bmatrix}\right) = 0$$

$$\Leftrightarrow (22-\lambda)(40-\lambda) - 28^2 = 0$$

$$\Leftrightarrow \left[\begin{array}{l} \lambda_1 = 56 \\ \lambda_2 = 6 \end{array}\right. \Rightarrow \left[\begin{array}{l} \sigma_1 = \sqrt{\lambda_1} = \sqrt{56} \\ \sigma_2 = \sqrt{\lambda_2} = \sqrt{6} \end{array}\right.$$

Step 4: Calculate eigenvectors $\Rightarrow$ form V

- case $\lambda_1 = 56$:

$$(X^TX)\, v_1 = \lambda_1 v_1$$

$$\Leftrightarrow \begin{bmatrix} 22 & 28 \\ 28 & 40 \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 56 \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\Rightarrow \begin{cases} 22x + 28y = 56x \\ 28x + 40y = 56y \end{cases} \Leftrightarrow \begin{cases} 22x + 28y = 56x \\ y = \frac{7}{4}x \end{cases}$$

$$\Rightarrow \begin{cases} x = 4 \\ y = 7 \end{cases}$$

Normalize $v_1 = \frac{v_1}{\|v_1\|} = \frac{1}{\sqrt{4^2 + 7^2}} \begin{bmatrix} 4 \\ 7 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.875 \end{bmatrix}$

- <u>Case $\lambda_2 = 6$:</u>

$$(X^T X) v_2 = \lambda_2 v_2$$

$$\Leftrightarrow \begin{bmatrix} 22 & 28 \\ 28 & 40 \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 6 \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\Rightarrow \begin{cases} 22x + 28y = 6x \\ 28x + 40y = 6y \end{cases}$$

$$\Leftrightarrow \begin{cases} x = -7 \\ y = 4 \end{cases}$$

Normalize $v_2 = \frac{v_2}{\|v_2\|} = \frac{1}{\sqrt{(-7)^2 + 4^2}} \begin{bmatrix} -7 \\ 4 \end{bmatrix} = \begin{bmatrix} -0.875 \\ 0.5 \end{bmatrix}$

- <u>Form V:</u> $V = (v_1 \mid v_2) = \begin{bmatrix} 0.5 & -0.875 \\ 0.875 & 0.5 \end{bmatrix}$

<u>Note:</u>

We could form matrix U by doing step 3 and 4 with matrix AA^T, but since we are trying to find principle components, we don't need U.

<u>Step 5:</u> Calculate principle components

$$X \cdot V = \begin{bmatrix} -3 & -4 \\ -1 & -2 \\ -1 & 0 \\ 1 & 0 \\ 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 0.5 & -0.875 \\ 0.875 & 0.5 \end{bmatrix} = \begin{bmatrix} \vdots & \vdots \\ \vdots & \vdots \end{bmatrix}$$