

2022.02.22

Singular Value Decomposition

$n \times m$ matrix 来表示 X . ($n \uparrow$ sample, $m \uparrow$ features)

Goal: 1. 用一个更小的 matrix 来 approximate X , 但同时存储了 similar info.

2. Dimensionality Reduction / Feature Extraction.

3. Anomaly Detection & Denoising

• $n \uparrow$ n -vector linearly independent iff 由这些 vectors 组成的 matrix 的 determinant 为 non-zero.

• 若 A 为 $n \times m$, 则需 ^存 \min n, m \uparrow values. 若 $\text{rank}(A) = k$, 则可将 $A = UV$.

U 为 $n \times k$, V 为 $k \times m$. 则 $k(m+n)$ 将小于 $m \cdot n$ (且更少 memory)

• Frobenius Distance

$$d_F(A, B) = \|A - B\|_F = \sqrt{\sum_{i,j} (a_{ij} - b_{ij})^2}$$

pairwise.

Goal: 找 B ($\text{rank}(B) = k \ll m/n$) 使 $d_F(A, B)$ 最小.

Def: When $k < \text{rank}(A)$, the rank k approximation of A 为

$$A^{(k)} = \arg \min_{\{B | \text{rank}(B) = k\}} d_F(A, B)$$

B 和 A 有同样 dimension. 但 B 的 rank 更小

Def: Singular Value Decomposition

of a rank- r matrix A has the form

$$A = U \Sigma V^T$$

$U^{n \times r}$ column orthonormal
 $V^{m \times r}$ column orthonormal
 $\Sigma = \begin{pmatrix} \sigma_1 & 0 & 0 & \dots \\ 0 & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{pmatrix}^{r \times r}$ transposed.

$$A = \begin{pmatrix} u_1 & u_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & \\ & \Sigma_2 \end{pmatrix} \begin{pmatrix} v_1 & v_2 \end{pmatrix}^T = A$$

$$A = \begin{pmatrix} u_1 & u_2 \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} v_1 & v_2 & 0 \end{pmatrix}^T = A$$

$$A = U \Sigma V^T$$

Property: $\|A - A^{(k)}\|_F^2 = \sum_{i=k+1}^r \sigma_i^2$ ($A^T A$ diagonal = $A A^T$)

The i th singular vector represents the direction of the i th most variance. U is the vector.

找 k 值
 1. 在 singular value plot 中找 elbow point
 2. 看不同 k 值的 residual error.

$$\begin{pmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \\ & & & & 0 \end{pmatrix} = \Sigma$$

$$(U \quad V) \begin{pmatrix} \Sigma & \\ & 0 \end{pmatrix} \begin{pmatrix} U^T & V^T \end{pmatrix} = A$$

words count
 brain
 CS1 0
 CS2 0
 Medicine 2

cell
 0
 0
 1

data
 4
 3
 0

data matrix $V^T \Sigma V$ singular value decomposition $A, A^T A$

Tf-idf

$\text{tf-idf} \rightarrow \log \left(\frac{\text{number of documents}}{\text{number of documents that contains that term}} \right)$
term frequency in the documents

• Determinant

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \det(A) = ad - bc$$

$$A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \quad \det(A) = a \cdot \det \begin{pmatrix} e & f \\ h & i \end{pmatrix} - b \cdot \det \begin{pmatrix} d & f \\ g & i \end{pmatrix} + c \cdot \det \begin{pmatrix} d & e \\ g & h \end{pmatrix}$$

• $\text{rank}(A) = \text{rank}(A^T)$

• Singular Value Decomposition

$$A = \cancel{U} \Sigma V^T \quad A_{n \times m} \quad U_{n \times n} \quad V_{m \times m}$$

orthonormal

$$\Sigma = \begin{pmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{pmatrix}$$

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r \geq 0$$

σ_i is the square root of the eigenvalues of $A^T A$, i.e. singular values.

$$A = (U_1 \ U_2) \begin{pmatrix} \Sigma_1 & \\ & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1 & V_2 \end{pmatrix}$$

$$A^{(k)} = U_1 \Sigma_1 V_1^T$$

$$\text{dF}(A, A^{(k)})^2 = \sum_{i=k+1}^r \sigma_i^2$$