

Lecture 8.1: Singular Value Decomposition

Optimization and Computational Linear Algebra for Data Science

PCA

- Data matrix $A \in \mathbb{R}^{n \times m}$
- “Covariance matrix” $S = A^T A \in \mathbb{R}^{m \times m}$.
- S is symmetric positive semi-definite.
- Spectral Theorem:** there exists an orthonormal basis v_1, \dots, v_m of \mathbb{R}^m such that the v_i 's are eigenvectors of S associated with the eigenvalues $\lambda_1 \geq \dots \geq \lambda_m \geq 0$.

Exercise: Show $\text{rank}(S) = \text{rank}(A) \stackrel{\text{(def)}}{=} r$

Consequence: $\begin{cases} \lambda_1 \geq \dots \geq \lambda_r > 0 \\ \lambda_{r+1} = \dots = \lambda_m = 0 \end{cases}$

Singular values/vectors

For $i = 1, \dots, m$:

square roots of eigenvalues of $A^T A$

- we define $\sigma_i = \sqrt{\lambda_i}$, called the i^{th} singular value of A .
- we call v_j the i^{th} right singular vector of A .

What about the left singular vectors?

We define

for $i = 1, \dots, r$

$$u_i \in \mathbb{R}^n = \frac{1}{\sigma_i} (A v_i)$$

the i^{th} left singular vector of A .

If $r < n$: we are going to add vectors $u_{r+1} \dots u_n$ in order to get an orthonormal basis $(u_1 \dots u_n)$ of \mathbb{R}^n

Singular Value decomposition

Theorem

Let $A \in \mathbb{R}^{n \times m}$. Then there exists two orthogonal matrices $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{m \times m}$ and a matrix $\Sigma \in \mathbb{R}^{n \times m}$ such that $\Sigma_{1,1} \geq \Sigma_{2,2} \geq \dots \geq 0$ and $\Sigma_{i,j} = 0$ for $i \neq j$, that verify

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

$A \propto m$

$$U \quad \left[\begin{array}{c|c|c|c} & & & \\ \hline u_1 & u_2 & \cdots & u_n \\ \hline & & & \end{array} \right] \quad n$$

$$\Sigma \quad \left[\begin{array}{cccccc} \sigma_1 & & & & & & \\ \hline & \ddots & & & & & \\ & & \sigma_r & & & & \\ \hline & & & 0 & \cdots & 0 & \\ & & & & \ddots & & \\ & & & & & 0 & \cdots & 0 \\ \hline & & & & & & \ddots & \\ & & & & & & & 0 \end{array} \right] \quad m$$

$$V^T \quad \left[\begin{array}{c|c|c|c} & & & \\ \hline v_1 & v_2 & \cdots & v_m \\ \hline & & & \end{array} \right] \quad m$$

Geometric interpretation of $U\Sigma V^T$

