

PCA

Dimensional Reduction

- Usually considered an unsupervised learning method
- Used for learning the low-dimensional structures in the data (e.g., topic vectors instead of bag-of-words vectors, etc.)
- Fewer dimensions \Rightarrow Less chances of overfitting \Rightarrow Better generalization.

Linear Dimensionality Reduction

- Projection matrix $U = [u_1, u_2, \dots, u_K]$ of size $D \times K$ defines K linear projection direction.
- U is to project $x^{(i)} \in \mathbb{R}^D$ to $z^{(i)} \in \mathbb{R}^K$

$$Z = U^T \cdot X, X = [x^{(1)} \dots x^{(N)}] \in \mathbb{R}^{D \times N} \quad Z = [z^{(1)} \dots z^{(N)}] \in \mathbb{R}^{K \times N}$$

PCA

- Usage: s dimensionality reduction, lossy data compression, feature extraction, and data visualization

Def. (2 commonly used definitions)

- Learning projection directions that capture maximum variance in data
- Learning projection directions that result in smallest reconstruction error
- Projection of $x^{(i)}$ along a one-dim subspace defined by $u_1 \in \mathbb{R}^D$, where $\|u_1\| = 1$.
- Mean of projections is $u_1^T \mu$, where $\mu = \frac{1}{N} \sum_{i=1}^N x^{(i)}$ is the mean of all data.
- Variance of projections is $u_1^T S u_1$

$$\begin{aligned} \frac{1}{N} \sum_{i=1}^N (u_1^T x^{(i)} - u_1^T \mu)^2 &= \frac{1}{N} \sum_{i=1}^N [u_1^T (x^{(i)} - \mu)]^2 \\ &= \frac{1}{N} \sum_{i=1}^N [u_1^T (x^{(i)} - \mu)] [u_1^T (x^{(i)} - \mu)]^T \\ &= E [u_1^T (X - \mu) (X - \mu)^T u_1] \\ &= u_1^T S u_1 \end{aligned}$$

- S is the $D \times D$ data covariance matrix

$$S = E [(X - \mu)(X - \mu)^T] = \frac{1}{N} \sum_{i=1}^N (x^{(i)} - \mu) (x^{(i)} - \mu)^T$$

Optimization

- We want u_1 s.t. the variance of the projected data is maximized

$$\begin{array}{ll} \max_{u_1} & u_1^T S u_1 \\ \text{s.t.} & u_1^T u_1 = 1 \end{array}$$

- The method of Lagrange multipliers

$$\mathcal{L}(u_1, \lambda_1) = u_1^T S u_1 - \lambda_1 (u_1^T u_1 - 1)$$

- where λ_1 is a Lagrange multiplier - Take the derivative w.r.t. u_1 and setting to zero

$$\frac{\partial}{\partial u_1} \mathcal{L}(u_1, \lambda_1) = (S + S^T)u_1 - 2\lambda_1 u_1 = 0 \Leftrightarrow S u_1 = \lambda_1 u_1, (S = S^T)$$

- Thus, u_1 is an eigenvector of S
- The variance of projection is $u_1^T S u_1 = \lambda_1$.
- Variance is maximized when u_1 is the top eigenvector with largest eigenvalue (so-called the first Principle Component, PC).

Steps

1. Center the data (subtract μ for each data)
2. Compute the covariance matrix $S = \frac{1}{N} X X^T$
3. Perform eigen decomposition of S and take first K leading eigenvectors $\{u_i\}_{i=1, \dots, K}$.
4. The projection is therefore given by $Z = U^T X$