

# 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

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

- 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  $\lambda_1$  is a Lagrange multiplier - Take the derivative w.r.t.  $u_1$  and setting to zero

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

- 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  $\mu$  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  $Z = U^T X$