

1. Minimum-error formulation of PCA

Consider a complete orthonormal set of D -dimensional basis vector $\{u_i\}$ that satisfy $u_i^T u_j = \delta_{ij}$. For any D -dimensional data point x_n , we can represent it with a linear combination of the basis vectors using

$$x_n = \sum_{i=1}^D (x_n^T u_i) u_i.$$

We want to approximate each data point x_n by

$$\tilde{x}_n = \sum_{i=1}^M z_{ni} u_i + \sum_{i=M+1}^D b_i u_i,$$

while minimizing

$$J = \frac{1}{N} \sum_{n=1}^N \|x_n - \tilde{x}_n\|^2.$$

Find the optimal u_i , z_{ni} and b_i .

Solution: We first consider the minimization with respect to z_{ni} by setting the derivative to be 0 and we get

$$z_{nj} = x_n^T u_j.$$

Similarly, setting the derivative of J with respect to b_i to zero, we get

$$b_j = \bar{x}^T u_j.$$

Substitute z_{ni} and b_i . We get

$$x_n - \tilde{x}_n = \sum_{i=M+1}^D [(x_n - \bar{x})^T u_i] u_i.$$

With this, we see that find that

$$J = \frac{1}{N} \sum_{n=1}^N \sum_{i=M+1}^D (x_n^T u_i - \bar{x}^T u_i)^2 = \sum_{i=M+1}^D u_i^T S u_i.$$

What remains is the constrained minimization with respect to $u_i, i = M + 1, \dots, N$. We get these base vectors should be the eigenvectors corresponding to the smallest eigenvalues by induction.

2. **Some intuition on bagging** Consider a regression problem in which we are trying to predict the value of a single continuous variable, and suppose we generate M bootstrap data sets and then use each to train a separate copy $y_m(x)$ of a predictive model where $m = 1, \dots, M$. The bagging prediction is given by

$$y_{\text{bagging}}(x) = \frac{1}{M} \sum_{m=1}^M y_m(x).$$

Suppose the true regression function that we are trying to predict is given by $h(x)$, so that the output of each of the models can be written as the true value plus an error in the form

$$y_m(x) = h(x) + \epsilon_m(x).$$

Assume $E[\epsilon_m(x)] = 0$ and $E[\epsilon_m(x)\epsilon_l(x)] = 0, i \neq l$. Find the average sum-of-squares error made by the models acting individually. Also find the expected error of the bagging predictor.

Solution:

$$E_{AV} = \frac{1}{M} \sum_{m=1}^M E[\epsilon_m(x)^2],$$

$$E_{\text{bagging}} = E \left[\left(\frac{1}{M} \sum_{m=1}^M \epsilon_m(x) \right)^2 \right] = \frac{1}{M} E_{AV}.$$