

Lecture 14. Principle Component Analysis

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1 Preliminary

1.1 Singular Value Decomposition

Definition 1. A set of vectors $\{\mathbf{v}_i\}_{i=1}^n$ in \mathbf{R}^d are called orthonormal if

$$\langle \mathbf{v}_i, \mathbf{v}_j \rangle = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{otherwise.} \end{cases}$$

A matrix $M \in \mathbb{R}^{d \times d}$ is orthogonal if

$$M^\top M = I,$$

where $I \in \mathbb{R}^{d \times d}$ is the identity matrix.

Theorem 1. Given a matrix $A \in \mathbb{R}^{m \times n}$. Suppose that $\text{rank}(A) = r$. Then, there exists n right singular vectors $\mathbf{v}_1, \dots, \mathbf{v}_n$ that are orthogonal in \mathbb{R}^n , and m left singular vectors $\mathbf{u}_1, \dots, \mathbf{u}_m$ that are orthogonal in \mathbb{R}^m , such that

$$A\mathbf{v}_i = \sigma_i \mathbf{u}_i, \quad i = 1, \dots, r, \quad (1)$$

$$A\mathbf{v}_i = 0, \quad i = r + 1, \dots, n, \quad (2)$$

where $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$ are the r positive singular values.

Remark 1.

1. The last $n - r$ \mathbf{v} 's span the null space of A . The last $m - r$ \mathbf{u} 's span the null space of A^\top .
2. Let $V = (\mathbf{v}_1, \dots, \mathbf{v}_r, \dots, \mathbf{v}_n)$, $U = (\mathbf{u}_1, \dots, \mathbf{u}_r, \dots, \mathbf{u}_m)$, and

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

We can write Eq. (1) as

$$AV = U\Sigma.$$

3. The singular value decomposition of A is

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

4. The singular value decomposition of A can be written as a sum of r rank 1 matrix:

$$A = U\Sigma V^\top = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^\top + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^\top + \dots + \sigma_r \mathbf{u}_r \mathbf{v}_r^\top.$$

5. Let $V_r = (\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r)$, $U_r = (\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r)$, and

$$\Sigma_r = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_r \end{pmatrix}$$

The reduced form of the SVD of A is

$$A = U_r \Sigma_r V_r^\top.$$

1.2 Random Vectors

A random vector X takes the form of

$$X = \begin{pmatrix} X_1 \\ \vdots \\ X_d \end{pmatrix}.$$

The mean of X is

$$\mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_d \end{pmatrix} = \begin{pmatrix} \mathbb{E}(X_1) \\ \vdots \\ \mathbb{E}(X_d) \end{pmatrix}. \quad (3)$$

The covariance matrix Σ , also written as $\mathbb{V}(X)$, is

$$\Sigma = \begin{pmatrix} \mathbb{V}(X_1) & \text{Cov}(X_1, X_2) & \cdots & \text{Cov}(X_1, X_d) \\ \text{Cov}(X_2, X_1) & \mathbb{V}(X_2) & \cdots & \text{Cov}(X_2, X_d) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(X_d, X_1) & \text{Cov}(X_d, X_2) & \cdots & \mathbb{V}(X_d) \end{pmatrix}.$$

Suppose that we randomly sample n data instances:

$$\mathbf{x}_i = \begin{pmatrix} x_{i,1} \\ \vdots \\ x_{i,d} \end{pmatrix}, i = 1, \dots, n. \quad (4)$$

The sample mean is

$$\bar{\mathbf{x}} = \begin{pmatrix} \bar{x}_1 \\ \vdots \\ \bar{x}_d \end{pmatrix} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i,$$

which implies that

$$\bar{x}_j = \frac{1}{n} \sum_{i=1}^n x_{i,j}, j = 1, \dots, d.$$

The sample variance matrix $S \in \mathbb{R}^{d \times d}$ is

$$S = \begin{pmatrix} s_{1,1} & s_{1,2} & \cdots & s_{1,d} \\ s_{2,1} & s_{2,2} & \cdots & s_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ s_{d,1} & s_{d,2} & \cdots & s_{d,d} \end{pmatrix},$$

where

$$s_{j,k} = \frac{1}{n-1} \sum_{i=1}^n (x_{i,j} - \bar{x}_j)(x_{i,k} - \bar{x}_k).$$

By simple algebraic manipulation, we can see that

$$S = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top = \frac{1}{n-1} \tilde{X} \tilde{X}^\top, \quad (5)$$

where $\tilde{X} \in \mathbb{R}^{d \times n}$ and its i^{th} column is $\mathbf{x}_i - \bar{\mathbf{x}}$.

2 Principle Component Analysis

The core idea of PCA is that, we would like to project the data instances into a subspace such that the projected data instances preserves as much information as possible.

2.1 The formulation

Suppose that we have a set of data instances $\mathbf{x}_i \in \mathbb{R}^d$, $i = 1, \dots, n$. Let $\mathbf{g}_k \in \mathbb{R}^d$, $k = 1, \dots, K$ with $K \leq d$, be a set of vectors such that

$$\langle \mathbf{g}_i, \mathbf{g}_j \rangle = \begin{cases} 1, & i \neq j; \\ 0, & \text{otherwise,} \end{cases}$$

and

$$G = (\mathbf{g}_1, \dots, \mathbf{g}_K).$$

Then, the projection of the \mathbf{x}_i into the subspace spanned by $\{\mathbf{g}_1, \dots, \mathbf{g}_K\}$, that is, the column space of G , is

$$\mathbf{z}_i = P_G(\mathbf{x}_i) = GG^\top \mathbf{x}_i. \quad (6)$$

We use the sample variance to measure the information carried by the data instances. Thus, the information preserved by the projected data instances is

$$\frac{1}{n-1} \sum_{i=1}^n \|\mathbf{z}_i - \bar{\mathbf{z}}\|^2,$$

where

$$\bar{\mathbf{z}} = \frac{1}{n} \sum_{i=1}^n \mathbf{z}_i. \quad (7)$$

By plugging Eq. (6) into Eq. (7), we have

$$\bar{\mathbf{z}} = \frac{1}{n} \sum_{i=1}^n \mathbf{z}_i = \frac{1}{n} \sum_{i=1}^n GG^\top \mathbf{x}_i = GG^\top \left(\frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \right) = GG^\top \bar{\mathbf{x}},$$

where

$$\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i.$$

Thus, the problem becomes

$$\begin{aligned} \max_{G \in \mathbb{R}^{d \times K}} \quad & \frac{1}{n-1} \sum_{i=1}^n \|GG^\top \mathbf{x}_i - GG^\top \bar{\mathbf{x}}\|^2, \\ \text{s.t.} \quad & G^\top G = I. \end{aligned} \tag{8}$$

Notice that

$$\begin{aligned} \frac{1}{n-1} \sum_{i=1}^n \|GG^\top \mathbf{x}_i - GG^\top \bar{\mathbf{x}}\|^2 &= \frac{1}{n-1} \sum_{i=1}^n \langle GG^\top (\mathbf{x}_i - \bar{\mathbf{x}}), GG^\top (\mathbf{x}_i - \bar{\mathbf{x}}) \rangle \\ &= \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^\top GG^\top GG^\top (\mathbf{x}_i - \bar{\mathbf{x}}) \\ &= \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^\top GG^\top (\mathbf{x}_i - \bar{\mathbf{x}}) \\ &= \frac{1}{n-1} \sum_{i=1}^n \text{tr} \left((\mathbf{x}_i - \bar{\mathbf{x}})^\top GG^\top (\mathbf{x}_i - \bar{\mathbf{x}}) \right) \\ &= \frac{1}{n-1} \sum_{i=1}^n \text{tr} \left(G^\top (\mathbf{x}_i - \bar{\mathbf{x}}) (\mathbf{x}_i - \bar{\mathbf{x}})^\top G \right) \\ &= \text{tr} \left(G^\top \left(\frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}}) (\mathbf{x}_i - \bar{\mathbf{x}})^\top \right) G \right) \\ &= \text{tr} \left(G^\top S G \right). \end{aligned}$$

Thus, the problem in (8) becomes

$$\begin{aligned} \max_{G \in \mathbb{R}^{d \times K}} \quad & \text{tr}(G^\top S G), \\ \text{s.t.} \quad & G^\top G = I. \end{aligned} \tag{9}$$

2.2 Solution to problem (9)

Recall from Eq. (5) that

$$S = \frac{1}{n-1} \tilde{X} \tilde{X}^\top.$$

Denote the SVD of \tilde{X} by

$$\tilde{X} = U\Sigma V^\top.$$

Thus,

$$S = \frac{1}{n-1} U\Sigma^2 U^\top. \quad (10)$$

Plugging Eq. (10) into the problem in (9) leads to

$$\begin{aligned} \max_{G \in \mathbb{R}^{d \times K}} \quad & \text{tr}(G^\top U\Sigma^2 U^\top G), \\ \text{s.t.} \quad & G^\top G = I. \end{aligned} \quad (11)$$

Denote

$$Q = U^\top G. \quad (12)$$

We can see that

$$Q^\top Q = I.$$

Thus, the problem in (11) reduces to

$$\begin{aligned} \max_{Q \in \mathbb{R}^{d \times K}} \quad & \text{tr}(Q^\top \Sigma^2 Q), \\ \text{s.t.} \quad & Q^\top Q = I. \end{aligned} \quad (13)$$

We can see that

$$\text{tr}(Q^\top \Sigma^2 Q) = \sum_{k=1}^K \sum_{j=1}^d \sigma_j^2 q_{k,j}^2 = \sum_{j=1}^d \sigma_j^2 \left(\sum_{k=1}^K q_{k,j}^2 \right).$$

Denote

$$\alpha_j = \sum_{k=1}^K q_{k,j}^2. \quad (14)$$

We can see that

$$\begin{aligned} \alpha_j &\in [0, 1], \quad j = 1, \dots, d, \\ \sum_{j=1}^d \alpha_j &= K. \end{aligned}$$

Thus, we can further transform the problem (13) to

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^d} \quad & \sum_{j=1}^d \alpha_j \sigma_j^2, \\ \text{s.t.} \quad & \alpha_j \in [0, 1], \quad j = 1, \dots, d, \\ & \sum_{j=1}^d \alpha_j = K. \end{aligned} \quad (15)$$

We can solve the above problem by the Lagrange multiplier method. However, we provide an alternative approach. Let

$$f(\alpha) = \sum_{j=1}^d \alpha_j \sigma_j^2.$$

Recall that we arrange the singular values in decending order, that is,

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_d \geq 0.$$

As $\sum_{j=1}^d \alpha_j = K$, we have

$$\sum_{j=K+1}^d \alpha_j = K - \sum_{j=1}^K \alpha_j.$$

Thus, for any α that is feasible with respect to problem (15)

$$\begin{aligned} f(\alpha) &= \sum_{j=1}^K \alpha_j \sigma_j^2 + \sum_{j=K+1}^d \alpha_j \sigma_j^2 \\ &\leq \sum_{j=1}^K \alpha_j \sigma_j^2 + \left(\sum_{j=K+1}^d \alpha_j \right) \sigma_{K+1}^2 \\ &= \sum_{j=1}^K \alpha_j \sigma_j^2 + \left(K - \sum_{j=1}^K \alpha_j \right) \sigma_{K+1}^2 \\ &= \sum_{j=1}^K \alpha_j \sigma_j^2 + \left(\sum_{j=1}^K (1 - \alpha_j) \right) \sigma_{K+1}^2 \\ &\leq \sum_{j=1}^K \alpha_j \sigma_j^2 + \sum_{j=1}^K (1 - \alpha_j) \sigma_j^2 \\ &= \sum_{j=1}^K \sigma_j^2 \\ &= f(\alpha^*), \end{aligned}$$

where $\alpha^* = (\alpha_1^*, \dots, \alpha_d^*)$ with

$$\alpha_j^* = \begin{cases} 1, & j = 1, \dots, K, \\ 0, & j = K + 1, \dots, d. \end{cases} \quad (16)$$

Moreover, it is easy to see that α^* is feasible. Thus, the vector α^* is the optimal solution to problem (15).

We denote the optimal solution to problem (13 by)

$$Q^* = (\mathbf{q}_1^*, \dots, \mathbf{q}_K^*).$$

In view of Eq. (14) and Eq. (16), we can see that the last $d - K$ entries of \mathbf{q}_j are 0 for all $j = 1, \dots, K$, that is

$$Q^* = \begin{pmatrix} \tilde{Q}^* \\ \mathbf{0} \end{pmatrix}_{d \times K},$$

where

$$\tilde{Q}^* \in \mathbb{R}^{K \times K} \text{ and } (\tilde{Q}^*)^\top \tilde{Q}^* = I.$$

Thus, by Eq. (12), we have

$$G^* = UQ^* = (\mathbf{u}_1, \dots, \mathbf{u}_K) \tilde{Q}^*. \quad (17)$$

That is, the optimal solution G^* to problem (9) is the matrix which shares the same column subspace spanned by the K left singular vectors of \tilde{X} corresponding to its first K largest singular values.

2.3 Principle components

Notice that, \tilde{Q}^* in Eq. (17) is an arbitrary $K \times K$ orthogonal matrix. Although G^* is a solution to problem (9) for any orthogonal matrix \tilde{Q}^* , the column vectors are not necessarily the so-called *principle component vectors* of the sampled data $\{\mathbf{x}_i\}_{i=1}^n$.

The column vectors of G^* are the *principle component vectors* of the data $\{\mathbf{x}_i\}_{i=1}^n$ only if $\tilde{Q}^* = I$, that is

$$G^* = (\mathbf{u}_1, \dots, \mathbf{u}_K),$$

and $\{\mathbf{u}_j\}_{j=1}^K$ are the first K principle component vectors.

Remark 2. *Commonly seen approach to derive the principle component vectors is to first set $K = 1$ and solve the problem in (9). By the same approach in the last section, we can get the first principle component vector as \mathbf{u}_1 . Then, we fix \mathbf{u}_1 and solve the problem in (9) by setting $K = 2$. We can get the second principle component vector \mathbf{u}_2 . Repeating this procedure, we can get the first K principle component vectors.*