Lecture 16. Principal 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* $\operatorname{rank}(A) = r$. *Then, there exists n right singular vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ that are orthonormal in $\mathbb{R}^n$, and m left singular vectors $\mathbf{u}_1, \ldots, \mathbf{u}_m$ that are orthonormal in $\mathbb{R}^m$, such that*

$$A\mathbf{v}_i = \sigma_i \mathbf{u}_i,\ i = 1, \ldots, r, \tag{1}$$

$$A\mathbf{v}_i = 0,\ i = r+1, \ldots, n, \tag{2}$$

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

***Remark** 1.*

1. The last $n - r$ right singular vectors $\mathbf{v}_i$, $i = r+1, \ldots, n$, span the null space of A. The last $m - r$ left singular vectors $\mathbf{u}_i$, $i = r+1, \ldots, m$, span the null space of $A^\top$.

2. Let $V = (\mathbf{v}_1, \ldots, \mathbf{v}_r, \ldots, \mathbf{v}_n)$, $U = (\mathbf{u}_1, \ldots, \mathbf{u}_r, \ldots, \mathbf{u}_m)$, and

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

   We can write Eq. (1) as

$$AV = U\Sigma.$$

3. The singular value decomposition of A is

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

4. Recall that, if $A = BCD^\top$, where $B \in \mathbb{R}^{m\times p}$, $C \in \mathbb{R}^{p\times q}$, and $D \in \mathbb{R}^{n\times q}$, then we can write A as the sum of a set of rank 1 matrix

$$A = \sum_{i=1}^{p}\sum_{j=1}^{q} c_{i,j}\mathbf{b}_i\mathbf{d}_j^\top,$$

where $\mathbf{b}_i$ and $\mathbf{d}_j$ are the i^{th} and j^{th} column vectors of B and D, respectively.

Therefore, by the singular value decomposition, we can write A as a sum of r rank 1 matrix:

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

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

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

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

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

Suppose that we randomly sample n data instances:

$$\mathbf{x}_i = \begin{pmatrix} x_{i,1} \\ \vdots \\ x_{i,d} \end{pmatrix}, i = 1, \ldots, n. \tag{4}$$

The **sample mean** is

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

Clearly,

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

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

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

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

2 Principal Component Analysis

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

2.1 The formulation

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

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

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

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

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

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

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

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

Notice that

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

Thus, the problem in (8) becomes

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

Question 1. Consider the problem in (9).

1. Does the problem always admit a solution?
2. If the problem admit a solution, is it unique?

2.2 Solution to problem (9)

Recall from Eq. (5) that

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

We denote the SVD of $\widetilde{X}$ by

$$\widetilde{X} = U\Sigma V^\top,$$

where $U \in \mathbb{R}^{d\times d}$, $\Sigma \in \mathbb{R}^{d\times n}$, and $V \in \mathbb{R}^{n\times n}$. Thus,

$$S = \frac{1}{n-1}U\Sigma_d^2 U^\top, \tag{10}$$

where $\Sigma_d^2 = \Sigma\Sigma^\top$. Plugging Eq. (10) into the problem in (9) leads to

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

Denote

$$Q = U^\top G. \tag{12}$$

We can see that

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

Thus, the problem in (11) reduces to

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

We can see that

$$\operatorname{tr}(Q^\top\Sigma^2 Q) = \sum_{k=1}^K\sum_{i=1}^d \sigma_i^2 q_{i,k}^2 = \sum_{i=1}^d \sigma_i^2\left(\sum_{k=1}^K q_{i,k}^2\right).$$

Notice that

$$\sum_{k=1}^K q_{i,k}^2 \tag{14}$$

is the square of the ℓ_2 norm of the i^{th} row of the matrix Q. Denote

$$\alpha_i = \sum_{k=1}^{K} q_{i,k}^2. \tag{15}$$

We can see that

$$\begin{aligned}
&\alpha_i \in [0,1],\ i = 1, \dots, d,\\
&\sum_{i=1}^{d} \alpha_i = \sum_{i=1}^{d}\sum_{k=1}^{K} q_{i,k}^2 = \sum_{k=1}^{K}\sum_{i=1}^{d} q_{i,k}^2 = \sum_{k=1}^{K} 1 = K.
\end{aligned}$$

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

$$\begin{aligned}
\max_{\alpha \in \mathbb{R}^d} &\sum_{i=1}^{d} \alpha_i \sigma_i^2, \\
\text{s.t.}\ &\alpha_i \in [0,1],\ i = 1, \dots, d,\\
&\sum_{i=1}^{d} \alpha_i = K.
\end{aligned} \tag{16}$$

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

$$f(\alpha) = \sum_{i=1}^{d} \alpha_i \sigma_i^2.$$

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

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

As $\sum_{i=1}^{d} \alpha_i = K$, we have

$$\sum_{i=K+1}^{d} \alpha_i = K - \sum_{i=1}^{K} \alpha_i.$$

Thus, for any α that is feasible with respect to problem (16)

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

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

$$\alpha_i^* = \begin{cases} 1, \; i = 1, \ldots, K, \\ 0, \; i = K+1, \ldots, d. \end{cases} \tag{17}$$

Moreover, it is easy to see that α^* is feasible. Thus, the vector α^* is the optimal solution to problem (16).

We denote the optimal solution to problem (13) by

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

In view of Eq. (15) and Eq. (17), we can see that the last $d - K$ entries of $\mathbf{q}_j^*$ are 0 for all $j = 1, \ldots, K$, that is

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

where

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

Thus, by Eq. (12), we have

$$G^* = UQ^* = U_K \widetilde{Q}^*, \tag{18}$$

where

$$U_K = (\mathbf{u}_1, \ldots, \mathbf{u}_K).$$

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 $\widetilde{X}$ corresponding to its first K largest singular values.

2.3 Principal components

Notice that, $\widetilde{Q}^*$ in Eq. (18) is an arbitrary $K \times K$ orthogonal matrix. Although G^* is a solution to problem (9) for any orthogonal matrix $\widetilde{Q}^*$, the column vectors are not necessarily the so-called *principal component vectors* of the sampled data $\{\mathbf{x}_i\}_{i=1}^n$.

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

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

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

Remark *2.* Commonly seen approach to derive the principal 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 principal 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 Principal component vector $\mathbf{u}_2$. Repeating this procedure, we can get the first K principal component vectors.

References