



Why

We want to find a low-dimensional affine set into which we can project some high-dimensional data.

Problem

For $a \in \mathbf{R}^n$ and $U \in \mathbf{R}^{n \times k}$, the set $W(a, U) = \{a + Uz \mid z \in \mathbf{R}^k\}$ is an affine set. Denote the projection of $x \in \mathbf{R}^n$ onto $W(a, U)$ by $\text{proj}_{W(a, U)}(x)$.

Problem 1. Given $x^{(1)}, \dots, x^{(m)} \in \mathbf{R}^n$, and a dimension k , find $a \in \mathbf{R}^n$ and $U \in \mathbf{R}^{n \times k}$ with $U^\top U = I$ to minimize

$$\sum_{i=1}^m \|x^{(i)} - \text{proj}_{W(a, U)}(x^{(i)})\|^2,$$

the sum of squared distances between $x^{(i)}$ and its projection on $W(a, U)$.

Express $\text{proj}_{W(a, U)}(x)$ as $UU^\top x + (I - UU^\top)a$ (see Projections on Affine Sets). We want to find $a \in \mathbf{R}^n$ and $U \in \mathbf{R}^{n \times k}$ to minimize

$$\sum_{i=1}^m \|x^{(i)} - UU^\top x^{(i)} - (I - UU^\top)a\|^2.$$

Fix $U \in \mathbf{R}^{n \times k}$. Define $A \in \mathbf{R}^{nm \times n}$, $B \in \mathbf{R}^{mn \times mn}$, and $\tilde{x} \in \mathbf{R}^{nm}$ by

$$A = \begin{bmatrix} I - UU^\top \\ \vdots \\ I - UU^\top \end{bmatrix}, \quad B = \begin{bmatrix} I - UU^\top & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & I - UU^\top \end{bmatrix}, \quad \text{and } \tilde{x} = \begin{bmatrix} x^{(1)} \\ \vdots \\ x^{(m)} \end{bmatrix}.$$

Then the objective is equivalent to

$$\|Aa - B\tilde{x}\|^2$$

Any minimizer a^* satisfies the normal equations

$$A^\top Aa^* = A^\top B\tilde{x}$$

Since $(I - UU^\top)^\top = I - UU^\top$ and $(I - UU^\top)^2 = I - UU^\top$,

$$A^\top A = \sum_{i=1}^m I - UU^\top = m(I - UU^\top)$$

and

$$A^\top B = \begin{bmatrix} I - UU^\top & \cdots & I - UU^\top \end{bmatrix}.$$

Consequently, we can express $A^\top A a^* = A^\top B \tilde{x}$ as

$$m(I - UU^\top) a^* = \sum_{i=1}^m (I - UU^\top) x^{(i)}.$$

So a^* is any vector satisfying

$$(I - UU^\top) a^* = (I - UU^\top) (1/m) \sum_{i=1}^m (I - UU^\top) x^{(i)}.$$

One such point satisfying the above is $\bar{x} = (1/m) \sum_{i=1}^m x^{(i)}$. An expedient choice, as it does not depend on U .

Now we want to find $U \in \mathbf{R}^{n \times k}$ to minimize

$$\sum_{i=1}^m \|(I - UU^\top)(x^{(i)} - \bar{x})\|^2.$$

Express the i th term of the sum as

$$\begin{aligned} \|(I - UU^\top)(x^{(i)} - \bar{x})\|^2 &= (x^{(i)} - \bar{x})(I - UU^\top)^\top (I - UU^\top)(x^{(i)} - \bar{x}) \\ &= (x^{(i)} - \bar{x})^\top (I - UU^\top)(x^{(i)} - \bar{x}) \\ &= \|x^{(i)} - \bar{x}\|^2 - \|U^\top (x^{(i)} - \bar{x})\|^2. \end{aligned}$$

The first term is a constant with respect to U . Define $\bar{X} \in \mathbf{R}^{n \times m}$ by

$$\bar{X} = \begin{bmatrix} x^{(1)} - \bar{x} & \cdots & x^{(m)} - \bar{x} \end{bmatrix}.$$

Express the sum of the second terms by

$$\|U^\top \bar{X}\|_F^2 = \text{tr} \bar{X}^\top U U^\top \bar{X} = \text{tr}(U^\top \bar{X} \bar{X}^\top U).$$

So we seek $U \in \mathbf{R}^{n \times k}$ with $U^\top U = I$ to maximize

$$\text{tr}(U^\top \bar{X} \bar{X}^\top U).$$

