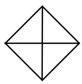

Why

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

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*

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

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

Express $\mathrm{proj}_{W(a,U)}(x)$ 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

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

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

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

Then the objective is equivalent to

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

Any minimizer $a^\star$ satisfies the normal equations

$$A^\top A a^\star = A^\top B \tilde{x}$$

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

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

and

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

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

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

So $a^\star$ is any vector satisfying

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

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

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

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

Express the ith term of the sum as

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

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

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

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

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


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Real Functions
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Intervals
Real Products
Square Numbers
Real Plane
Real Line
Real Additive Inverses
Greatest Lower Bounds
Real Sequences
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Rational Multiplicative Inverses
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Set Powers
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Partitions
Intersection of Empty Set
Successor Sets
Unordered Triples
Set Dualities
Set Unions and Intersections
Set Complements
Set Intersections
Pair Unions
Ordered Pairs
Set Differences
Set Unions
Pair Intersections
Empty Set
Unordered Pairs
Set Specification
Set Equality
Set Inclusion
Standardized Accounts
Accounts
Deductions
Quantified Statements
Logical Statements
Statements
Sets
Identities
Names
Letters
Objects