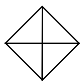


## Why

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 $\mathbf{proj}_{W(a,U)}(x)$.

**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*

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

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

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

$$A^\top B = \left[ \begin{array}{ccc} I - UU^\top & \cdots & I - UU^\top \end{array} \right].$$

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 $i$th 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

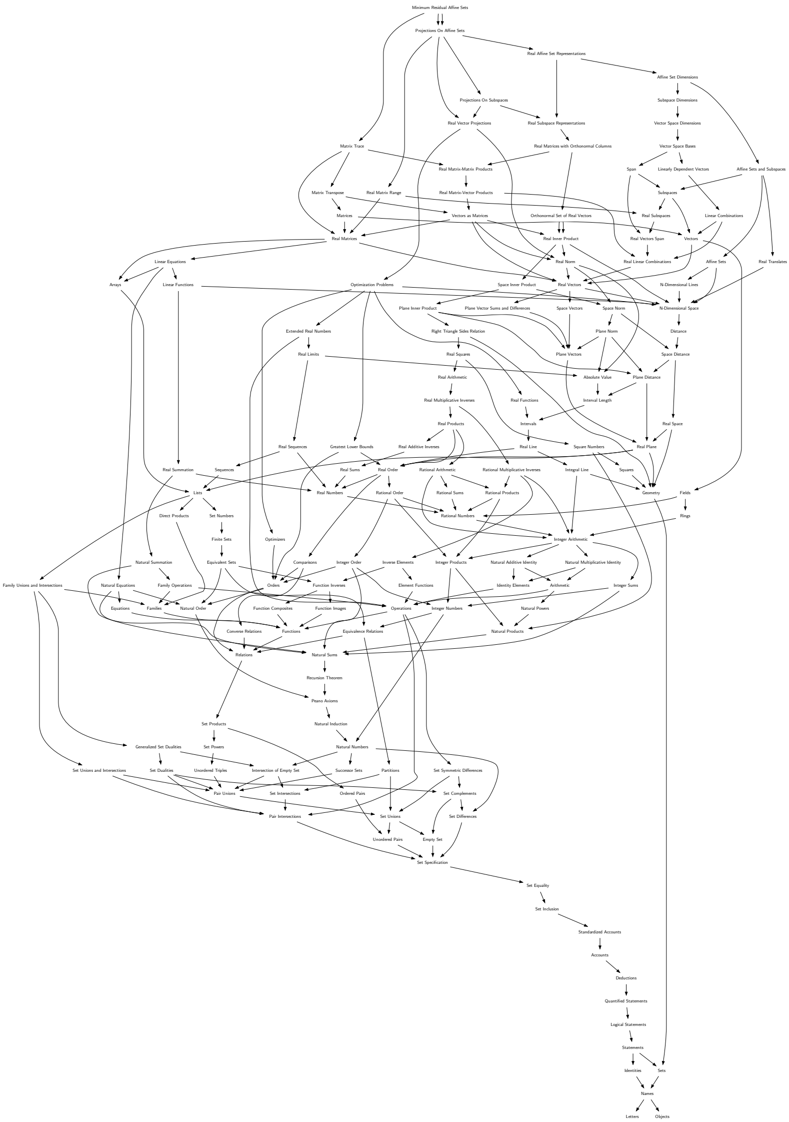
$$\bar{X} = \left[ \begin{array}{ccc} x^{(1)} - \bar{x} & \cdots & x^{(m)} - \bar{x} \end{array} \right].$$

Express the sum of the second terms by

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

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

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


Minimum Residual Affine Sets
Projections On Affine Sets
Real Affine Set Representations
Affine Set Dimensions
Projections On Subspaces
Subspace Dimensions
Real Vector Projections
Real Subspace Representations
Vector Space Dimensions
Matrix Trace
Real Matrices with Orthonormal Columns
Vector Space Bases
Real Matrix-Matrix Products
Span
Linearly Dependent Vectors
Affine Sets and Subspaces
Matrix Transpose
Real Matrix Range
Real Matrix-Vector Products
Subspaces
Matrices
Vectors as Matrices
Orthonormal Set of Real Vectors
Real Subspaces
Linear Combinations
Real Matrices
Real Inner Product
Real Vectors Span
Vectors
Linear Equations
Real Norm
Real Linear Combinations
Affine Sets
Real Translates
Arrays
Linear Functions
Optimization Problems
Space Inner Product
Real Vectors
N-Dimensional Lines
Plane Inner Product
Plane Vector Sums and Differences
Space Vectors
Space Norm
N-Dimensional Space
Extended Real Numbers
Right Triangle Sides Relation
Plane Norm
Distance
Real Limits
Real Squares
Plane Vectors
Space Distance
Real Arithmetic
Absolute Value
Plane Distance
Real Multiplicative Inverses
Real Functions
Interval Length
Real Products
Intervals
Real Space
Real Sequences
Greatest Lower Bounds
Real Additive Inverses
Real Line
Square Numbers
Real Plane
Real Summation
Sequences
Real Sums
Real Order
Rational Arithmetic
Rational Multiplicative Inverses
Integral Line
Squares
Lists
Real Numbers
Rational Order
Rational Sums
Rational Products
Geometry
Fields
Direct Products
Set Numbers
Rational Numbers
Rings
Finite Sets
Optimizers
Integer Arithmetic
Natural Summation
Equivalent Sets
Comparisons
Integer Order
Inverse Elements
Integer Products
Natural Additive Identity
Natural Multiplicative Identity
Family Unions and Intersections
Natural Equations
Family Operations
Orders
Function Inverses
Element Functions
Identity Elements
Arithmetic
Integer Sums
Equations
Families
Natural Order
Function Composites
Function Images
Operations
Integer Numbers
Natural Powers
Converse Relations
Functions
Equivalence Relations
Natural Products
Relations
Natural Sums
Recursion Theorem
Peano Axioms
Natural Induction
Set Products
Generalized Set Dualities
Set Powers
Natural Numbers
Set Unions and Intersections
Set Dualities
Unordered Triples
Intersection of Empty Set
Successor Sets
Partitions
Set Symmetric Differences
Pair Unions
Set Intersections
Ordered Pairs
Set Complements
Pair Intersections
Set Unions
Set Differences
Unordered Pairs
Empty Set
Set Specification
Set Equality
Set Inclusion
Standardized Accounts
Accounts
Deductions
Quantified Statements
Logical Statements
Statements
Identities
Sets
Names
Letters
Objects