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 $x^{(1)}, \ldots, x^{(m)} \in \mathbf{R}^n$, 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

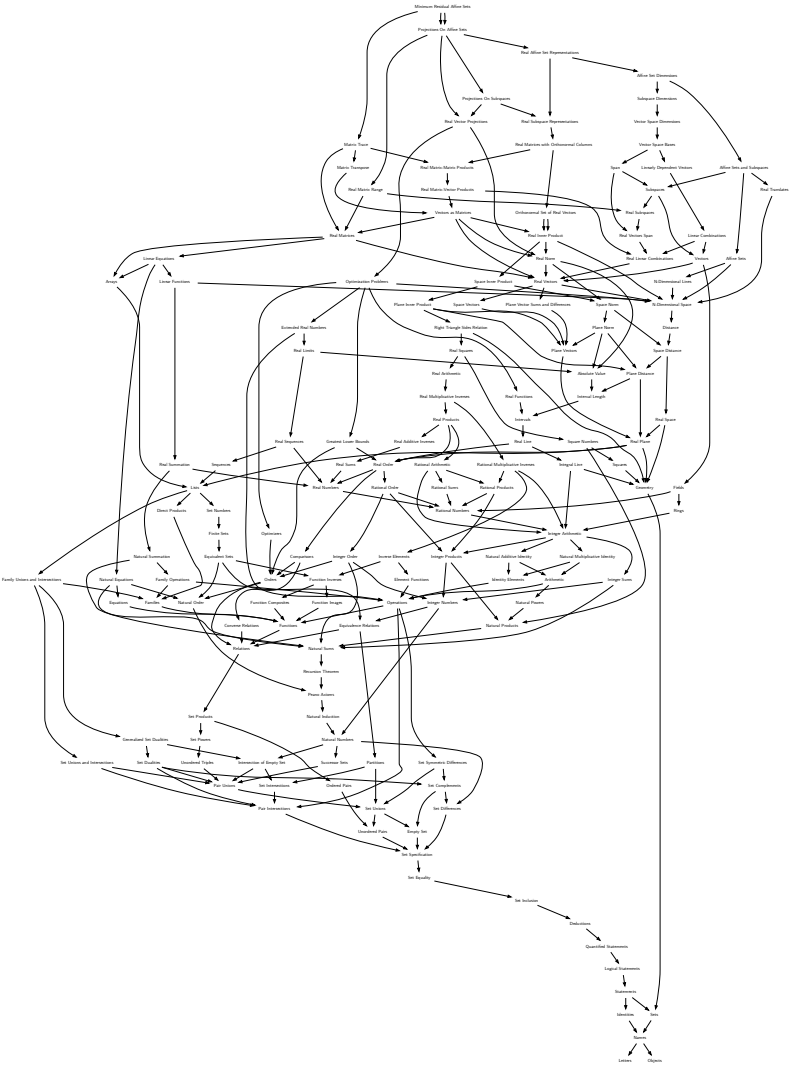
$$\bar{X} = \begin{bmatrix} x^{(1)} - \bar{x} & \cdots & x^{(m)} - \bar{x} \end{bmatrix}.$$

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

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


Moreover Residual Affine Sets
Projections On Affine Sets
Real Affine Set Representations
Affine Set Dimensions
Subspace Dimensions
Projections On Subspaces
Real Subspace Representations
Vector Space Dimensions
Real Vector Projections
Matrix Trace
Real Matrices with Orthonormal Columns
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Real Matrix-Vector Products
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Space Distance
Real Arithmetic
Euclidean Norm
Plane Distance
Real Multiplicative Inverses
Real Functions
Internal Length
Real Products
Intersect
Real Square
Real Sequences
Greatest Lower Bounds
Real Addition Inverses
Real Line
Square Numbers
Real Plane
Real Intervalue
Inequation
Real Sums
Real Order
Rational Arithmetic
Rational Multiplicative Inverses
Integral Line
Square
Line
Real Numbers
Rational Order
Rational Sums
Rational Products
Complex
Polar
Direct Products
Set Numbers
Rational Numbers
Rings
Finite Sets
Integer Arithmetic
Optimizers
Natural Intervalue
Equivalence Sets
Commutative
Integer Order
Inverse Elements
Integer Products
Natural Addition Identity
Natural Multiplicative Identity
Family Unions and Intersections
Natural Equations
Family Operations
Order
Function Inverses
Identity Elements
Associative
Integer Lines
Equations
Cardinal
Natural Order
Function Composition
Function Images
Optimizers
Integer Numbers
Natural Powers
Common Relations
Functions
Equivalence Relations
Natural Products
Relations
Natural Sums
Recursive Theorems
Power Arrows
Set Products
Natural Induction
Set Powers
Natural Numbers
Generalized Set Duality
Set Unions and Intersections
Set Duality
Unordered Triples
Intersection of Sets
Successor Sets
Positives
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
Deductions
Quantified Statements
Logical Statements
Statements
Identities
Sets
Numbers
Lattices
Objects