Feature Selection

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For CMSC 828K:
Algorithms and Data Structures
for Information Retrieval

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Introduction

Information retrieval for multimedia and other non-text databases:

- **Image and multimedia:** Images, video, audio.
- **Medical databases:** ECGs, X-rays, MRI scans.
- **Time series data:** Financial data, sales, meteorological, geological data.
- **Biology:** Genome, proteins.

Query-by-example: Find objects that are similar to a given query object.

Distance and Metrics

Similarity is defined in terms of a **distance function**. An important subclass are **metrics**.

Metric Space: A pair (X,d) where X is a set and d is a distance function such that for x,y in X:

$d(x,y) = d(y,x) \geq 0$

$d(x,y) = 0 \Leftrightarrow x = y$

$d(x,y) + d(y,z) \geq d(x,z)$ (Triangle Inequality)

Hilbert Space: A vector space and a norm $|v|$, which defines a metric $d(u,v)=|v-u|$.

Examples of Metrics

Minkowski L_p Metric: Let $X = \mathbf{R}^k$.

$$d(x, y) = \left[\sum_i |x_i - y_i|^p \right]^{1/p}$$

L_1 (Manhattan): $$d(x, y) = \sum |x_i - y_i|$$

L_2 (Euclidean): $$d(x, y) = \sqrt{\sum (x_i - y_i)^2}$$

L_{inf} (Chessboard): $$d(x, y) = \max_i |x_i - y_i|$$

More Metrics

Hamming Distance: Let $X = \{0,1\}^k$. Number of 1-bits in the exclusive-or

$$x \oplus y.$$

Edit Distance: Let $X = \Sigma^*$. Minimum number of single character changes (insert, delete, swap) to convert x into y.

Objective

Efficiency issues:

- **Edit distance** requires **quadratic time** to compute.
- **Data structures:** There are many data structures for storing vector data.
- **Curse of dimensionality:** Most nearest neighbor algorithms have running times that grow **exponentially** with dimension.

Objective: Embed objects into a low-dimensional space and use a Minkowski metric, allowing for a small **distortion** in distances.

Isometries and Embeddings

Isometry: A **distance preserving** mapping f from metric space (A, d_A) to (B, d_B):

$$d_B(f(x), f(y)) = d_A(x, y)$$

Contractive: A mapping f that **does not increase** distances:

$$\frac{1}{c} d_A(x, y) \leq d_B(f(x), f(y)) \leq d_A(x, y)$$

c is the **distortion** of the embedding.

Feature Selection

Main Problem: Given some finite metric space (X, d), where $|X|=n$, map it to some Hilbert space, say, $(\mathbf{R}^k, L_p)$. Ideally both the dimension and the distortion should be as low as possible.

Feature Selection: We can think of each coordinate of the resulting vector as describing some feature of the object. Henceforth, feature means coordinate.

Overview

We present methods for mapping a metric space (X, d) to $(\mathbf{R}^k, L_p)$. Let $|X| = n$.

Multidimensional Scaling: A classical method for embedding metric spaces into Hilbert spaces.

Lipschitz Embeddings: From any finite metric space to $(\mathbf{R}^k, L_p)$ where k is $O(\log^2 n)$ with $O(\log n)$ distortion.

SparseMap: A practical variant of LLR embeddings.

KL-transform and FastMap: Methods based on projections to lower dimensional spaces.

Multidimensional Scaling

Finding the best mapping of a metric space (X,d) to a k-dimensional Hilbert space $(\mathbf{R}^k,d')$ is a nonlinear optimization problem. The objective function is the **stress** between the distances:

$$\text{Stress}(d,d') = \sqrt{\frac{\sum (d'(f(x),f(y)) - d(x,y))^2}{\sum d(x,y)^2}}$$

Standard incremental methods (e.g., **steepest descent**) can be used to search for a mapping of minimal stress.

Limitations

MDS has a number of limitations that make it difficult to apply to information retrieval.

- All **O(n^2) distances** in the database need to be computed in the embedding process. Too large for most real databases.
- In order to map a query point into the embedded space, a similar optimization problem needs to be solved, requiring computation of **O(n) distances**.

Lipschitz Embeddings

Each coordinate or **feature** is the distance to the closest point of a subset of X.

Bourgain (1985) Any n-point metric space (X, d) can be embedded into O(log n)-dimensional Euclidean space with O(log n) distortion.

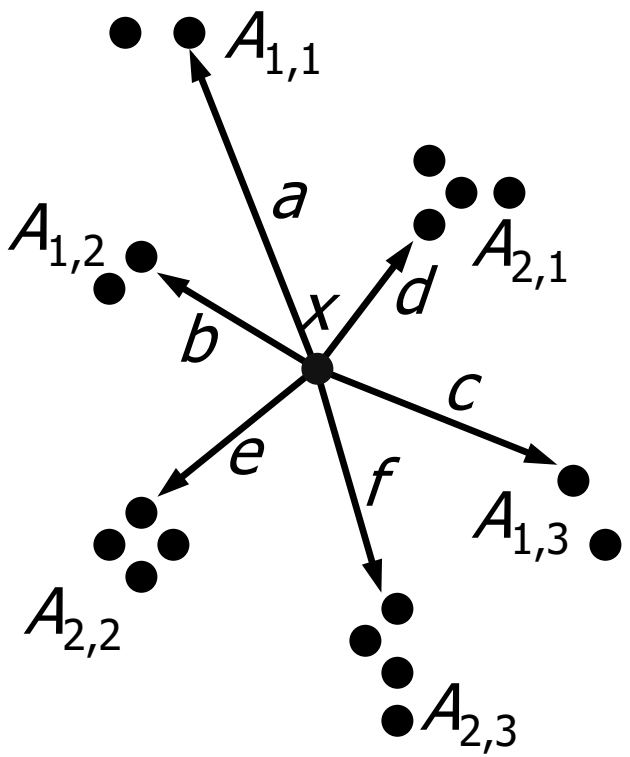
Linial, London, and Rabinovich (1995) Generalized to any L_p metric, and showed how it to compute it by a **randomized** algorithm. Dimension increases to $O(\log^2 n)$.

LLR Embedding Algorithm

Let q = O(log n). [Constant affects prob of success.]

For i = 1,2,…,lg n do
  For j = 1 to q do
    $A_{i,j}$ = random subset of X of size 2^i.

Map x to the vector $\{d_{i,j}\}/Q$ where $d_{i,j}$ is the distance from x to the closest point in $A_{i,j}$ and Q is the total number of subsets.



$$x \to \frac{1}{6}(a,b,c,d,e,f)$$

Why does it work?

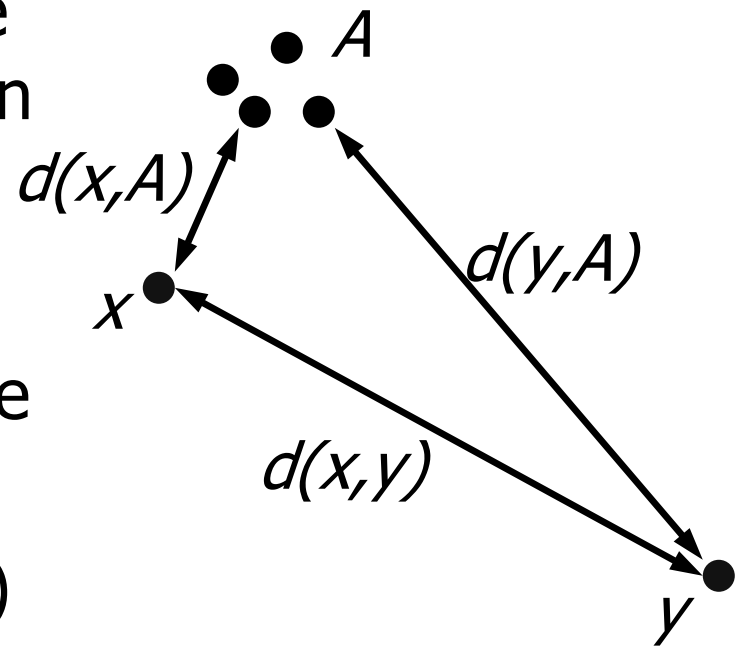
Assume L_1 metric.

Let *d(x,A)* denote the distance from *x* to the closest point in *A*.

Observe that for any *x,y* and any subset *A*, by the triangle inequality we have

$$\left|d(x,A) - d(y,A)\right| \leq d(x,y)$$

The mapping is **contractive**.



Why does it work?

Let $B(x, r_x)$ denote the set of points within distance r_x of x. Suppose $r_y < r_x$ and A is a subset such that

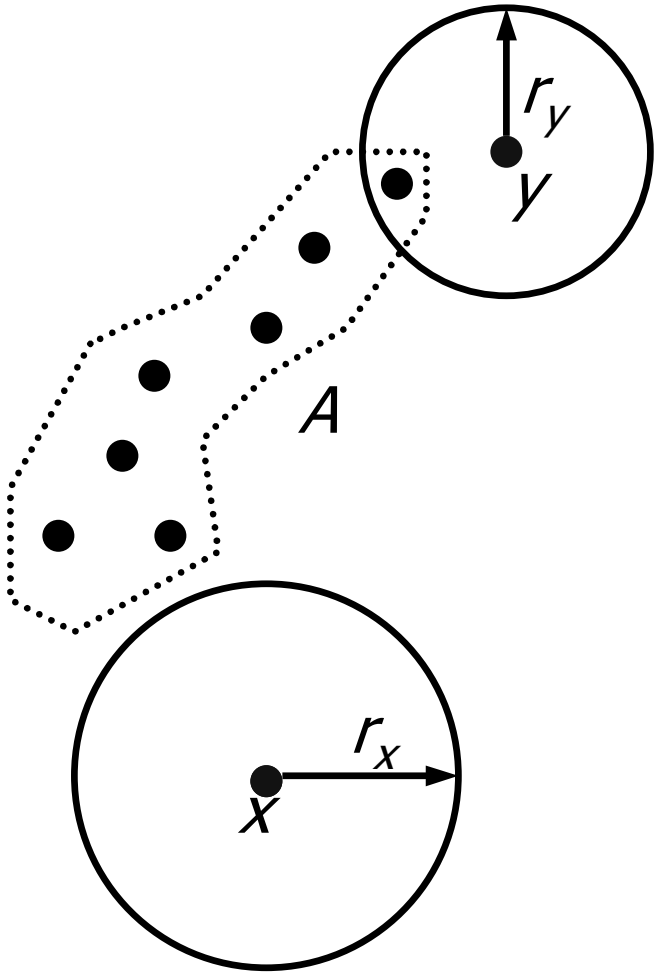
$$\left(A \cap B(x, r_x) = \emptyset\right) \wedge$$

$$\left(A \cap B(y, r_y) \neq \emptyset\right)$$

then

$$\left|d(x, A) - d(y, A)\right| \geq r_x - r_y$$

Will show this happens often.



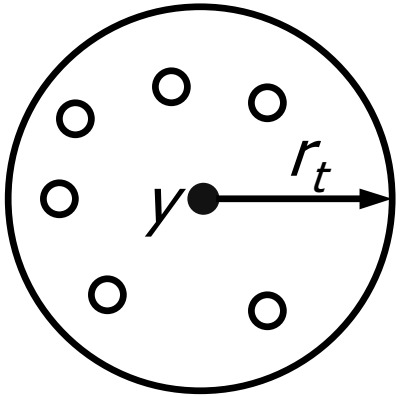
Why does it work?

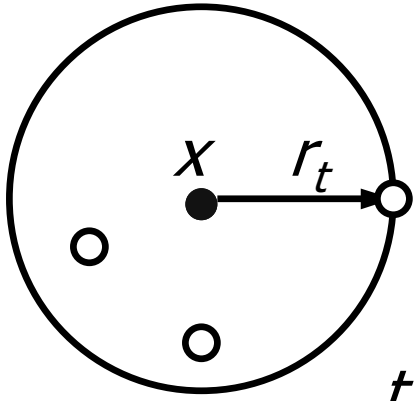
Fix points x and y. For t = 1,2,… let r_t be the smallest value such that

$$\min\left(\left|B(x, r_t)\right|, \left|B(y, r_t)\right|\right) \geq 2^t$$

Repeat as long as $r_t < d(x,y)/2$.

Note that for all r_t, $B(x, r_t)$ and $B(y, r_t)$ are disjoint.





$t = 2$

Why does it work?

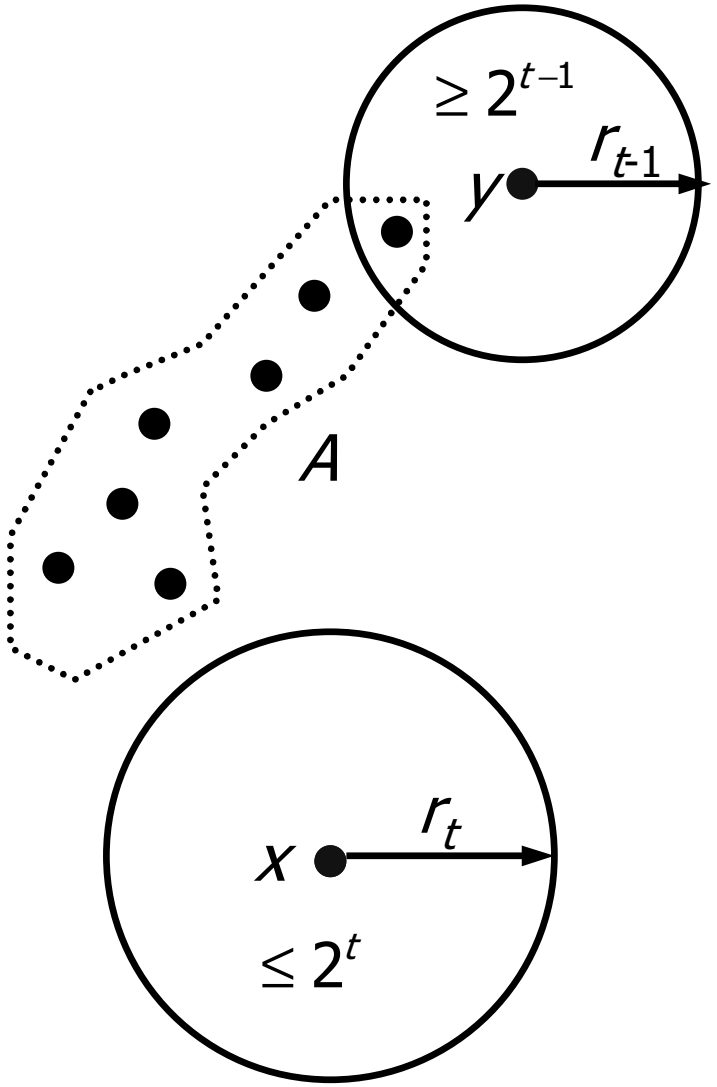
When the algorithm picks a random subset A of size roughly $n/2^t$, with constant probability (>1/10):

$$\left(A \cap B(x, r_t) = \emptyset\right) \wedge$$

$$\left(A \cap B(y, r_{t-1}) \neq \emptyset\right)$$

or vice versa.

Repeating this $q = O(\log n)$ times the expected number of such sets is at least $q/10$.



Why does it work?

Repeating over all q subsets in this group, with high probability we have:

$$\sum_{i=1}^{q} \left| d(x, A_i) - d(y, A_i) \right| \geq \frac{\log n}{10} \left(r_t - r_{t-1} \right)$$

Repeating this for all the size groups t=1,2,…, with high probability we have

$$d_{\mathrm{L1}}(x', y') = \sum_{i,j}^{Q} \left| d(x, A_{i,j}) - d(y, A_{i,j}) \right| / Q$$

$$\geq \frac{\log n}{10 \cdot Q} \sum_{t} \left(r_t - r_{t-1} \right) \geq \frac{\log n}{20 \cdot Q} d(x, y)$$

Review of the proof

Since $Q = O(\log^2 n)$ the final distortion is $O(\log n)$.

When we sample subsets of size $n/2^t$, we have a **constant probability** of finding subsets whose corresponding coordinate differs by at least $r_t - r_{t-1}$.

We repeat the sample $O(\log n)$ times so that this occurs with **high probability**. There are $O(\log n)$ size groups so the total dimension is $O(\log^2 n)$.

The sum of the $r_t - r_{t-1}$ terms **telescope** totaling to $d(x,y)/2$, and repeated sampling adds an $O(\log n)$ factor.

How low can you go?

Folklore: Any *n*-point metric space can be embedded into ($\mathbf{R}^n$, L_{inf}) with distortion **1**. (A point is mapped to a vector of distances to the other points.)

Bourgain: There is an *n*-point metric space such that any embedding in ($\mathbf{R}^k$,L_2) has distortion of at least **O(log *n* / log log *n*)**.

Johnson-Lindenstrauss: You can embed *n* points in ($\mathbf{R}^t$, L_2) into ($\mathbf{R}^k$, L_2) where $k = O((\log n)/\varepsilon^2)$ with distortion **1+**ε. (Select *k* unit vectors from $\mathbf{R}^t$ at random. Each coordinate is the length of the orthogonal projection onto each vector.)

Limitations

Limitations of the LLR embedding:

- **O(log *n*) distortion**: Experiments show that the actual distortions may be much smaller.
- **O(log^2 *n*) dimension**: This is a real problem.
- **O(*n* ^{2}) distance computations** must be performed in the process of embedding and embedding a query point requires **O(n) distance computations**: Too high if distance function is complex.

SparseMap

SparseMap (Hristescu and Farach-Colton) is a variant of the LLR-embedding:

Incremental construction of features: Once the first k coordinates have been computed, we can use these (rather than the distance function) to perform...

Distance Approximation: For computing the distance from a point x to a subset $A_{i,j}$.

Greedy Resampling: Keep only the best (most discriminating) coordinates.

Distance Approximation

Suppose that the first *k'* coordinates have been selected. This gives a partial distance estimate

$$d'_{k'}(x,y) = \sqrt{\sum_{i=1}^{k'} (x_i - y_i)^2}$$

To compute *d(x,A)* for a new subset *A*:

- Compute $d'_{k'}(x,y)$ for each *y* in *A*.
- Select *y* with the smallest such distance estimate.
- Return *d(x,y)*.

Only 1 distance calculation, as opposed to |*A*|. Total number is of distances is O(*kn*).

Greedy Resampling

Suppose that k coordinates have been computed. Want to keep only the **best** coordinates.

- **Sample** some number of random pairs (x,y) from the database, and compute their distances $d(x,y)$.
- **Select** the coordinate (subset A) that minimizes the **stress** between the true and estimated distances:

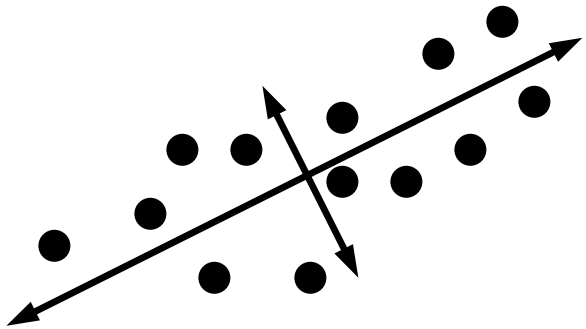
$$\text{Stress}(d,d') = \sqrt{\frac{\sum (d(x,y) - d'(x,y))^2}{\sum d'(x,y)^2}}$$

- **Repeat** selecting the coordinate which together with the previous coordinates minimizes stress.

KL-Transform

Karhunen-Loeve transform:

Given n points (vectors) in $\mathbf{R}^t$, project them into a lower dimensional space $\mathbf{R}^k$, so as to minimize the mean squared error.



KL-Transform

- Translate the points so that their mean coincides with the origin.
- Let X denote the matrix whose columns are the resulting vectors. Compute the **covariance matrix** $\Sigma = XX^{\mathsf{T}}$.
- Compute the **eigenvectors** Φ_i and the **eigenvalues** λ_i of Σ in decreasing order.
- Project the columns of X orthogonally onto the subspace spanned by Φ_i, $i = 1,\ldots,k$.

FastMap

The KL-transform assumes that points are in $\mathbf{R}^t$. What if we have a finite metric space (X, d)?

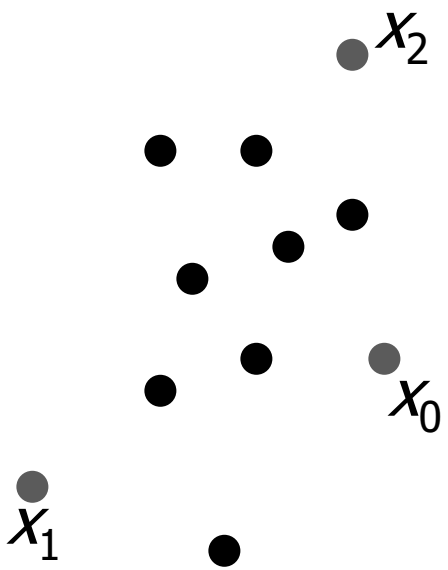
Faloutsos and Lin (1995) proposed FastMap as metric analogue to the KL-transform. Imagine that the points are in a Euclidean space.

- Select two **pivot points** x_a and x_b that are far apart.
- Compute a **pseudo-projection** of the remaining points along the "line" $x_a x_b$.
- **"Project"** the points to an orthogonal subspace and **recurse**.

Selecting the Pivot Points

The pivot points should lie along the principal axes, and hence should be far apart.

- Select any point x_0.
- Let x_1 be the furthest from x_0.
- Let x_2 be the furthest from x_1.
- Return (x_1, x_2).



Pseudo-Projections

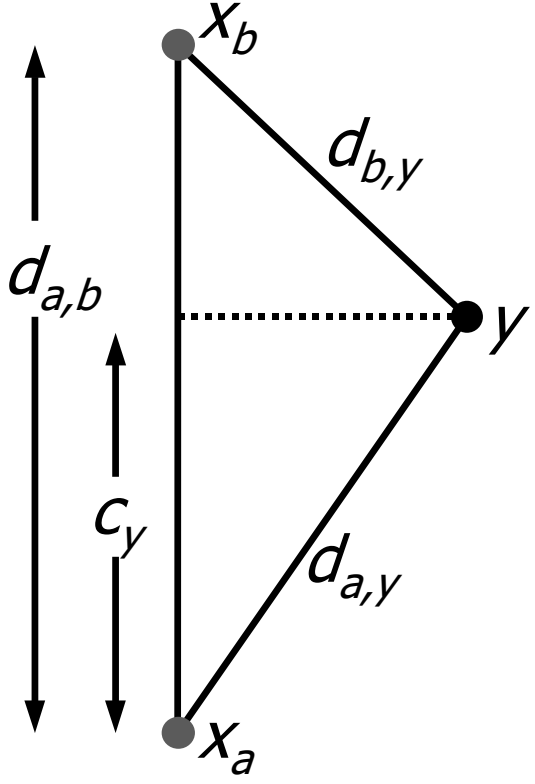
Given pivots (x_a , x_b), for any third point y, we use the **law of cosines** to determine the relation of y along $x_a x_b$.

$$d_{by}^2 = d_{ay}^2 + d_{ab}^2 - 2c_y d_{ab}$$

The **pseudo-projection** for y is

$$c_y = \frac{d_{ay}^2 + d_{ab}^2 - d_{by}^2}{2d_{ab}}$$

This is first coordinate.

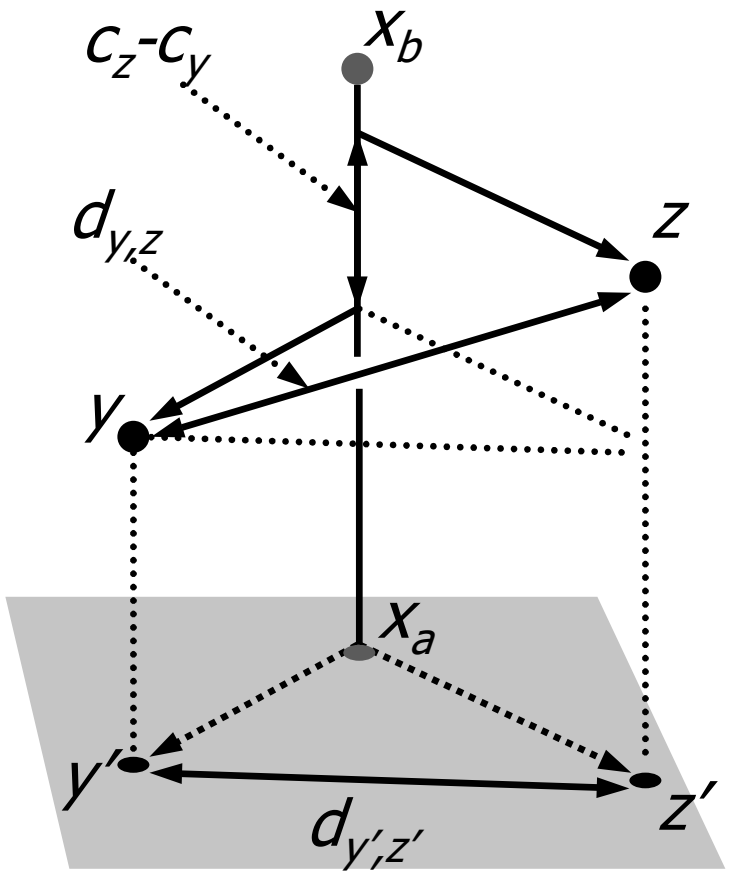


"Project to orthogonal plane"

Given distances along $x_a x_b$ we can compute distances within the "orthogonal hyperplane" using the Pythagorean theorem.

$$d'(y', z') = \sqrt{d^2(y, z) - (c_z - c_y)^2}$$

Using $d'(.,.)$, recurse until k features chosen.



Experimental Results

Faloutsos and Lin present experiments showing that FastMap is **faster** than MDS for a given level of stress, but has **much higher** stress than MDS. All data sets were relatively small.

Hristescu and Farach-Colton present experiments on protein data showing that SparseMap is considerably **faster** than FastMap, and it performs marginally **better** with respect to stress and cluster preservation.

Summary

- **Lipschitz Embeddings:** Embedding metric spaces using distances to subsets.
  - $O(\log^2 n)$ dimensions and $O(\log n)$ distortion.
  - Likely the best from a theoretical point of view.
  - SparseMap, a practical variant of this idea.
- **Johnson-Lindenstrauss:** Can embed any n-point set in Euclidean space into $O(\log n)$ dimensions.
- **KL-transform:** Embedding that minimizes squared errors. FastMap mimics this idea in metric spaces.

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