CSE 332
Introduction to Visualization

Data Reduction & Similarity metrics

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Stony Brook University
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Recall: The Rectangular Dataset

The variables → the attributes or properties we measured

The data items → the samples (observations) we obtained from the population of all instances

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Each data item is an N-dimensional vector (N variables)
- recall 2D and 3D vectors in 2D and 3D space, respectively

Now we have N-D attribute space
- now the data axes extend into more than 3 orthogonal directions
- hard to imagine?
- that’s why need good visualization methods (will see some soon...)
Data Reduction
Because...
- need to reduce the data so they can be feasibly stored
- need to reduce the data so a mining algorithm can be feasibly run

What else could we do
- buy more storage
- buy more computers or faster ones
- develop more efficient algorithms (look beyond O-notation)

However, in practice, all of this is happening at the same time
- unfortunately, the growth of data and complexities is always faster
- and so, data reduction will always be important
Data Reduction – How?

Reduce the number of data items (samples):
  • random sampling
  • stratified sampling

Reduce the number of attributes (dimensions):
  • dimension reduction by transformation
  • dimension reduction by elimination

Usually do both

Utmost goal
  • keep the gist of the data
  • only throw away what is redundant or superfluous
  • it’s a one way street – once it’s gone, it’s gone
Good candidates are *redundant* data

- how many cans of ravioli will you buy?
Keep a representative number of samples:
- pick one of each
- or maybe a few more depending on importance
You are faced with collections of many different data

- they are usually not nicely organized like this:

- but more like this:
Are all of these items pants?

- need a measure of similarity
- it’s a distance measure in high-dimensional feature space
We did not consider color, texture, size, etc...
- this would have brought more differentiation (blue vs. tan pants)
- the more features, the better the differentiation
How Many Features Do We Need?

Measuring similarity can be difficult
quantize each person into a vector
each vector element is a feature measurement
compare the vectors in terms of similarity
similarity is also called a distance function
Pant:
<length, ornateness, color>

Food delivery customer:
<type-pizza, type-salad, type-drink>

Examples:
- pants: <long, plain, tan>, <short, ornate, blue>, ...
  expressed in numbers: <30”, 1, 2>, <15”, 2, 5>
- food: <pepperoni, tossed, none>, <pepperoni, tossed, coke>, ...
  expressed in numbers: <1, 1, 0>, <1, 1, 3>
**Metric Distances**

**Manhattan distance**

\[ \text{dist}(a, b) = \|a - b\|_1 = \sum_i |a_i - b_i| \]

**Euclidian distance**

\[ \text{dist}(a, b) = \|a - b\|_2 = \sqrt{\sum_i (a_i - b_i)^2} \]
Cosine Similarity

\[ s(x, y) = \frac{\mathbf{x} \cdot \mathbf{y}}{\|\mathbf{x}\| \|\mathbf{y}\|} = \frac{\sum_{i=0}^{n-1} x_i y_i}{\sqrt{\sum_{i=0}^{n-1} (x_i)^2} \times \sqrt{\sum_{i=0}^{n-1} (y_i)^2}} \]

how is this related to correlation?
What is correlation

- correlation is a statistical measure that indicates the extent to which two or more variables fluctuate together
- a positive correlation indicates the extent to which those variables increase or decrease in parallel
- a negative correlation indicates the extent to which one variable increases as the other decreases
Cosine Similarity

\[ s(x, y) = \frac{x \cdot y}{\|x\| \|y\|} = \frac{\sum_{i=0}^{n-1} x_i y_i}{\sqrt{\sum_{i=0}^{n-1} (x_i)^2} \times \sqrt{\sum_{i=0}^{n-1} (y_i)^2}} \]

how is this related to correlation?

Pearson’s Correlation = correlation similarity

\[ r = r_{xy} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^{n} (y_i - \bar{y})^2}} \]

mean across all variable values for data items x, y

e.g. the “average looking” pair of pants or shoes
Correlation Demonstration

Correlations: \((5 \times 5 - 5)/2 = 10\) pairs

- positively correlated: shoes 1 and 2, shoes 4 and 5
- negatively correlated: shoes 1 and 4, 1 and 5, 2 and 4, 2 and 5
- fairly uncorrelated: shoe 3 with all others 1, 2, 4, 5
Correlation distance is invariant to addition of a constant
- subtracts out by construction
- green and blue curve have correlation of 1
- but cosine similarity is < 1
- correlated vectors just vary in the same way
- cosine similarity is stricter

Both correlation and cosine similarity are invariant to multiplication with a constant
- invariant to scaling

green = blue + 0.1
What’s the Jaccard similarity of the two baskets A and B?
3/13 = 0.23
This process is called **clustering**

- and in contrast to a real store, we can make the computer do it for us
Note:

- in data mining similarity and distance are the same thing
- so we will use these terms interchangeably
A cluster is a group of objects that are similar
- and dissimilar from other groups of objects at the same time

We need an objective function to capture this mathematically
- the computer will evaluate this function within an algorithm
- one such function is the mean-squared error (MSE)
- and the objective is to minimize the MSE

It’s not that easy in practice
- there is only one global minimum
- but often there are many local minima
- need to find the global minimum
In this case

- \( n=12 \) (blue points)
- \( k=2 \) (red points, the computed centroids)
- distance metric used: Euclidean
- minimization seems to be achieved
The K-Means Clustering Algorithm

1. Decide on a value for \( k \)

2. Initialize the \( k \) cluster centers (randomly, if necessary)

3. Decide the class memberships of the \( N \) objects by assigning them to the nearest cluster center

4. Re-estimate the \( k \) cluster centers, by assuming the memberships found above are correct

5. If none of the \( N \) objects changed membership in the last iteration, exit. Otherwise goto 3

The last slide and the next 8 slides contain figures courtesy of Eamonn Keogh, UC Riverside
K-means Clustering: Step 1

Algorithm: k-means, Distance Metric: Euclidean Distance
K-means Clustering: Step 2

Algorithm: k-means, Distance Metric: Euclidean Distance
K-means Clustering: Step 3

Algorithm: k-means, Distance Metric: Euclidean Distance
**K-means Clustering: Step 4**

Algorithm: k-means, Distance Metric: Euclidean Distance
K-means Clustering: Step 5

Algorithm: k-means, Distance Metric: Euclidean Distance
K-Means Algorithm – Comments

Strengths:
- relatively efficient: $O(tkn)$, where $n$ is # objects, $k$ is # clusters, and $t$ is # iterations. Normally, $k, t << n$.
- simple to code

Weaknesses:
- need to specify $k$ in advance which is often unknown
- find the best $k$ by trying many different ones and picking the one with the lowest error
- often terminates at a local optimum
- the global optimum may be found by trying many times and using the best result
How Can We Find the Best K?

- k=1, MSE=873.0
- k=2, MSE=173.1
- k=3, MSE=133.6
Is there a principled way we can know when to stop looking? Yes...

- we can plot the objective function values for $k$ equals 1 to 6...
- then check for a flattening of the curve

The abrupt change at $k = 2$ is highly suggestive of two clusters.

This technique is known as “knee finding” or “elbow finding.”
What is sampling?

- pick a **representative** subset of the data
- discard the remaining data
- pick as many you can afford to keep
- recall: once it’s gone, it’s gone
- be smart about it

Simplest: random sampling

- pick sample points at random
- will work if the points are distributed uniformly
- this is usually not the case
- outliers will likely be missed
- so the sample will not be representative
Pick the samples according to some knowledge of the data distribution

- cluster the data (outliers will form clusters as well)
- these clusters are also called *strata* (hence, stratified sampling)
- the size of each cluster represents its percentage in the population
- guides the number of samples – bigger clusters get more samples

**Better: Adaptive Sampling**

![Histogram of Black Cherry Tree Heights](image)

- **Sampling rate ~ bin height**
- **Sampling rate ~ cluster size**
Good candidates for elimination are *redundant* data

- how many cans of ravioli will you buy?
Eliminate redundant attributes
  - eliminate correlated attributes
    - km vs. miles
    - \( a + b + c = d \) \( \rightarrow \) can eliminate ‘c’ (or ‘a’ or ‘b’)

Eliminate redundant data
  - cluster the data with small ranges
  - only keep the cluster centroids
  - store size of clusters along to keep importance
SAMPLING OF WELL-SCATTERED POINTS

Used in the CURE high-dimensional clustering algorithm

Algorithm
- initialize the point set $S$ to empty
- pick the point farthest from the mean as the first point for $S$
- then iteratively pick points that are furthest from the points in $S$ collected so far

Complexity is $O(m \cdot n^2)$
- $n$ is the total number of points, $m$ is the number of desired points
- can find arbitrarily shaped clusters and preserve outliers, too
- need some good data structures to run efficiently: kd-tree, heap
- can get really expensive when the dimensionality $d$ is large because each pairwise distance has $O(d)$
Learned about

- distance metrics to evaluate similarity among data points
- correlation, cosine, Euclidian, Jacquard, Manhattan distance
- used it for clustering that can identify groups in data
- these groups can be used for unbiased data reduction and augmentation
- the k-means algorithm as a simple yet effective clustering scheme
- the elbow method to pick a good $k = \text{number of clusters}$
- advanced sampling methods: well-scattered points, Reservoir sampling for streaming data