# DATA MINING SIMILARITY & DISTANCE

Similarity and Distance

Recommender Systems

## SIMILARITY AND DISTANCE

Thanks to:

Tan, Steinbach, and Kumar, "Introduction to Data Mining" Rajaraman and Ullman, "Mining Massive Datasets"

### Similarity and Distance

- For many different problems we need to quantify how close two objects are.
- Examples:
  - For an item bought by a customer, find other similar items
  - Group together the customers of a site so that similar customers are shown the same ad.
  - Group together web documents so that you can separate the ones that talk about politics and the ones that talk about sports.
  - Find all the near-duplicate mirrored web documents.
  - Find credit card transactions that are very different from previous transactions.
- To solve these problems we need a definition of similarity, or distance.
  - The definition depends on the type of data that we have

## **Similarity**

- Numerical measure of how alike two data objects are.
  - A function that maps pairs of objects to real values
  - Higher when objects are more alike.
- Often falls in the range [0,1], sometimes in [-1,1]
- Desirable properties for similarity
  - 1. s(p, q) = 1 (or maximum similarity) only if p = q. (Identity)
  - 2. s(p, q) = s(q, p) for all p and q. (Symmetry)

## Similarity between sets

Consider the following documents

apple releases new ipod apple releases new ipad new apple pie recipe

Which ones are more similar?

How would you quantify their similarity?

### Similarity: Intersection

Number of words in common

apple releases new ipod

apple releases new ipad

new apple pie recipe

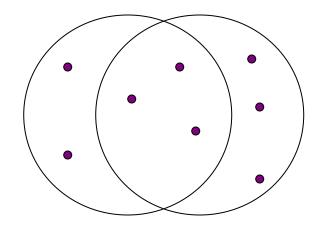
- Sim(D,D) = 3, Sim(D,D) = Sim(D,D) = 2
- What about this document?

Vefa releases new book with apple pie recipes

• Sim(D,D) = Sim(D,D) = 3

#### **Jaccard Similarity**

- The Jaccard similarity (Jaccard coefficient) of two sets  $S_1$ ,  $S_2$  is the size of their intersection divided by the size of their union.
  - JSim  $(S_1, S_2) = |S_1 \cap S_2| / |S_1 \cup S_2|$ .



3 in intersection.

8 in union.

Jaccard similarity = 3/8

- Extreme behavior:
  - Jsim(X,Y) = 1, iff X = Y
  - Jsim(X,Y) = 0 iff X,Y have no elements in common
- JSim is symmetric

#### Jaccard Similarity between sets

The distance for the documents

apple releases new ipod

apple releases new ipad

new apple pie recipe Vefa releases new book with apple pie recipes

- JSim(D,D) = 3/5
- JSim(D,D) = JSim(D,D) = 2/6
- JSim(D,D) = JSim(D,D) = 3/9

#### Similarity between vectors

Documents (and sets in general) can also be represented as vectors

document	Apple	Microsoft	Obama	Election
D1	10	20	0	0
D2	30	60	0	0
D3	60	30	0	0
D4	0	0	10	20

How do we measure the similarity of two vectors?

- We could view them as sets of words. Jaccard Similarity will show that D4 is different form the rest
- But all pairs of the other three documents are equally similar

We want to capture how well the two vectors are aligned

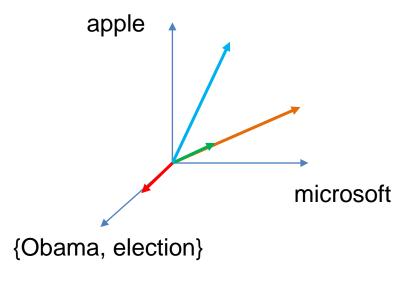
### Example

document	Apple	Microsoft	Obama	Election
D1	10	20	0	0
D2	30	60	0	0
<b>D3</b>	60	30	0	0
D4	0	0	10	20

Documents D1, D2 are in the "same direction"

Document D3 is on the same plane as D1, D2

Document D4 is orthogonal to the rest



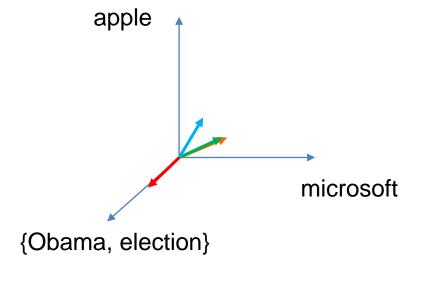
## Example

document	Apple	Microsoft	Obama	Election
D1	10	20	0	0
D2	30	60	0	0
<b>D3</b>	60	30	0	0
D4	0	0	10	20

Documents D1, D2 are in the "same direction"

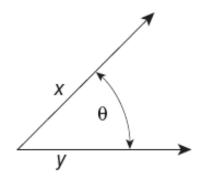
Document D3 is on the same plane as D1, D2

Document D4 is orthogonal to the rest



## **Cosine Similarity**

- Sim(X,Y) = cos(X,Y)
  - The cosine of the angle betweer



**Figure 2.16.** Geometric illustration of the cosine measure.

- If the vectors are aligned (correlated) angle is zero degrees and cos(X,Y)=1
- If the vectors are orthogonal (no common coordinates) angle is 90 degrees and cos(X,Y) = 0
- Cosine is commonly used for comparing documents, where we assume that the vectors are normalized by the document length, or words are weighted by tf-idf.

### Cosine Similarity - math

 $\cos(d_1, d_2) = .3150$ 

If d₁ and d₂ are two vectors, then
 cos(d₁, d₂) = (d₁ • d₂) / ||d₁|| ||d₂||,
 where • indicates vector dot product and || d || is the length of vector d.

Example:

$$d_1 = 3 2 0 5 0 0 0 2 0 0$$

$$d_2 = 1 0 0 0 0 0 1 0 2$$

$$d_1 \bullet d_2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$$

$$||d_1|| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$$

$$||d_2|| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.245$$

Note: We only need to consider the non-zero entries of the vectors

What if we have 0/1 vectors?

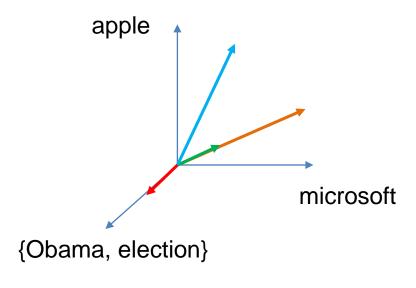
#### Example

document	Apple	Microsoft	Obama	Election
D1	10	20	0	0
D2	30	60	0	0
<b>D3</b>	60	30	0	0
D4	0	0	10	20

$$Cos(D1,D2) = 1$$

$$Cos(D3,D1) = Cos(D3,D2) = 4/5$$

$$Cos(D4,D1) = Cos(D4,D2) = Cos(D4,D3) = 0$$



#### **Correlation Coefficient**

- The correlation coefficient measures correlation between two random variables.
- If we have observations (vectors)  $X = (x_1, \dots, x_n)$  and  $Y = (y_1, \dots, y_n)$  is defined as

$$CorrCoeff(X,Y) = \frac{\sum_{i} (x_i - \mu_X)(y_i - \mu_Y)}{\sqrt{\sum_{i} (x_i - \mu_X)^2} \sqrt{\sum_{i} (y_i - \mu_Y)^2}}$$

- This is essentially the cosine similarity between the normalized vectors (where from each entry we remove the mean value of the vector.
- The correlation coefficient takes values in [-1,1]
  - -1 negative correlation, +1 positive correlation, 0 no correlation.
- Most statistical packages also compute a p-value that measures the statistical importance of the correlation
  - Lower value higher statistical importance

#### **Correlation Coefficient**

#### Normalized vectors

document	Apple	Microsoft	Obama	Election
D1	-5	+5	0	0
<b>D2</b>	-15	+15	0	0
<b>D3</b>	+15	-15	0	0
D4	0	0	-5	+5

$$CorrCoeff(X,Y) = \frac{\sum_{i}(x_i - \mu_X)(y_i - \mu_Y)}{\sqrt{\sum_{i}(x_i - \mu_X)^2}\sqrt{\sum_{i}(y_i - \mu_Y)^2}}$$

CorrCoeff(D1,D2) = 1

CorrCoeff(D1,D3) = CorrCoeff(D2,D3) = -1

CorrCoeff(D1,D4) = CorrCoeff(D2,D4) = CorrCoeff(D3,D4) = 0

#### Distance

- Numerical measure of how different two data objects are
  - A function that maps pairs of objects to real values
  - Lower when objects are more alike
  - Higher when two objects are different
- Minimum distance is 0, when comparing an object with itself.
- Upper limit varies

#### Distance Metric

- A distance function d is a distance metric if it is a function from pairs of objects to real numbers such that:
  - 1.  $d(x,y) \ge 0$ . (non-negativity)
  - 2. d(x,y) = 0 iff x = y. (identity)
  - 3. d(x,y) = d(y,x). (symmetry)
  - 4.  $d(x,y) \le d(x,z) + d(z,y)$  (triangle inequality).

## Triangle Inequality

- Triangle inequality guarantees that the distance function is wellbehaved.
  - The direct connection is the shortest distance
- It is useful also for proving useful properties about the data.

### Example

- We have a set of objects  $X = \{x_1, ..., x_n\}$  of a universe U (e.g.,  $U = \mathbb{R}^d$ ), and a distance function d that is a metric.
- We want to find the object  $z \in U$  that minimizes the sum of distances from X.
  - For some distance metrics this is easy, for some it is an NP-hard problem.
- It is easy to find the object  $x^* \in X$  that minimizes the distances from all the points in X.
- But how good is this? We can prove that

$$\sum_{x \in X} d(x, x^*) \le 2 \sum_{x \in X} d(x, z)$$

We are a factor 2 away from the best solution.

#### Distances for real vectors

• Vectors  $x = (x_1, ..., x_d)$  and  $y = (y_1, ..., y_d)$ 

L<sub>D</sub> norms are known to be distance metrics

• *L<sub>p</sub>*-norms or Minkowski distance:

$$L_p(x,y) = [|x_1 - y_1|^p + \dots + |x_d - y_d|^p]^{1/p}$$

L<sub>2</sub>-norm: Euclidean distance:

$$L_2(x,y) = \sqrt{|x_1 - y_1|^2 + \dots + |x_d - y_d|^2}$$

• *L*<sub>1</sub>-norm: Manhattan distance:

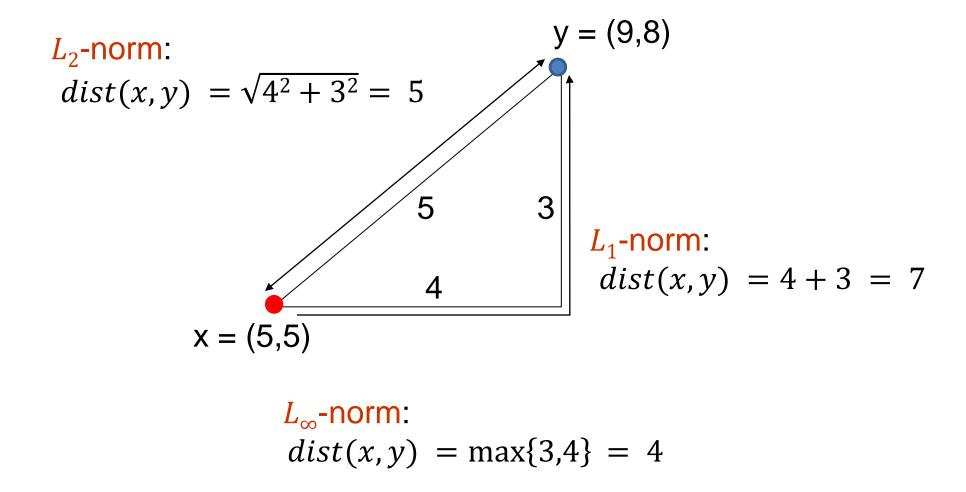
$$L_1(x,y) = |x_1 - y_1| + \dots + |x_d - y_d|$$

• **L**<sub>∞</sub>-norm:

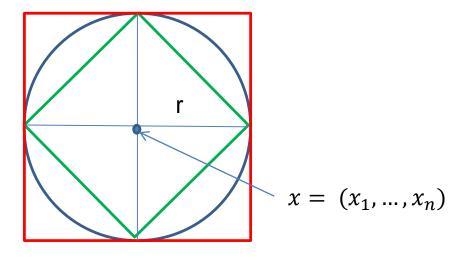
$$L_{\infty}(x, y) = \max\{|x_1 - y_1|, ..., |x_d - y_d|\}$$

The limit of L<sub>p</sub> as p goes to infinity.

#### **Example of Distances**



## Example



Green: All points y at distance  $L_1(x, y) = r$  from point x

Blue: All points y at distance  $L_2(x, y) = r$  from point x

Red: All points y at distance  $L_{\infty}(x,y) = r$  from point x

## $L_p$ distances for sets

- We can apply all the L<sub>p</sub> distances to the cases of sets of attributes, with or without counts, if we represent the sets as vectors
  - E.g., a transaction is a 0/1 vector
  - E.g., a document is a vector of counts.

#### Similarities into distances

Jaccard distance:

$$JDist(X,Y) = 1 - JSim(X,Y)$$

Jaccard Distance is a metric

Cosine distance:

$$Dist(X,Y) = 1 - \cos(X,Y)$$

Cosine distance is a metric

### Hamming Distance

- Hamming distance is the number of positions in which bit-vectors differ.
  - Example:
    - $p_1 = 10101$
    - $p_2 = 10011$ .
    - $d(p_1, p_2) = 2$  because the bit-vectors differ in the 3<sup>rd</sup> and 4<sup>th</sup> positions.
    - The L₁ norm for the binary vectors
- Hamming distance between two vectors of categorical attributes is the number of positions in which they differ.
  - Example:
    - x = (married, low income, cheat)
    - y = (single, low income, not cheat)
    - $\bullet \ d(x,y) = 2$

#### Why Hamming Distance Is a Distance Metric

- d(x,x) = 0 since no positions differ.
- d(x,y) = d(y,x) by symmetry of "different from."
- $d(x,y) \ge 0$  since strings cannot differ in a negative number of positions.
- Triangle inequality: changing x to z and then to y is one way to change x to y.

For binary vectors if follows from the fact that L<sub>1</sub> norm is a metric

#### Distance between strings

How do we define similarity between strings?

weird wierd intelligent unintelligent Athena Athina

 Important for recognizing and correcting typing errors and analyzing DNA sequences.

#### Edit Distance for strings

- The edit distance of two strings is the number of inserts and deletes of characters needed to turn one into the other.
- Example: x = abcde; y = bcduve.
  - Turn x into y by deleting a, then inserting u and v after d.
  - Edit distance = 3.
- Minimum number of operations can be computed using dynamic programming
- Common distance measure for comparing DNA sequences

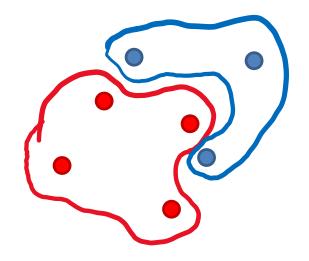
#### Why Edit Distance Is a Distance Metric

- d(x,x) = 0 because 0 edits suffice.
- d(x,y) = d(y,x) because insert/delete are inverses of each other.
- $d(x,y) \ge 0$ : no notion of negative edits.
- Triangle inequality: changing x to z and then to y is one way to change x to y. The minimum is no more than that

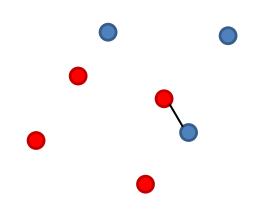
#### Variant Edit Distances

- Allow insert, delete, and mutate.
  - Change one character into another.
- Minimum number of inserts, deletes, and mutates also forms a distance measure.

- Same for any set of operations on strings.
  - Example: substring reversal or block transposition OK for DNA sequences
  - Example: character transposition is used for spelling

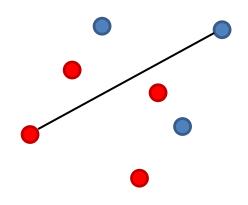


How do we measure the distance between the two sets?



How do we measure the distance between the two sets?

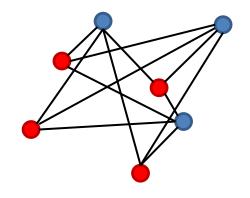
Minimum distance over all pairs



How do we measure the distance between the two sets?

Minimum distance over all pairs

Maximum distance over all pairs

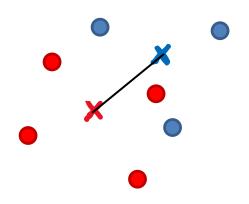


How do we measure the distance between the two sets?

Minimum distance over all pairs

Maximum distance over all pairs

Average distance over all pairs



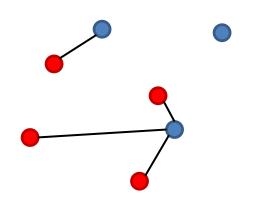
How do we measure the distance between the two sets?

Minimum distance over all pairs

Maximum distance over all pairs

Average distance over all pairs

Distance between averages



How do we measure the distance between the two sets?

Minimum distance over all pairs

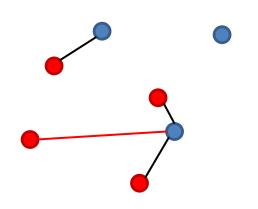
Maximum distance over all pairs

Average distance over all pairs

Distance between averages

#### Hausdorff distance:

• For each red point x compute the distance to the closest Blue point:  $d(x, Blue) = \min_{y \in Blue} d(x, y)$ 



How do we measure the distance between the two sets?

Minimum distance over all pairs

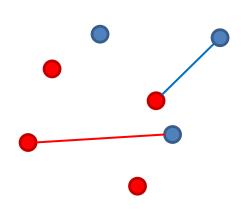
Maximum distance over all pairs

Average distance over all pairs

Distance between averages

#### Hausdorff distance:

- For each red point x compute the distance to the closest Blue point:  $d(x, Blue) = \min_{y \in Blue} d(x, y)$
- Find the maximum: this is the distance from Red to Blue:  $d(Red, Blue) = \max_{x \in Red} d(x, Blue)$



How do we measure the distance between the two sets?

Minimum distance over all pairs

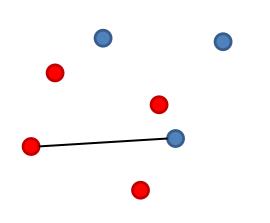
Maximum distance over all pairs

Average distance over all pairs

Distance between averages

#### Hausdorff distance:

- For each red point x compute the distance to the closest Blue point:  $d(x, Blue) = \min_{y \in Blue} d(x, y)$
- Find the maximum: this is the distance from Red to Blue:  $d(Red, Blue) = \max_{x \in Red} d(x, Blue)$
- Compute the *d*(*Blue*, *Red*)



How do we measure the distance between the two sets?

Minimum distance over all pairs

Maximum distance over all pairs

Average distance over all pairs

Distance between averages

#### Hausdorff distance:

- For each red point x compute the distance to the closest Blue point:  $d(x, Blue) = \min_{y \in Blue} d(x, y)$
- Find the maximum: this is the distance from Red to Blue:  $d(Red, Blue) = \max_{x \in Red} d(x, Blue)$
- Compute the *d*(*Blue*, *Red*)
- Take the maximum of the two

$$d_H(Red, Blue) = \max \left\{ \max_{x \in Red} \min_{y \in Blue} d(x, y), \max_{x \in Red} \min_{y \in Blue} d(x, y) \right\}$$

## Distances between distributions

 Some times data can be represented as a distribution (e.g., a document is a distribution over the words)

document	Apple	Microsoft	Obama	Election
D1	0.35	0.5	0.1	0.05
D2	0.4	0.4	0.1	0.1
D3	0.05	0.05	0.6	0.3

How do we measure distance between distributions?

## Variational distance

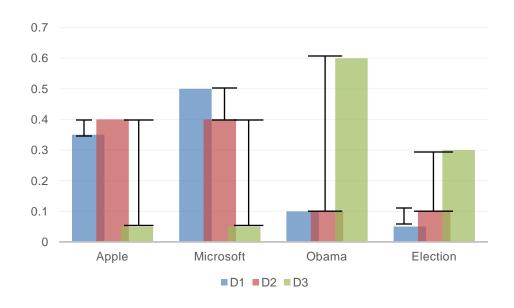
• Variational distance: The  $L_1$  distance between the distribution vectors

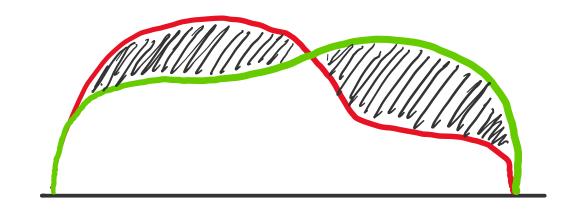
document	Apple	Microsoft	Obama	Election
D1	0.35	0.5	0.1	0.05
D2	0.4	0.4	0.1	0.1
D3	0.05	0.05	0.6	0.3

$$Dist(D1,D2) = 0.05+0.1+0.05 = 0.2$$

$$Dist(D2,D3) = 0.35+0.35+0.5+0.2 = 1.4$$

$$Dist(D1,D3) = 0.3+0.45+0.5+0.25 = 1.5$$





Information	theoretic	distances
		alotal 1000

document	Apple	Microsoft	Obama	Election
D1	0.35	0.5	0.1	0.05
D2	0.4	0.4	0.1	0.1
D3	0.05	0.05	0.6	0.3

KL-divergence (Kullback-Leibler) for distributions P,Q

$$D_{KL}(P||Q) = \sum_{x} p(x) \log \frac{p(x)}{q(x)}$$

 KL-divergence is asymmetric. We can make it symmetric by taking the average of both sides

$$\frac{1}{2} (D_{KL}(P||Q) + D_{KL}(Q||P))$$

JS-divergence (Jensen-Shannon)

$$JS(P,Q) = \frac{1}{2}D_{KL}(P||M) + \frac{1}{2}D_{KL}(Q||M)$$

$$M = \frac{1}{2}(P+Q)$$
 Average distribution

# Ranking distances

The input in this case is two rankings/orderings of the same n items. For example:

$$R_1 = \langle x, y, z, w \rangle$$
  

$$R_2 = \langle y, w, z, x \rangle$$

- How do we define distance in this case?
- Kendal's tau: Number of pairs of items that are in different order:

$$|\{(x,y),(x,z),(x,w),(z,w)\}| = 4$$

- Defines a metric.
- Maximum:  $\frac{n(n-1)}{2}$  when rankings are reversed.
- Spearman rank distance:  $L_1$  distance between the ranks

• 
$$SR(R_1, R_2) = |1 - 4| + |2 - 1| + |3 - 3| + |4 - 2| = 6$$

	X	у	z	w
$R_1$	1	2	3	4
$R_2$	4	1	3	2

# Why is similarity important?

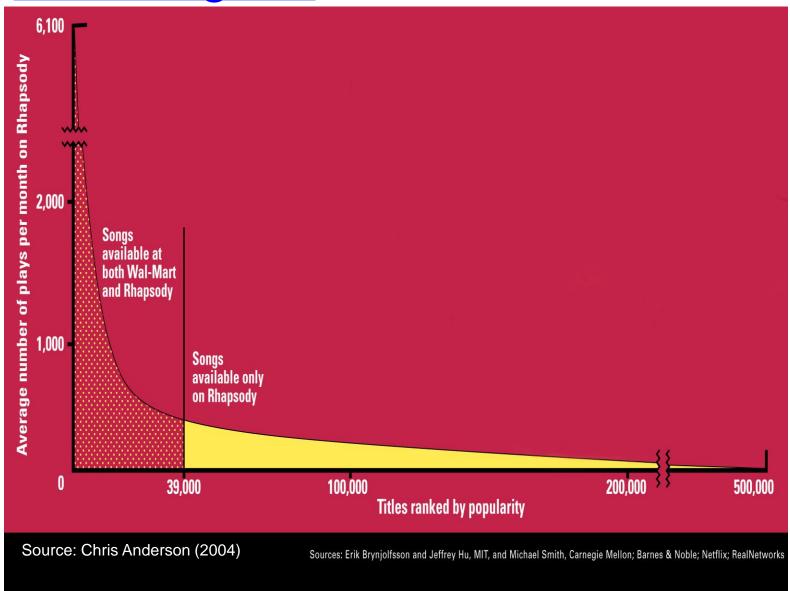
- We saw many definitions of similarity and distance
- How do we make use of similarity in practice?
- What issues do we have to deal with?

# APPLICATIONS OF SIMILARITY: RECOMMENDATION SYSTEMS

# An important problem

- Recommendation systems
  - When a user buys an item (initially books) we want to recommend other items that the user may like
  - When a user rates a movie, we want to recommend movies that the user may like
  - When a user likes a song, we want to recommend other songs that they
    may like
- A big success of data mining
- Exploits the long tail
  - How Into Thin Air made Touching the Void popular

# The Long Tail



# Utility (Preference) Matrix

	Harry Potter 1	Harry Potter 2	Harry Potter 3	Twilight	Star Wars 1	Star Wars 2	Star Wars 3
Α	4			5	1		
В	5	5	4				
С				2	4	5	
D		3					3

**Rows: Users** 

Columns: Movies (in general Items)

Values: The rating of the user for the movie

How can we fill the empty entries of the matrix?

# Recommendation Systems

#### Content-based:

- Represent the items into a feature space and recommend items to customer
   C similar to previous items rated highly by C
  - Movie recommendations: recommend movies with same actor(s), director, genre, ...
  - Websites, blogs, news: recommend other sites with "similar" content

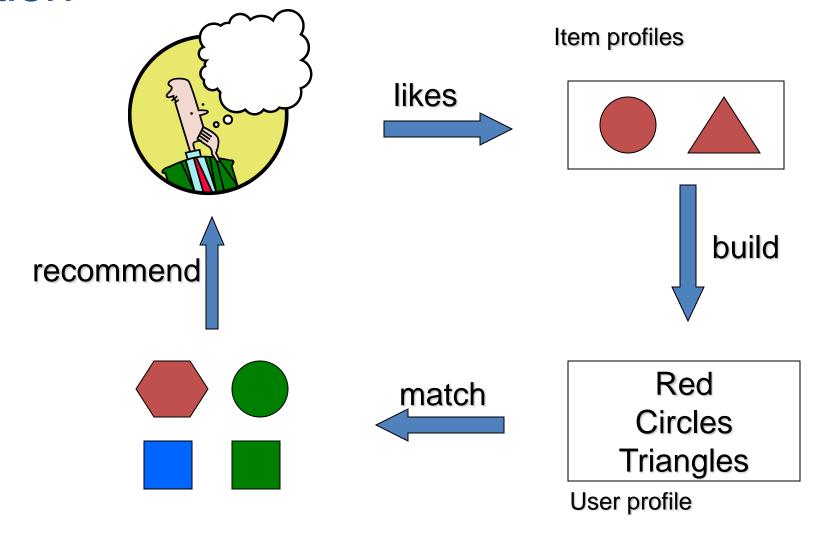
# Content-based prediction

	Harry Potter 1	Harry Potter 2	Harry Potter 3	Twilight	Star Wars 1	Star Wars 2	Star Wars 3
Α	4			5	1		
В	5	5	4				
С				2	4	5	
D		3					3

Someone who likes one of the Harry Potter (or Star Wars) movies is likely to like the rest

Same actors, similar story, same genre

## Intuition



# Approach

- Map items into a feature space:
  - For movies:
    - Actors, directors, genre, rating, year,...
    - Challenge: make all features compatible.
  - For documents?
- To compare items with users we need to map users to the same feature space. How?
  - Take all the movies that the user has seen and take the average vector
    - Other aggregation functions are also possible.
- Recommend to user C the most similar item i computing similarity in the common feature space
  - Distributional distance measures also work well.

## Limitations of content-based approach

- Finding the appropriate features
  - e.g., images, movies, music
  - Embeddings and deep learning can help
- Overspecialization
  - Never recommends items outside user's content profile
  - People might have multiple interests
- Recommendations for new users
  - How to build a profile?

# Collaborative filtering

	Harry Potter 1	Harry Potter 2	Harry Potter 3	Twilight	Star Wars 1	Star Wars 2	Star Wars 3
Α	4			5	1		
В	5	5	4				
С				2	4	5	
D		3					3

Two users are similar if they rate the same items in a similar way

Recommend to user C, the items liked by many of the most similar users.

	Harry Potter 1	Harry Potter 2	Harry Potter 3	Twilight	Star Wars 1	Star Wars 2	Star Wars 3
Α	4			5	1		
В	5	5	4				
С				2	4	5	
D		3					3

Which pair of users do you consider as the most similar?

What is the right definition of similarity?

	Harry Potter 1	Harry Potter 2	Harry Potter 3	Twilight	Star Wars 1	Star Wars 2	Star Wars 3
Α	1			1	1		
В	1	1	1				
С				1	1	1	
D		1					1

Jaccard Similarity: users are sets of movies

Disregards the ratings.

Jsim(A,B) = 1/5

Jsim(A,C) = 1/2

Jsim(B,D) = 1/4

	Harry Potter 1	Harry Potter 2	Harry Potter 3	Twilight	Star Wars 1	Star Wars 2	Star Wars 3
Α	4			5	1		
В	5	5	4				
С				2	4	5	
D		3					3

### **Cosine Similarity:**

Assumes zero entries are negatives:

Cos(A,B) = 0.38

Cos(A,C) = 0.32

	Harry Potter 1	Harry Potter 2	Harry Potter 3	Twilight	Star Wars 1	Star Wars 2	Star Wars 3
Α	2/3			5/3	-7/3		
В	1/3	1/3	-2/3				
С				-5/3	1/3	4/3	
D		0					0

#### Normalized Cosine Similarity:

 Subtract the mean rating per user (without the zeros) and then compute Cosine (correlation coefficient)

$$Corr(A,B) = 0.092$$
  
 $Corr(A,C) = -0.559$ 

# User-User Collaborative Filtering

- For a user u, find the set TopK(u) of the K users whose ratings are most "similar" to u's ratings
- Estimate u's ratings based on ratings of users in TopK using some aggregation function. For item i:

$$\widehat{r_{ui}} = \frac{1}{Z} \sum_{v \in TopK(u)} sim(u, v) r_{vi}$$

$$Z = \sum_{v \in TopK(u)} sim(u, v)$$

Modeling deviations:

Deviation from mean for v

Mean rating of u 
$$\widehat{r_{ui}} = \overline{r_u} + \frac{1}{Z} \sum_{v \in TopK(u)} \sin(u, v) (r_{vi} - \overline{r_v})$$
 Mean deviation of similar users

Advantage: for each user we have small amount of computation.

# Item-Item Collaborative Filtering

- We can transpose (flip) the matrix and perform the same computation as before to define similarity between items
  - Intuition: Two items are similar if they are rated in the same way by many users.
  - Better defined similarity since it captures the notion of genre of an item
    Users may have multiple interests.
- Algorithm: For each user u and item i not rated by u
  - Find the set  $TopK_u(i)$  of most similar items to item i that have been rated by user u.
  - Aggregate their ratings to predict the rating for item i.
- Disadvantage: we need to consider each user-item pair separately

# Implementation details

- When removing the mean rating make sure to not take into account the non-rated entries
- When trying to compute the rating for pair (u, i):
  - When looking for the k most similar users to a user u:
    - Take the k most similar users regardless
    - Take the k most similar users that have rated the item i
  - When looking for the k most similar items to an item i:
    - Take the k most similar items regardless
    - Take the k most similar items that have been rated by user u

## **Evaluation**

- Split the data into train and test set
  - Keep a fraction of the ratings to test the accuracy of the predictions
- Metrics:
  - Root Mean Square Error (RMSE) for measuring the quality of predicted ratings:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i,j} (\widehat{r_{ij}} - r_{ij})^2}$$

- Precision/Recall for measuring the quality of binary (action/no action) predictions:
  - Precision = fraction of predicted actions that were correct
  - Recall = fraction of actions that were predicted correctly
  - We may also consider the top-k recommendations for the evaluation
- Kendal' tau for measuring the quality of predicting the ranking of items:
  - The fraction of pairs of items that are ordered correctly (or incorrectly)

# Pros and cons of collaborative filtering

- Works for any kind of item
  - No feature selection needed
- New user problem
- New item problem
- Sparsity of rating matrix
  - Cluster-based smoothing?

# The Netflix Challenge

1M prize to improve the prediction accuracy by 10%



