Similarity:

Beyond numerical Data

Mining Massive Datasets

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Main Sources

- Data Mining, The Textbook (2015) by Charu Aggarwal (Chapter 3) + slides by Lijun Zhang
- Data Mining Concepts and Techniques, 3rd edition (2011) by Han et al. (Section 2.4)
- Introduction to Data Mining 2nd edition (2019) by Tan et al. (Chapter 2)
- Mining of Massive Datasets 2nd edition (2014) by Leskovec et al. (Chapter 3)

Categorical and mixed data

Simple similarity for categorical data

- Given $\overline{X} = (x_1, \ldots, x_d); \overline{Y} = (y_1, \ldots, y_d)$
- Compute similarity as

$$\text{sim}(\overline{X}, \overline{Y}) = \sum_{i=1}^{d} S(x_i, y_i)$$

- Simple coordinate wise similarity

$$S(x_i, y_i) = \begin{cases} 1, & \text{if } x_i = y_i \\ 0, & \text{otherwise} \end{cases}$$

Weighing feature values by how rare they are

- Compute similarity as $$\text{sim}(\overline{X}, \overline{Y}) = \sum_{i=1}^{d} S(x_i, y_i)$$

- Inverse occurrence frequency

$p_i(z)$ is the probability that feature i takes value z

$$S(x_i, y_i) = \begin{cases} 1/p_i(x_i)^2, & \text{if } x_i = y_i \\ 0, & \text{otherwise} \end{cases}$$

$$S(x_i, y_i) = \begin{cases} 1 - p_i(x_i), & \text{if } x_i = y_i \\ 0, & \text{otherwise} \end{cases}$$

Goodall measure

Mixture of quantitative and categorical data

- Given $\overline{X} = (\overline{X_c}, \overline{X_n}); \overline{Y} = (\overline{Y_c}, \overline{Y_n});$
- Where c denotes the subset of categorical data and n the subset of numerical data

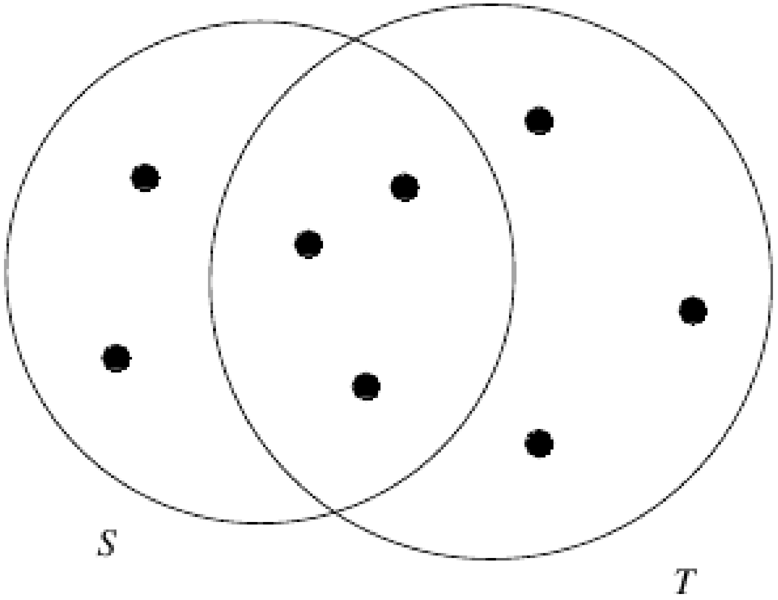
$$\mathrm{sim}(\overline{X}, \overline{Y}) = \lambda\,\mathrm{CatSim}(\overline{X_c}, \overline{Y_c}) + (1-\lambda)\,\mathrm{NumSim}(\overline{X_n}, \overline{Y_n})$$

- In general λ is difficult to set, and additionally we should have variables with similar variances or normalize by variance

Binary and set data

Jaccard coefficient

Example: J(S,T) = 3/8



$$J(S,T) = \frac{|S \cap T|}{|S \cup T|}$$

Binary variables can be set as set inclusion variables

- If $\overline{X}=(x_1, \ldots, x_d)$ is such that $x_i = 1$, this can be seen as element $\overline{X}$ belonging to set i
- Alternatively, $\overline{X}$ can be seen as $S_{\overline{X}}$ the set of all variables i such that $x_i = 1$
- Extended Jaccard coefficient (Tanimoto)

$$J(\overline{X},\overline{Y}) = \frac{\sum_{i=1}^{d} x_i \cdot y_i}{\sum_{i=1}^{d} x_i^2 + \sum_{i=1}^{d} y_i^2 - \sum_{i=1}^{d} x_i \cdot y_i}$$

Exercise

Answer in
Nearpod open-ended question
Code to be given in class

- Compute Tanimoto and Jaccard* coefficient between:

  $(0, 2, 1, 0, 3)$

  $(1, 2, 0, 0, 0)$

  * For the Jaccard coefficient, binarize the vectors

$$J(\overline{X}, \overline{Y}) = \frac{\sum_{i=1}^{d} x_i \cdot y_i}{\sum_{i=1}^{d} x_i^2 + \sum_{i=1}^{d} y_i^2 - \sum_{i=1}^{d} x_i \cdot y_i}$$

Similarity != Distance

- When using Jaccard:
  - The similarity between an object and itself is 1.0
  - The distance between an object and itself is 0.0
- Hence:
  - Jaccard **similarity** = Jaccard_coefficient
  - Jaccard **distance** = 1 - Jaccard_coefficient

Text data

Text documents as vectors: L_p norms

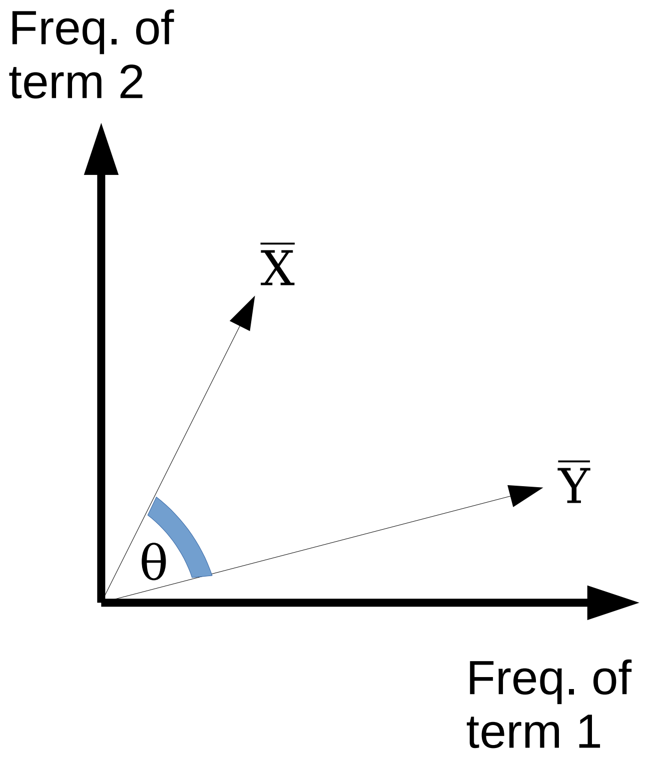
- As Quantitative Multidimensional Data
  - Bag of words model
  - They are very sparse
  - L_p norm does not work well
  - Long documents have long distance
- Dimensionality Reduction (A Possible Solution)
  - Latent Semantic Analysis (equivalent to SVD)
  - L_p norm in the new space

Text documents as vectors: angles

- What we care about is the relative frequency of terms

$$\mathrm{sim}(\overline{X}, \overline{Y}) = \cos\theta$$

$$\mathrm{sim}(\overline{X}, \overline{Y}) = \frac{\sum_{i=1}^{d} x_i \cdot y_i}{\sqrt{\sum_{i=1}^{d} x_i^2} \cdot \sqrt{\sum_{i=1}^{d} y_i^2}}$$



However, some terms are very common and others are very rare …

Text documents as vectors: tf-idf weighting (idf)

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- $\mathrm{idf}(t) = \log \frac{n}{n_t}$
  - Global inverse document frequency of term t
  - Where n_t is the number of documents where term t appears, n is the total number of documents
- Typical variation (i.e. Okapi BM25)

$$\mathrm{idf}(t) = \log \frac{n - n_t + 0.5}{n_t + 0.5}$$

Text documents as vectors: tf-idf weighting (tf)

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- $tf(x_i)$
  - Frequency in a document of term x_i
  - Log frequency, square root of frequency, or similar to reduce the impact of terms of very high frequency

Text documents as vectors: tf-idf weighting (cont.)

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- $h(x_i) = tf(x_i) \times idf(x_i)$

$$\mathrm{sim}(\overline{X}, \overline{Y}) = \frac{\sum_{i=1}^{d} h(x_i) \cdot h(y_i)}{\sqrt{\sum_{i=1}^{d} h(x_i)^2} \cdot \sqrt{\sum_{i=1}^{d} h(y_i)^2}}$$

- Or Tanimoto like:

$$J(\overline{X}, Y) = \frac{\sum_{i=1}^{d} h(x_i) \cdot h(y_i)}{\sum_{i=1}^{d} h(x_i)^2 + \sum_{i=1}^{d} h(y_i)^2 - \sum_{i=1}^{d} h(x_i) \cdot h(y_i)}$$

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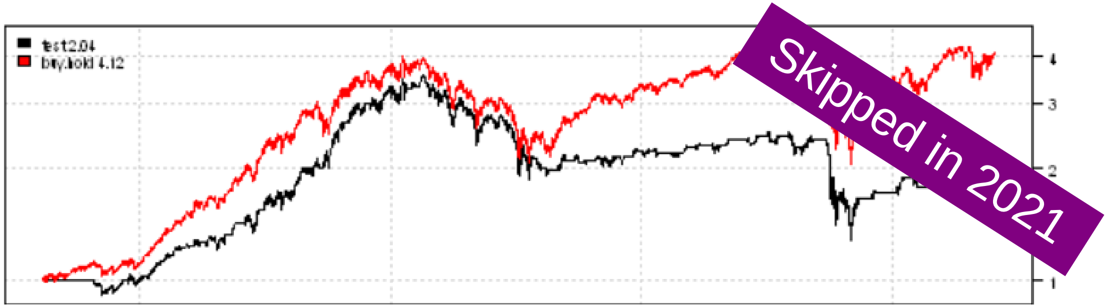
Continuous time series data

Misalignment between series



- Behavioral attributes
  - Scaling (range is larger or narrower)
  - Translation (series is shifted up or down)
- Contextual attribute (typically, time)
  - Scaling (time is stretched or compressed)
  - Translation or shift (starting time changes)
- Matches might not be contiguous (noisy segments)

Example of scaling, translation, noise

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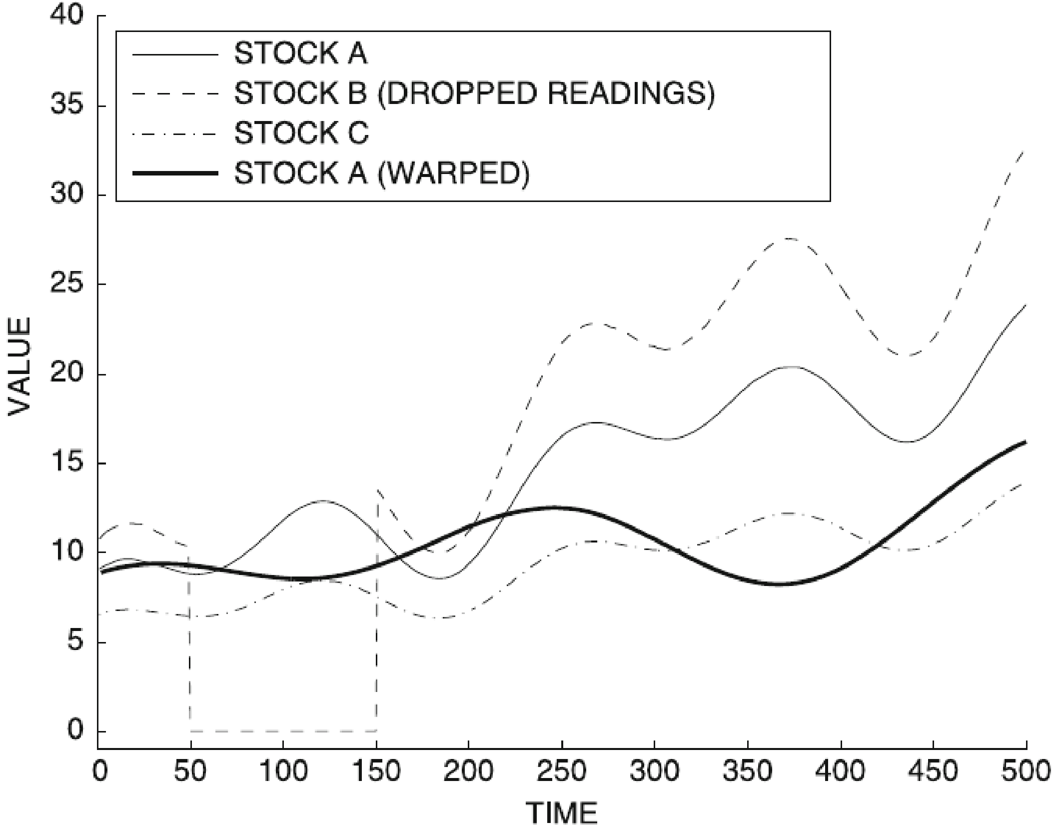

More on this later in the course, in the sequence mining topic

Data Mining, The Textbook (2015) by Charu Aggarwal (Chapter 3).

Warping means stretching or compressing time.

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Discrete sequence data

Discrete sequences can be treated as strings

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- Compute edit distance
- Compute longest common sub-sequence
- In genetic sequences, use PAM (*Point Accepted Mutation*) matrices
  - Indicate rarity (cost) of replacement

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Example PAM matrix

		Ala	Arg	Asn	Asp	Cys	Gln	Glu	Gly	His	Ile	Leu	Lys	Met	Phe	Pro	Ser	Thr	Trp	Tyr	Val
		A	R	N	D	C	Q	E	G	H	I	L	K	M	F	P	S	T	W	Y	V
Ala	A	9867	2	9	10	3	8	17	21	2	6	4	2	6	2	22	35	32	0	2	18
Arg	R	1	9913	1	0	1	10	0	0	10	3	1	19	4	1	4	6	1	8	0	1
Asn	N	4	1	9822	36	0	4	6	6	21	3	1	13	0	1	2	20	9	1	4	1
Asp	D	6	0	42	9859	0	6	53	6	4	1	0	3	0	0	1	5	3	0	0	1
Cys	C	1	1	0	0	9973	0	0	0	1	1	0	0	0	0	1	5	1	0	3	2
Gln	Q	3	9	4	5	0	9876	27	1	23	1	3	6	4	0	6	2	2	0	0	1
Glu	E	10	0	7	56	0	35	9865	4	2	3	1	4	1	0	3	4	2	0	1	2
Gly	G	21	1	12	11	1	3	7	9935	1	0	1	2	1	1	3	21	3	0	0	5
His	H	1	8	18	3	1	20	1	0	9912	0	1	1	0	2	3	1	1	1	4	1
Ile	I	2	2	3	1	2	1	2	0	0	9872	9	2	12	7	0	1	7	0	1	33
Leu	L	3	1	3	0	0	6	1	1	4	22	9947	2	45	13	3	1	3	4	2	15
Lys	K	2	37	25	6	0	12	7	2	2	4	1	9926	20	0	3	8	11	0	1	1
Met	M	1	1	0	0	0	2	0	0	0	5	8	4	9874	1	0	1	2	0	0	4
Phe	F	1	1	1	0	0	0	0	1	2	8	6	0	4	9946	0	2	1	3	28	0
Pro	P	13	5	2	1	1	8	3	2	5	1	2	2	1	1	9926	12	4	0	0	2
Ser	S	28	11	34	7	11	4	6	16	2	2	1	7	4	3	17	9840	38	5	2	2
Thr	T	22	2	13	4	1	3	2	2	1	11	2	8	6	1	5	32	9871	0	2	9
Trp	W	0	2	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	9976	1	0
Tyr	Y	1	0	3	0	3	0	1	0	4	1	1	0	0	21	0	1	1	2	9945	1
Val	V	13	2	1	1	3	2	2	3	3	57	11	1	17	1	3	2	10	0	2	9901

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Graph data

Distance/similarity in graph data

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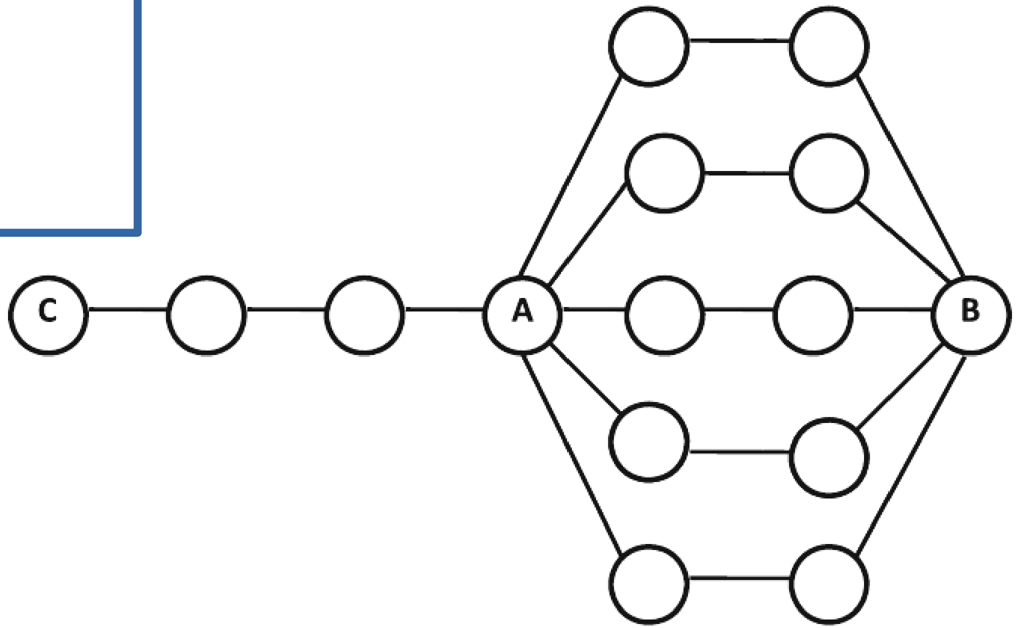
- Comparing A-B and A-C?
  - A-B should be closer
  - A-C should be closer
  - Both should be equal



Distance/similarity in graph data

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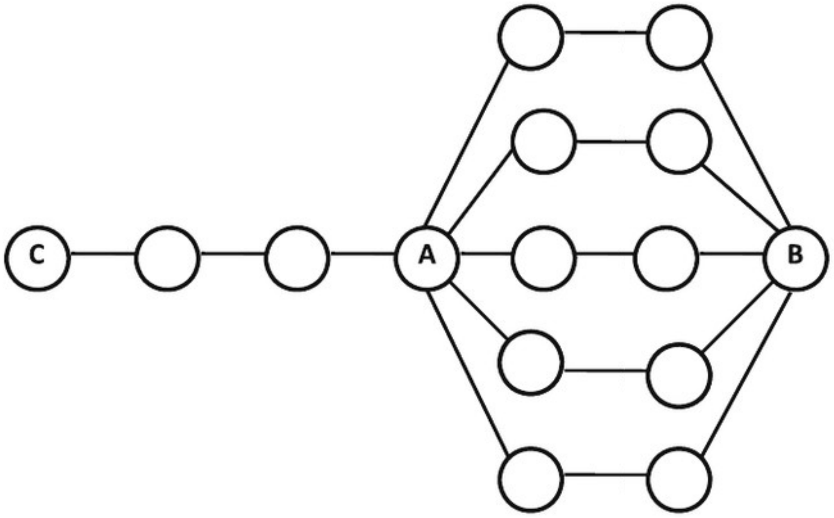
- Distance-Based Measure
  - Shortest-path on the graph
  - Dijkstra algorithm
- Random Walk-Based Similarity
  - (e.g. personalized PageRank)
  - Accounts for multiplicity in paths during similarity computation



Under random walk similarity, A-B are closer than A-C

Supervised similarity functions

Learning a distance function through supervised ML

- Suppose you have data from experts, annotators, or user feedback:

$$\mathcal{S} = \{O_i, O_j : O_i \text{ is similar to } O_j\}$$

$$\mathcal{D} = \{O_i, O_j : O_i \text{ is dissimilar to } O_j\}$$

$$\min_{\theta} \sum_{(O_i, O_j) \in \mathcal{S}} (f(O_i, O_j, \theta) - 0)^2 + \sum_{(O_i, O_j) \in \mathcal{D}} (f(O_i, O_j, \theta) - 1)^2$$

Summary

Things to remember

- For similarity/distance computation, there are different solutions for different data types

Exercises for this topic

- **Data Mining, The Textbook (2015) by Charu Aggarwal**
  - **Exercises 3.9 on similarity measures**
- Introduction to Data Mining 2nd edition (2019) by Tan et al.
  - Exercises 2.6 $\rightarrow$ 14-28
- Mining of Massive Datasets 2nd edition (2014) by Leskovec et al.
  - Exercises 3.5.7 on distance measures
- Data Mining Concepts and Techniques, 3rd ed. (2011) by Han et al.
  - Exercises 2.6 $\rightarrow$ 2.5-2.8