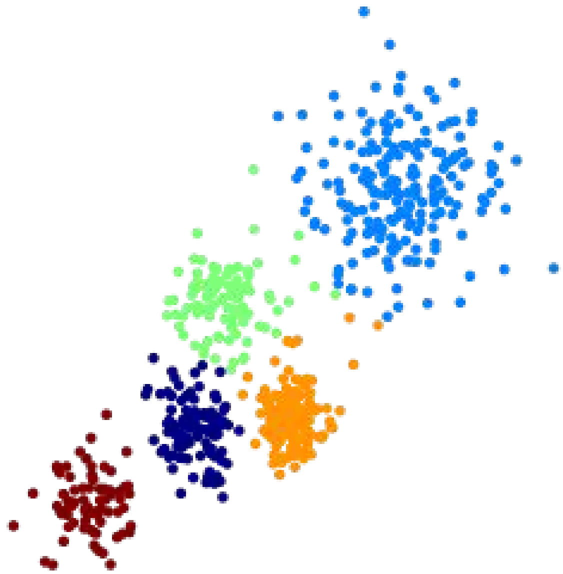
Clustering

K-means
& hierarchical clustering

DSI SEA5, jf.omhover, Oct 10 2016



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OBJECTIVES

- **Relate** clustering to unsupervised learning
- **Illustrate** the utility of clustering in real-world problems
- **Describe** and **implement** the k-means algorithm
- **Describe** and **implement** the HAC algorithm
- **Compare** purpose and utility of k-means and HAC
- **Discuss** the role of metrics for applying clustering to different problems
- **Analyze** how the (high) dimensionality of data impacts metrics based clustering techniques

K-Means

Objective: minimize WCSS
"within cluster sum of squares"

$$\underset{C_1,\dots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

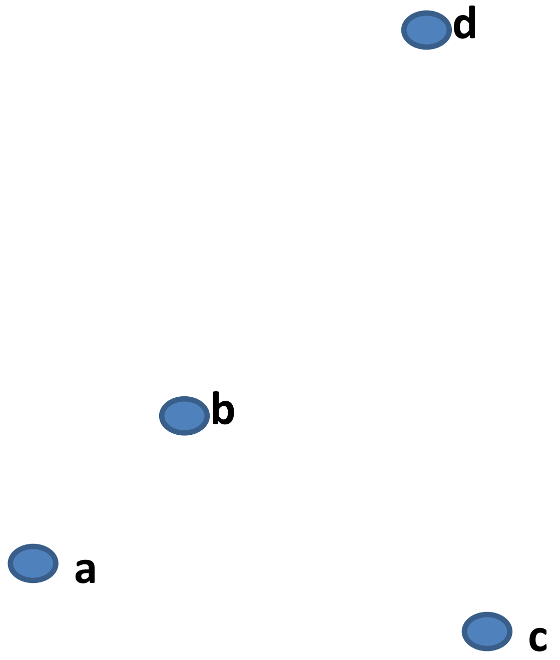
1. Randomly assign a number, from 1 to K, to each of the observations.
2. **Iterate** until the cluster assignments stop changing:
   a. For each of the K clusters, compute the cluster ***centroid***: the vector of the *p* features **means** for the observations in the k-th cluster
   b. **Assign** each observation to the cluster whose centroid is **closest** (defined using Euclidian distance)

K-Means in a nutshell :

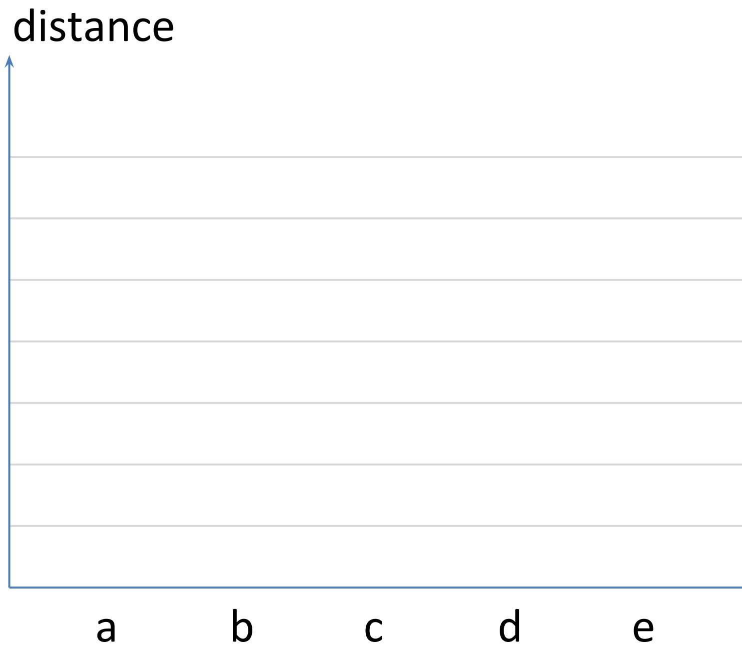
- **Computing distances**
- **Computing means**

Hierarchical Clustering (step by step)

1 - Computing distances between observations
2 – Identification / choose a minimum
3 – Fusion of observations



Observations



Dendrogram

1 - Computing distances between observations
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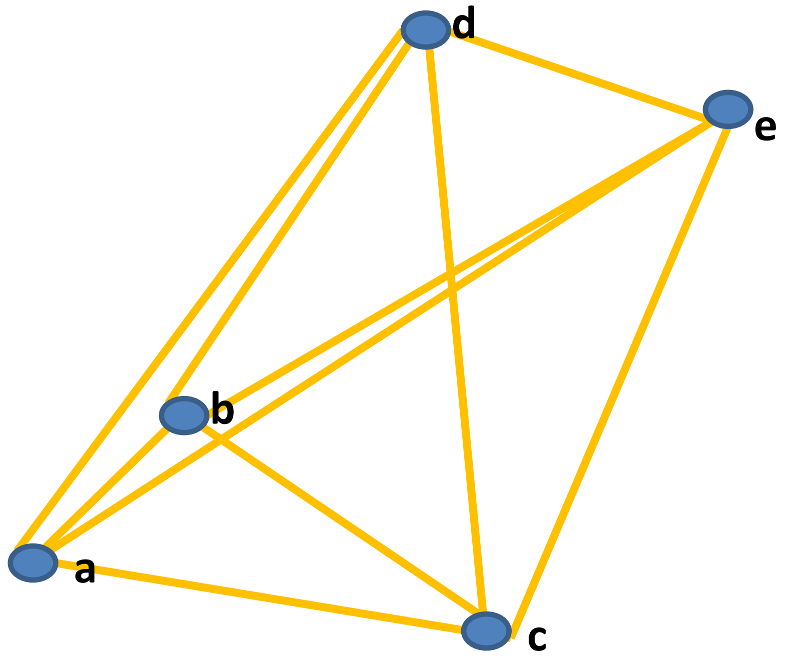

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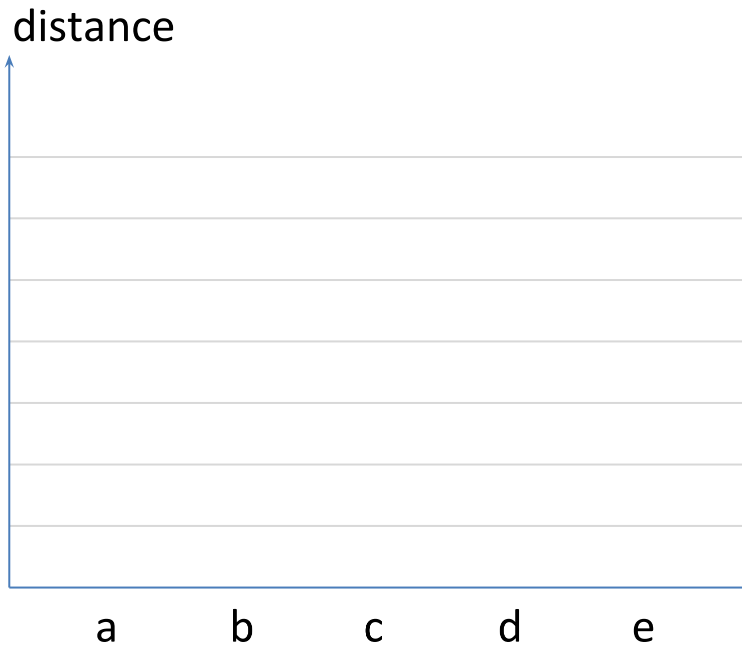

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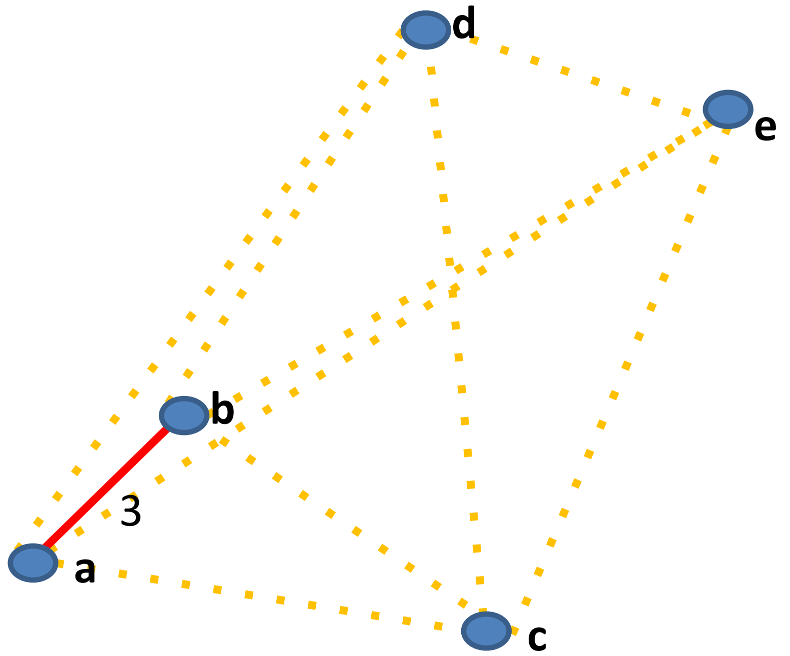

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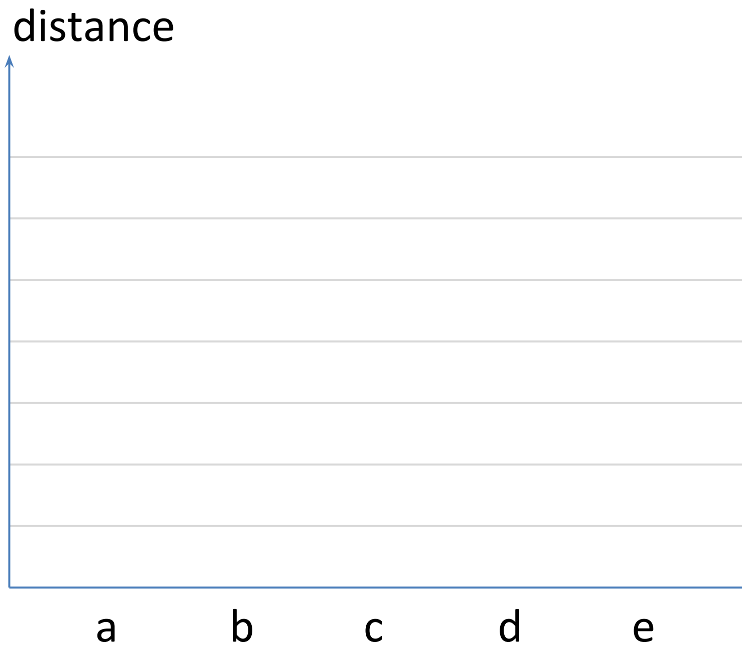

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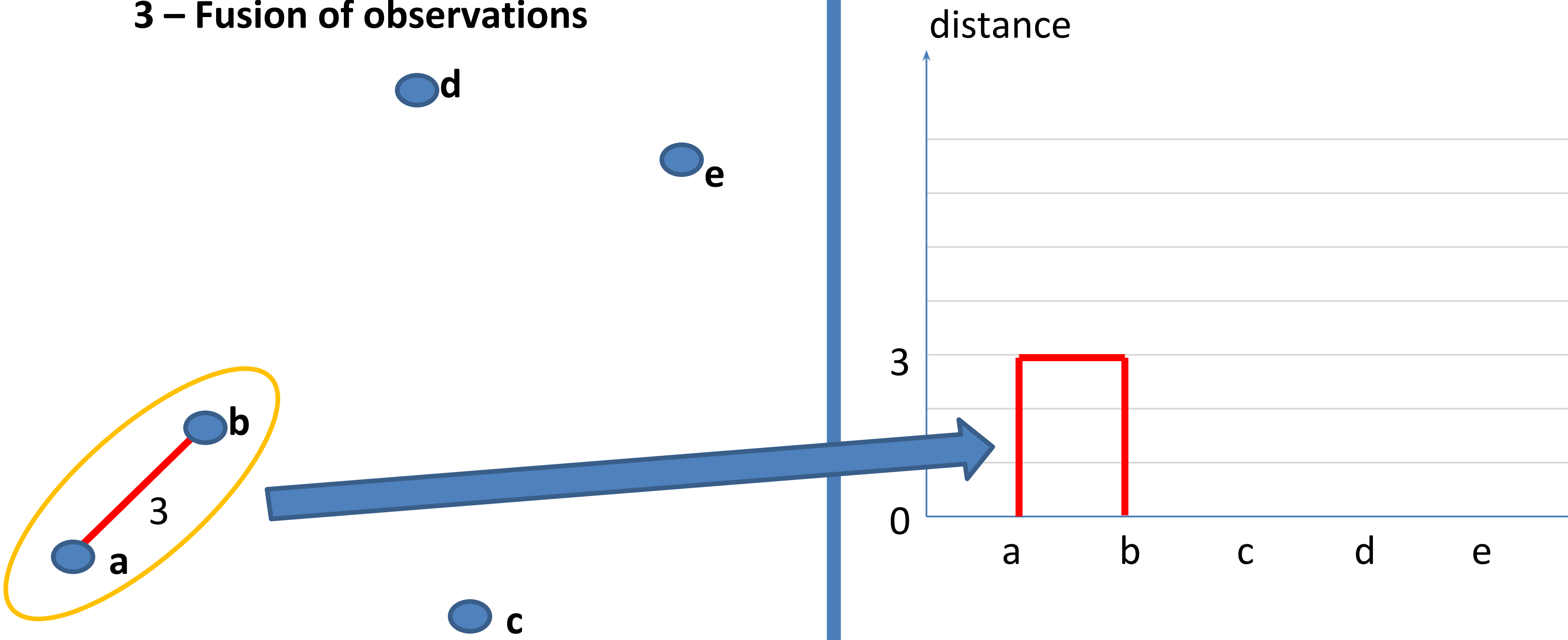

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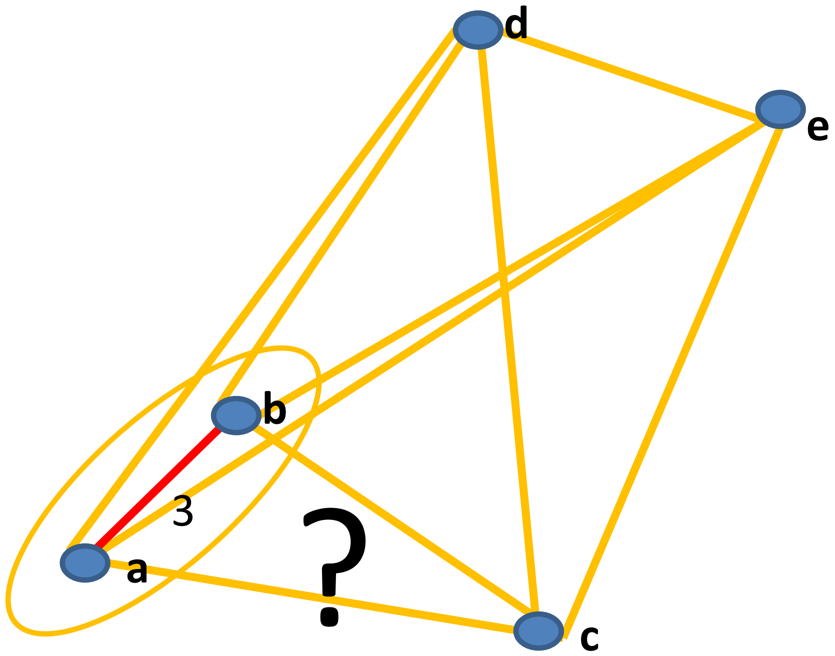

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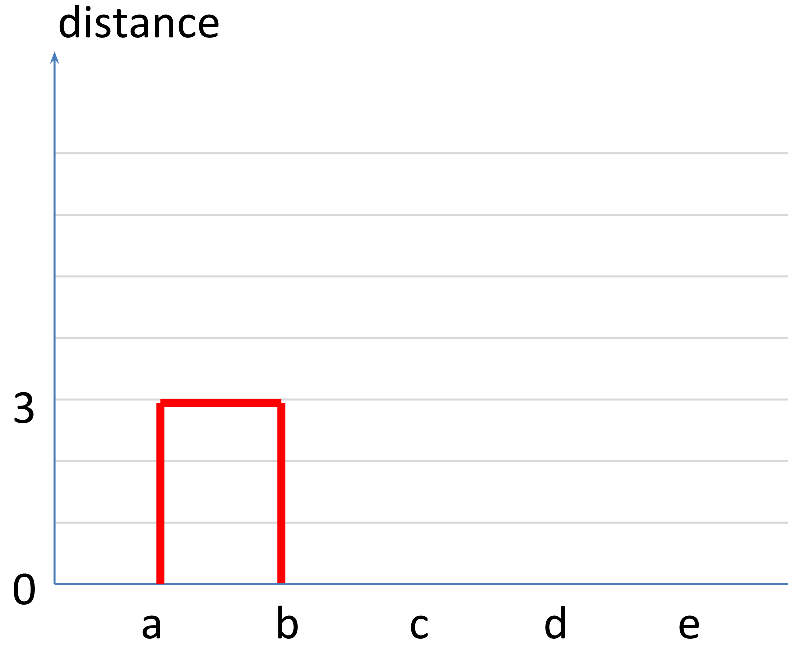

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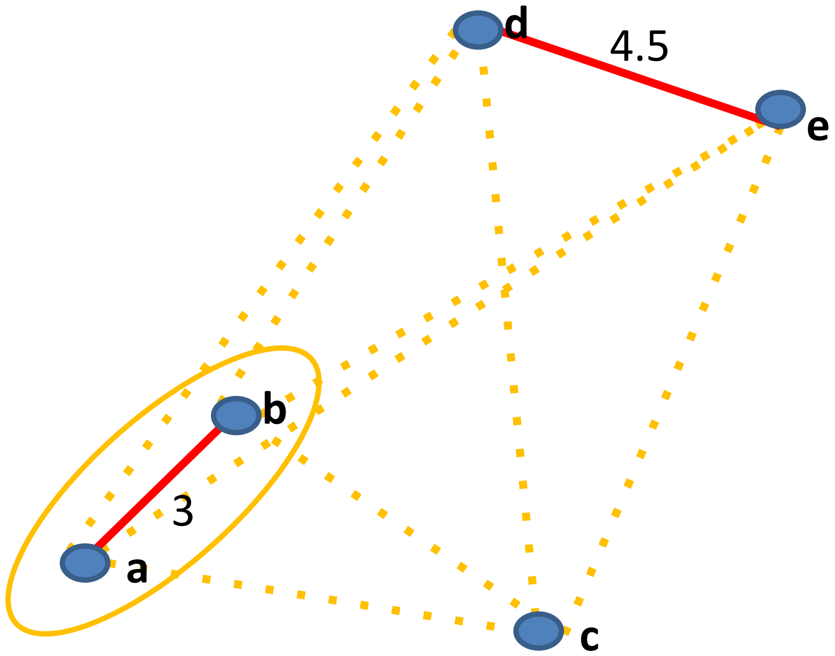

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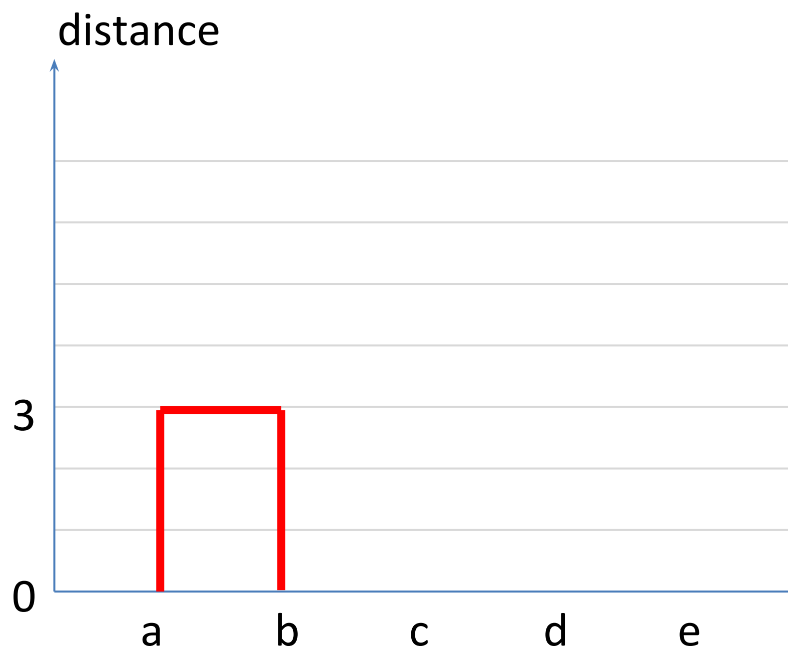

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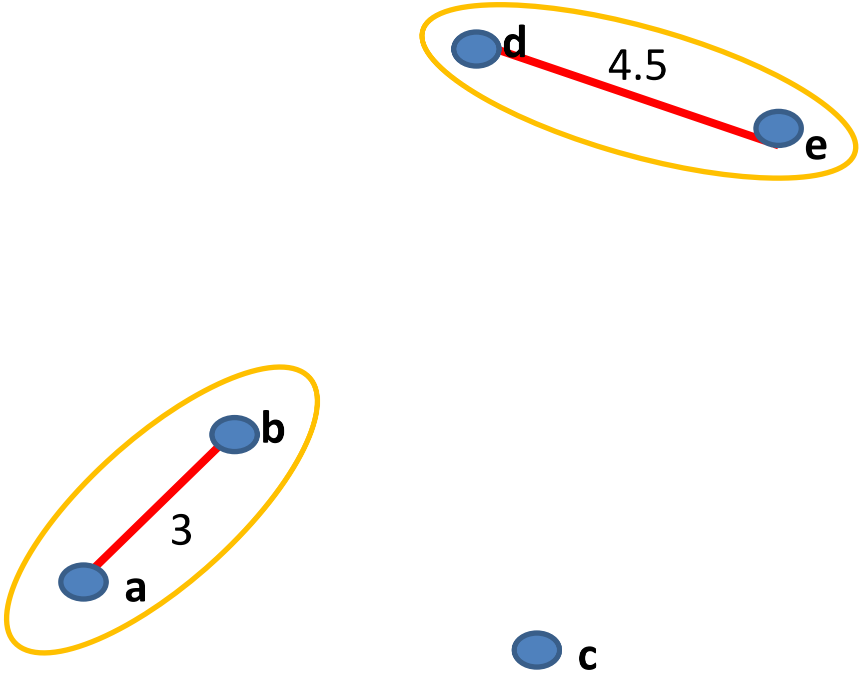

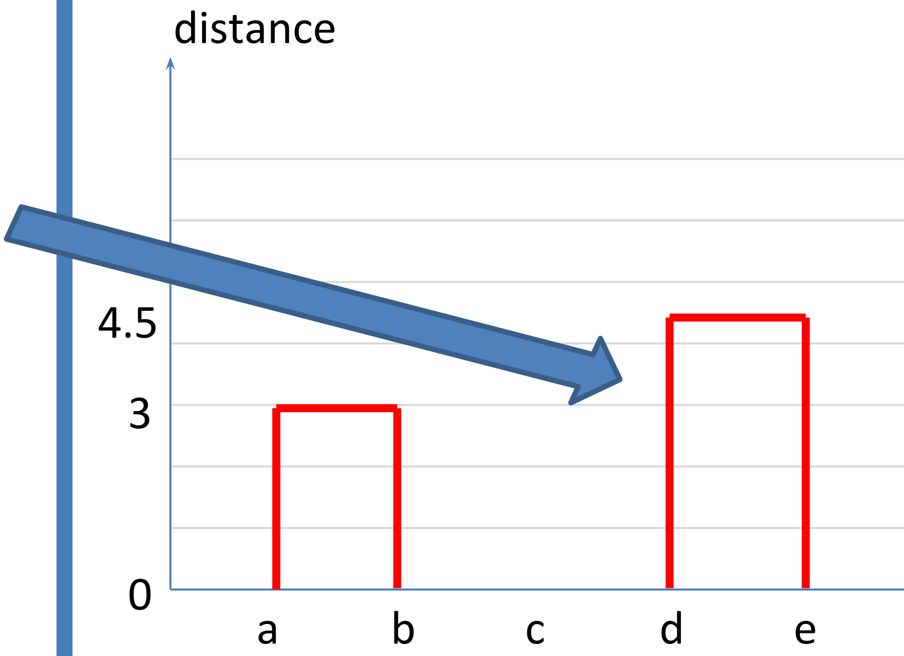

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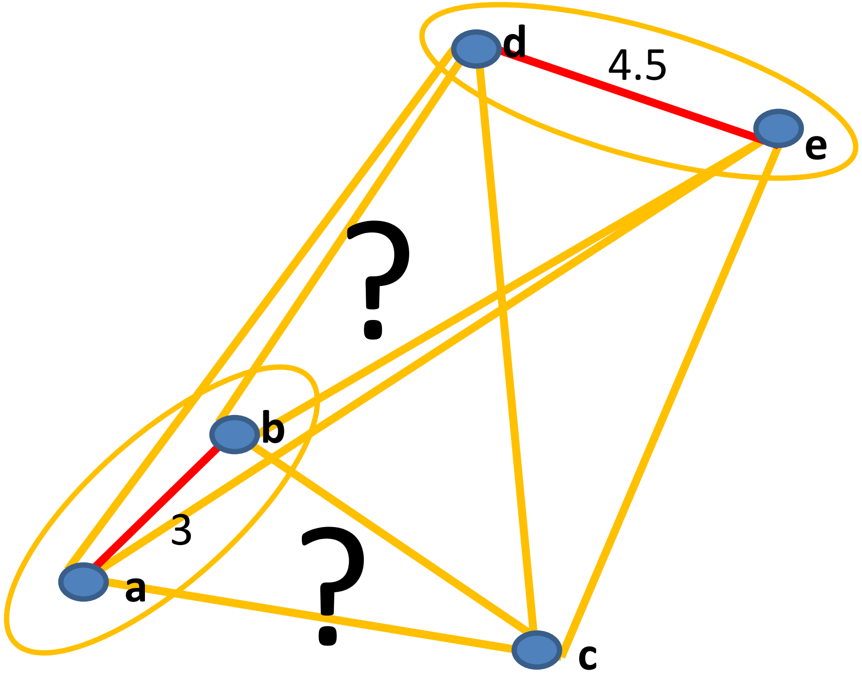

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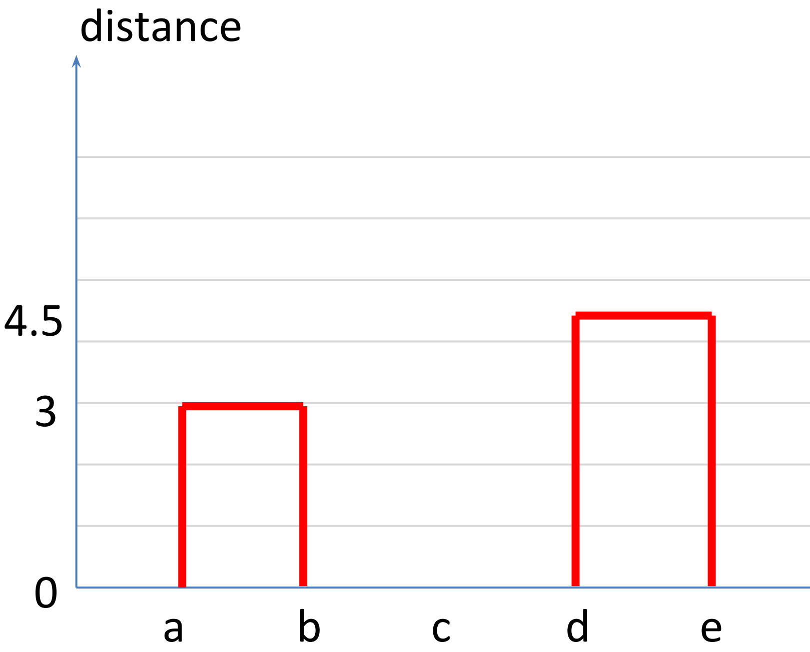

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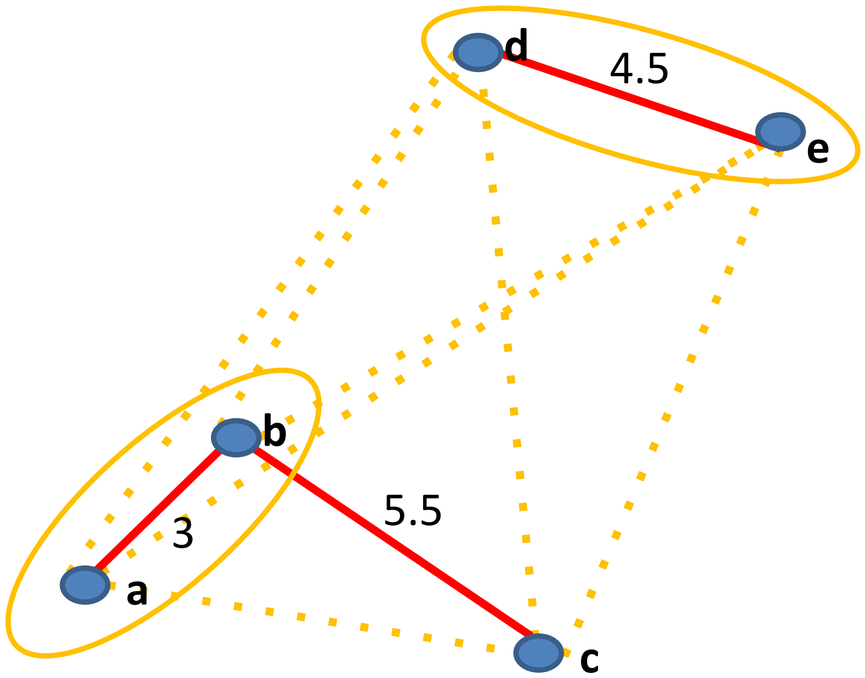

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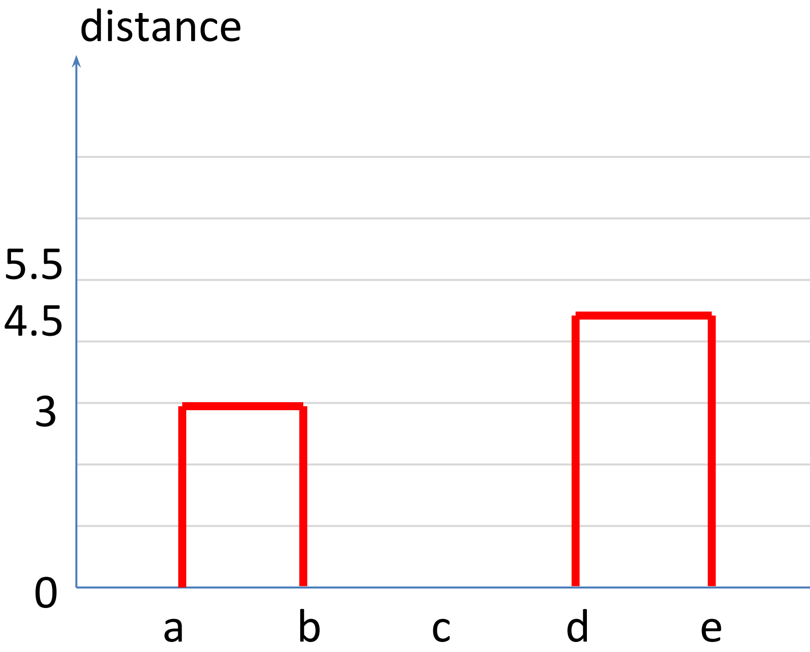

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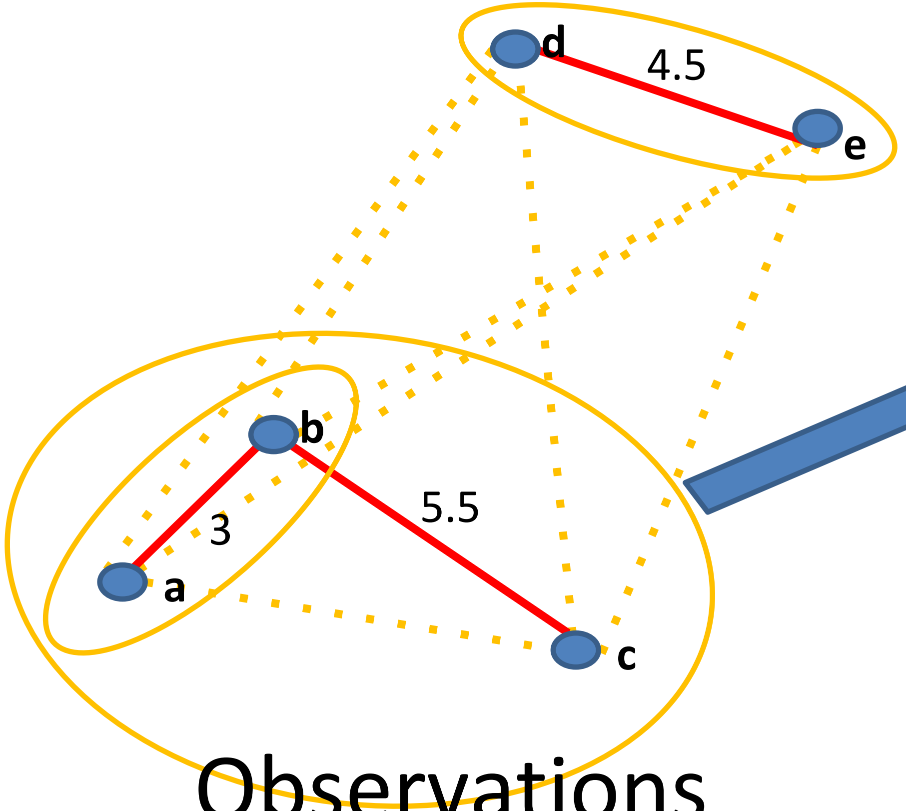

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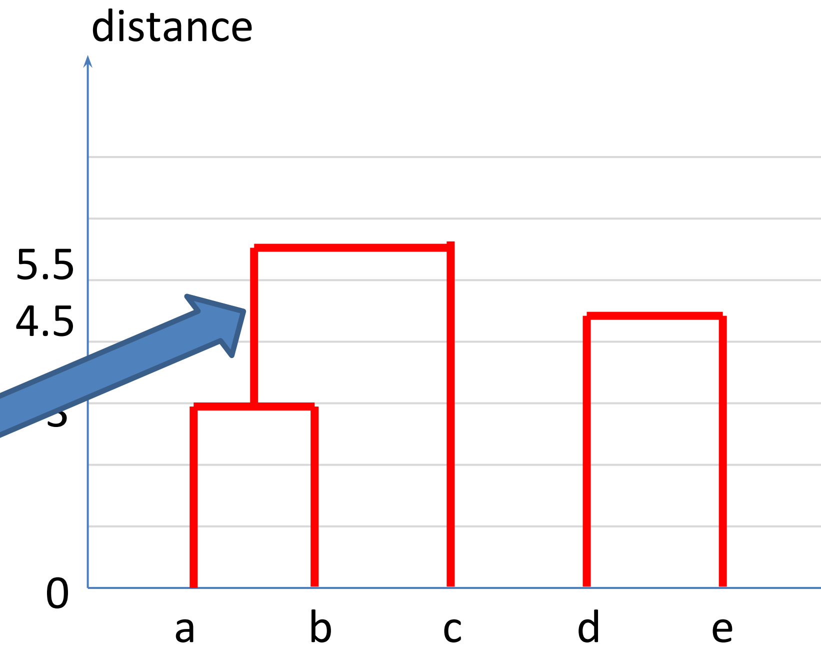

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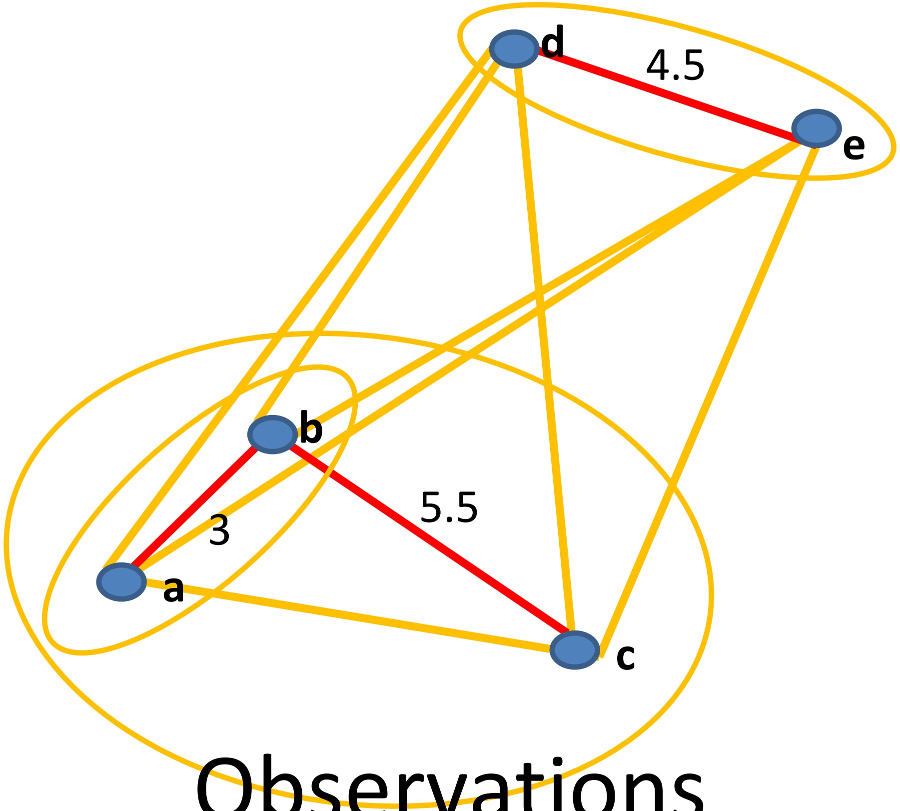

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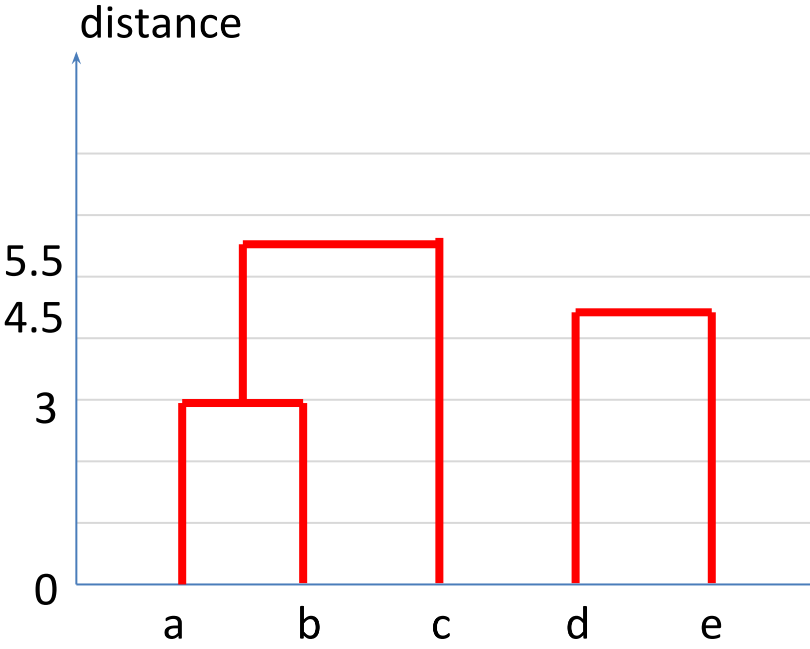

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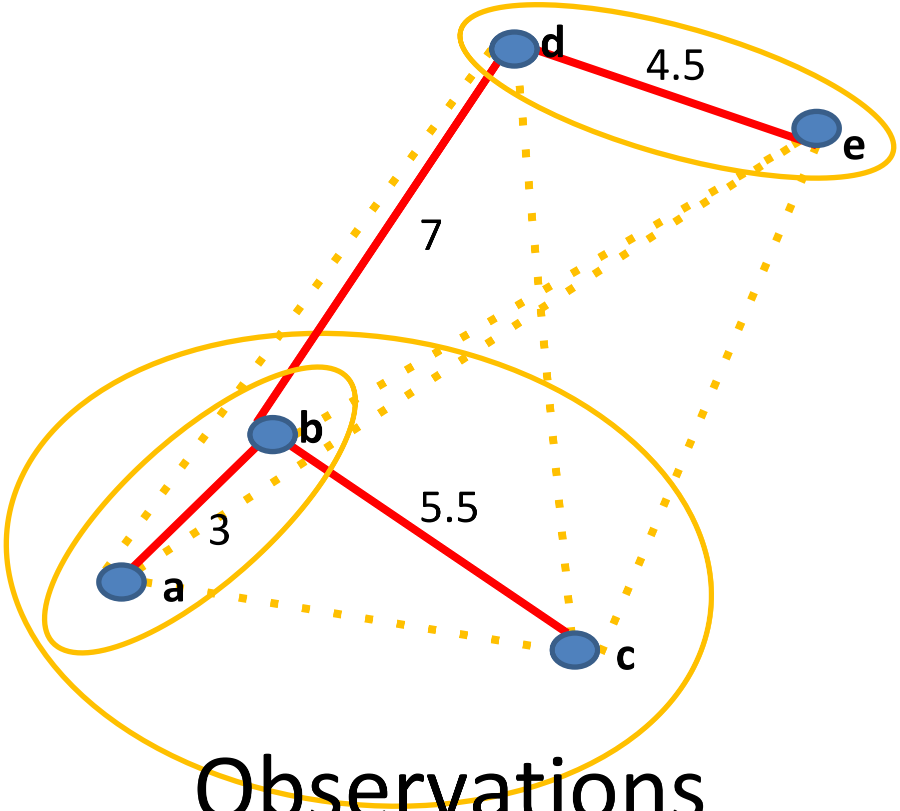

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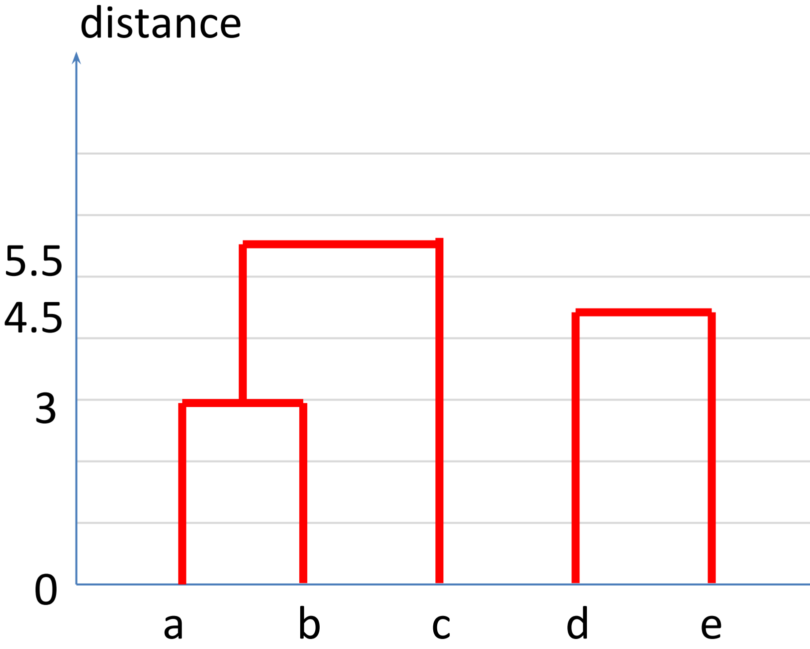

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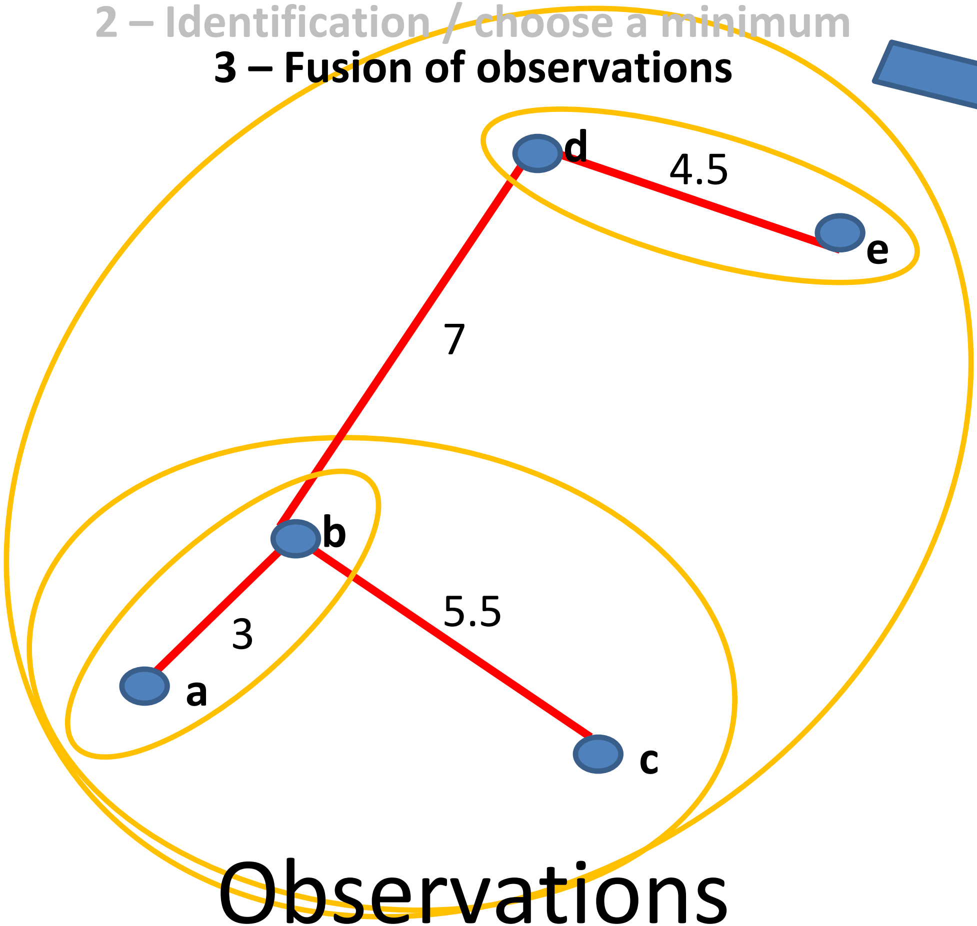

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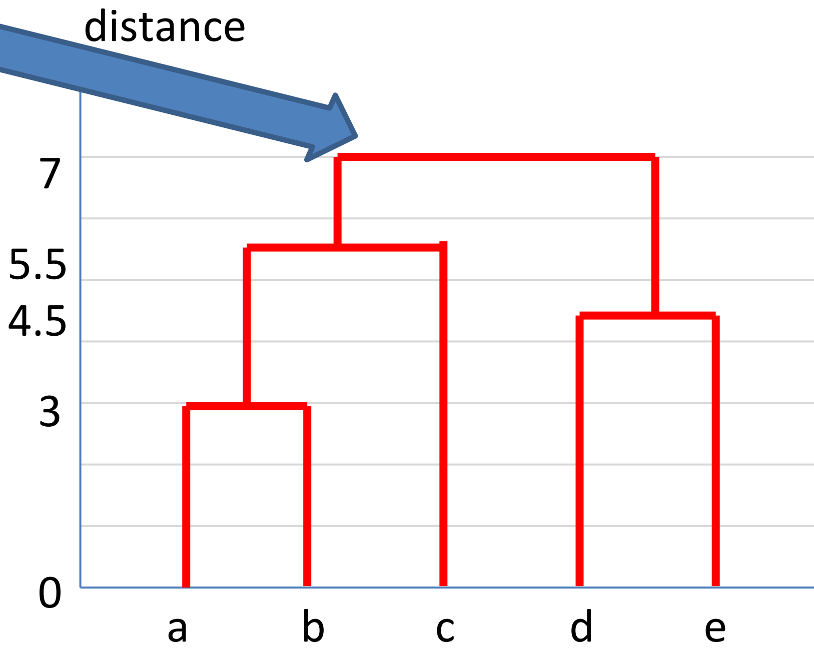
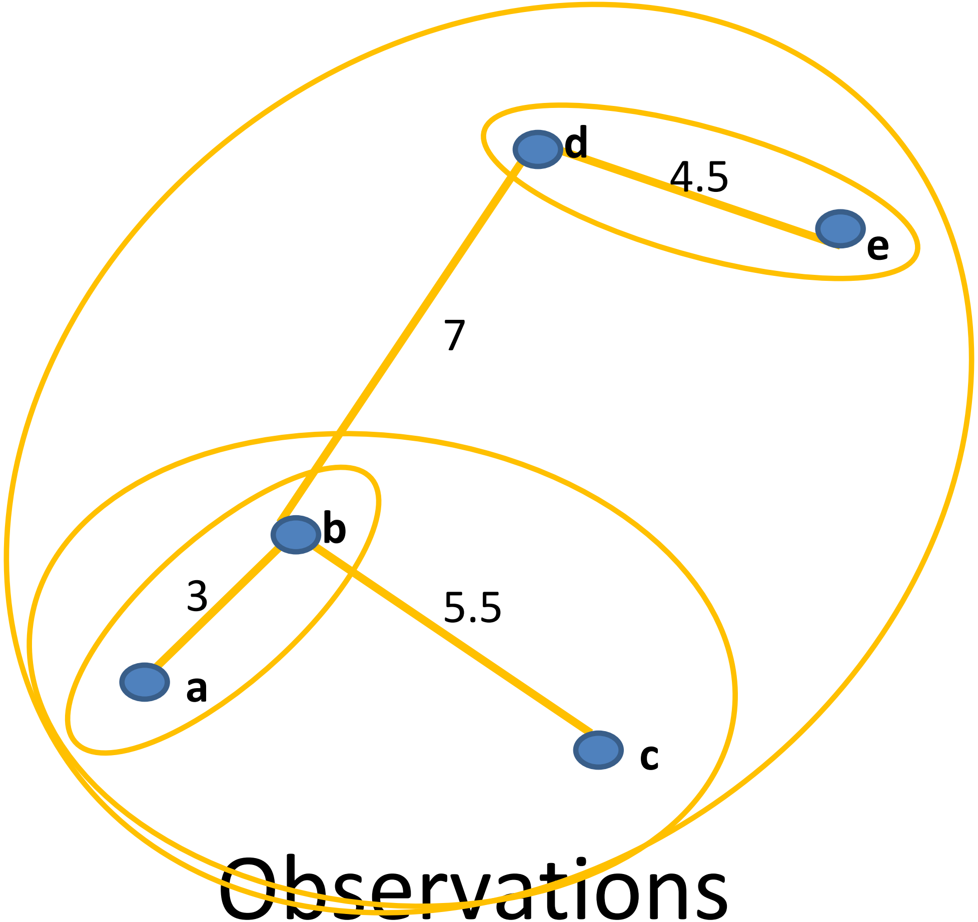


STOP !

Dendrogram



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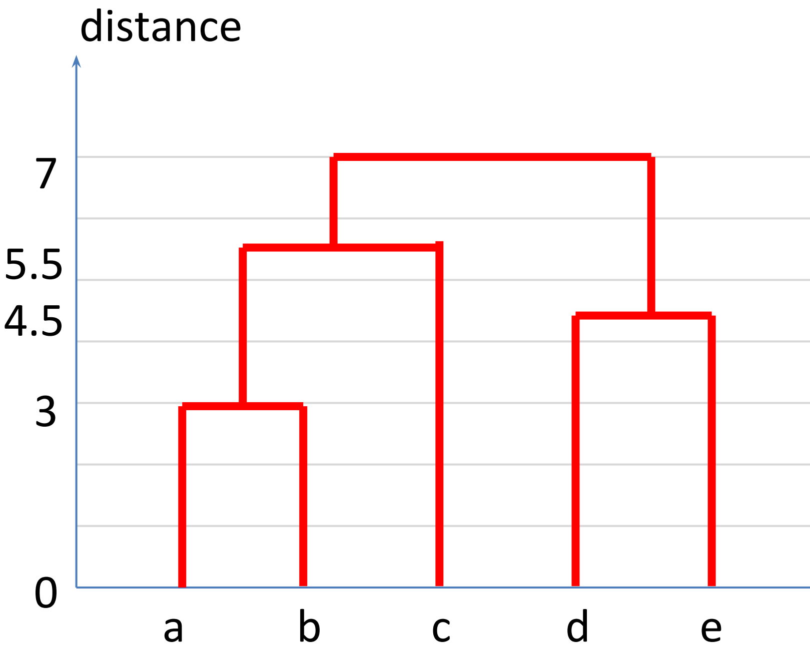


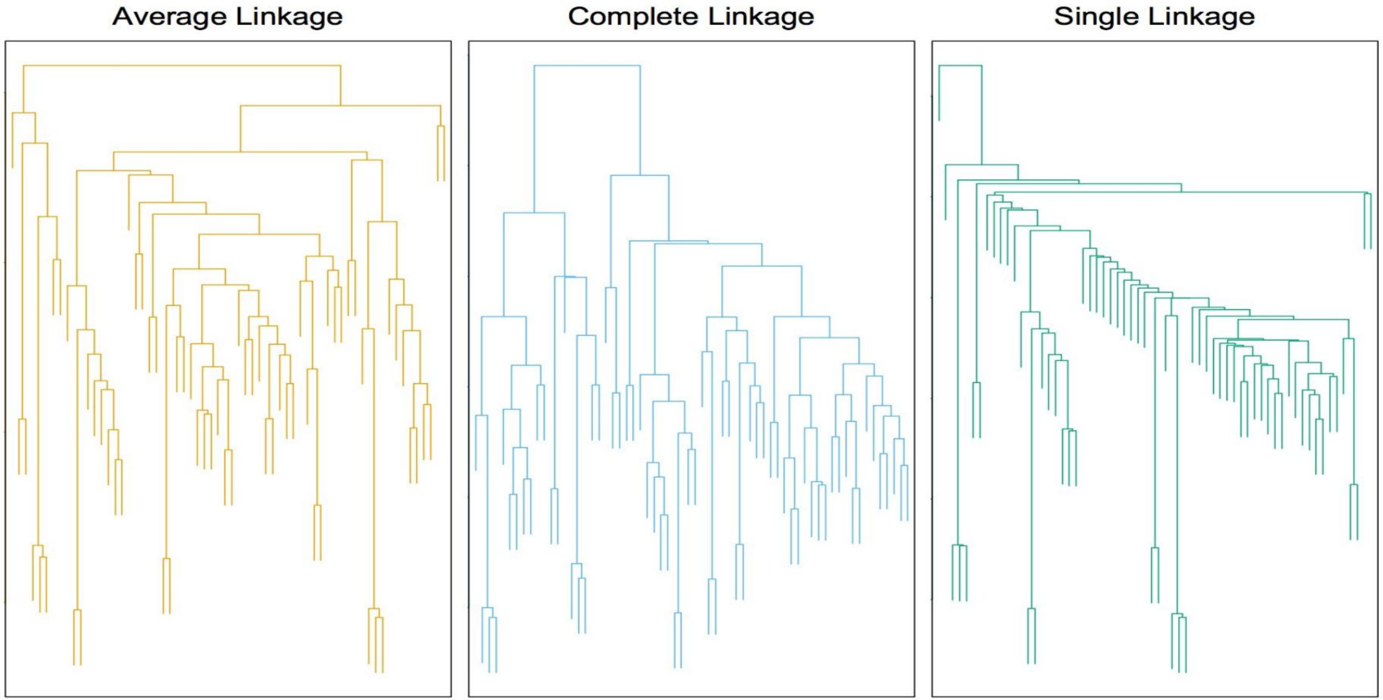
Dendrogram

HAC Linkage

How do we define dissimilarity between clusters?

- **Complete:** Maximum pairwise dissimilarity between points in clusters – good
- **Average:** Average of pairwise dissimilarity between points in clusters – also good
- **Single:** Minimum pairwise dissimilarity between points in clusters – not as good; can lead to long narrow clusters

Linkage on Dendrograms



- Not too sensitive to outliers
- Compromise between complete linkage and single

- More sensitive to outliers
- May violate “closeness”

- Less sensitive to outliers
- Handles irregular shapes fairly naturally

Metrics / Distances / Similarities

Metrics

Distance

$$d : X \times X \to [0, \infty),$$

1. $d(x, y) \geq 0$ non-negativity or separation axiom
2. $d(x, y) = 0 \Leftrightarrow x = y$ identity of indiscernibles
3. $d(x, y) = d(y, x)$ symmetry
4. $d(x, z) \leq d(x, y) + d(y, z)$ subadditivity or triangle inequality

Similarity Measure [Tversky]

Increases with the quantity of common features between A and B
Decreases with the quantity of features that are specific to A, specific to B

How would you measure the similarity between...

- Vectors in an data array
- TFIDF vectors
- Sets (Bags / Transactions)
- Time series
- Strings
- Trees
- Images
- ...

Similarity between… TFIDF vectors

- Occurences / tfidf
- Only positive values

- Cosine Similarity

$$\frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = \frac{\sum_{i=1}^{n} A_i B_i}{\sqrt{\sum_{i=1}^{n} A_i^2} \sqrt{\sum_{i=1}^{n} B_i^2}}$$

Similarity between… sets

- Tverksy Index

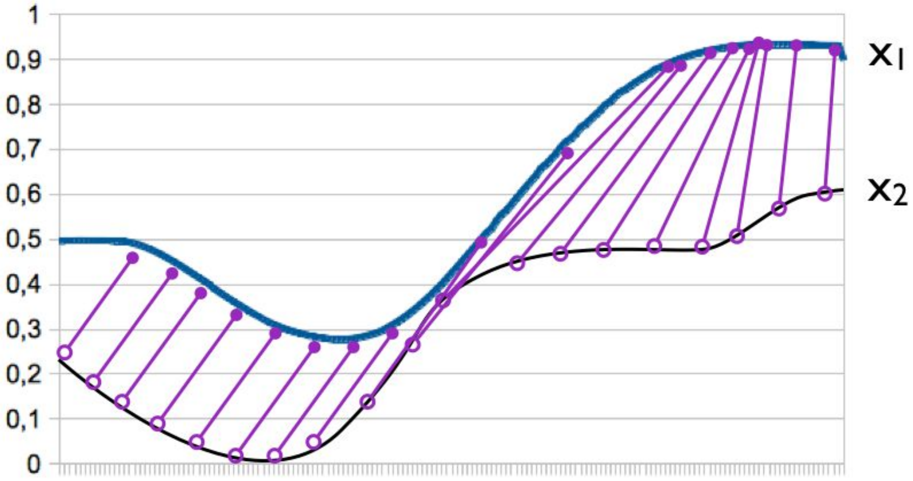
$$S(X,Y) = \frac{|X \cap Y|}{|X \cap Y| + \alpha|X - Y| + \beta|Y - X|}$$

- Jaccard Measure

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}.$$

Similarity between… time series

- Dynamic Time Warp



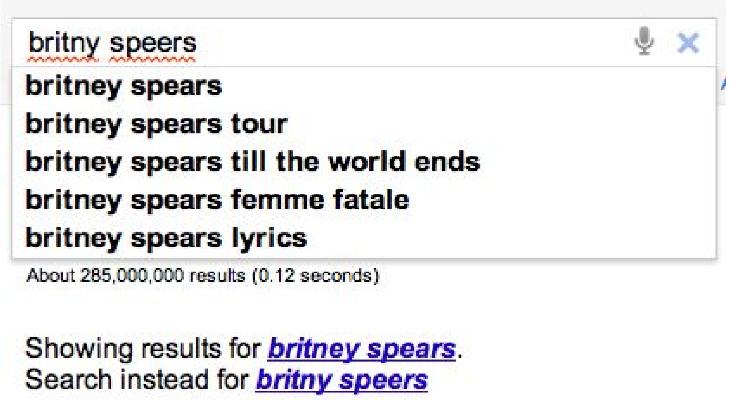
[source]

Similarity between… strings

488941	britney spears
40134	brittany spears
36315	brittney spears
24342	britany spears
7331	britny spears
6633	briteny spears
2696	britteny spears
1807	briney spears
1635	brittny spears

...

[source]

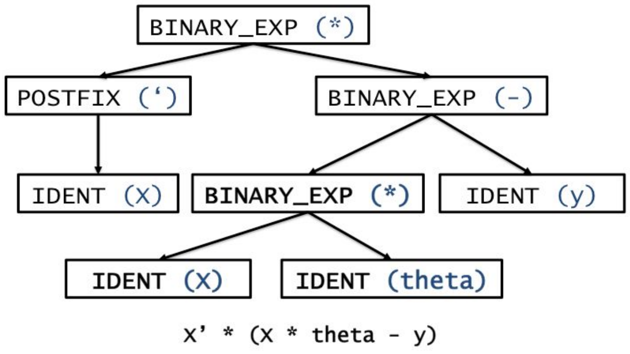


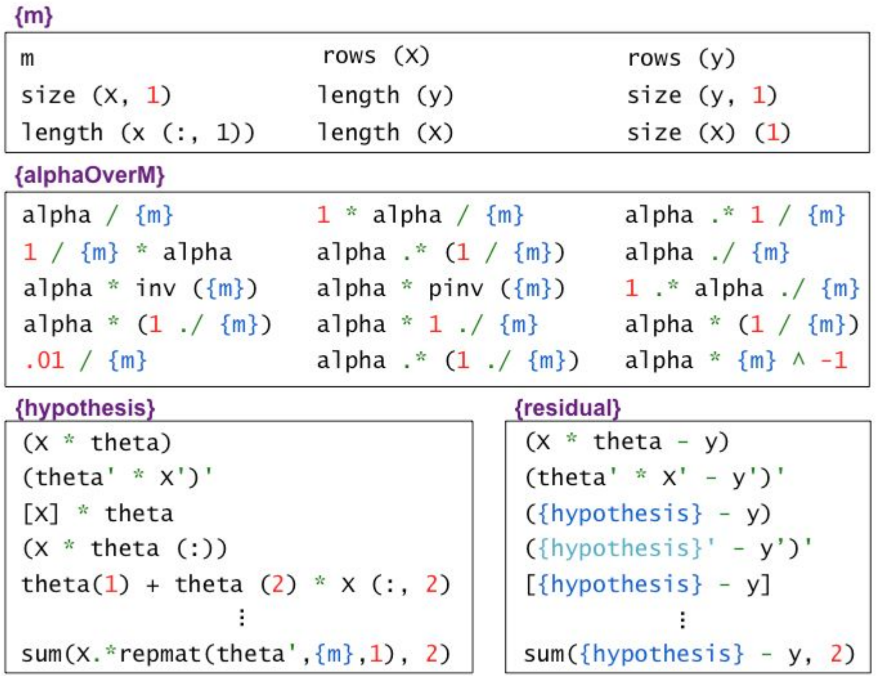
[source]

=> EDIT DISTANCE
How many editions (add/sub/switch) are needed at the least to transform one string into another ?

! Can be applied to sequences of clicks

Similarity between… trees





[J. Huang source]

Similarity between… images

Create image signatures / feature vectors: color / texture / shape features

Semantic Gap : distortion between feature distance and cognitive distance

Curse of Dimensionality

(see notebook)

Pair Assignment