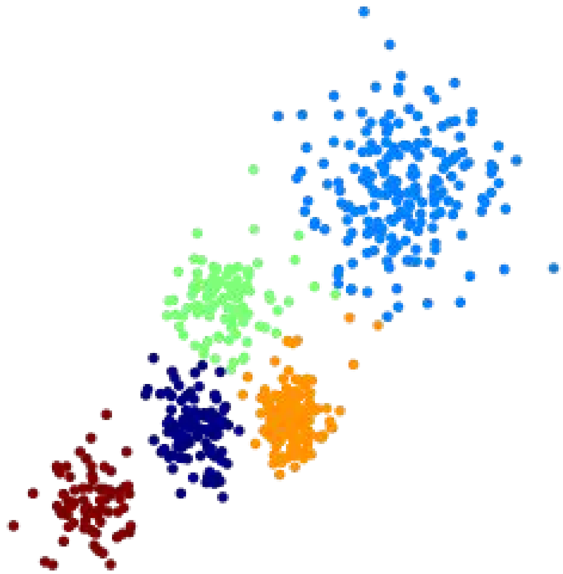
# Clustering

## K-means
## & hierarchical clustering

DSI SEA, jf.omhover, Oct 10 2016



# Clustering

## K-means
## & hierarchical clustering

DSI SEA, jf.omhover

## 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"

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

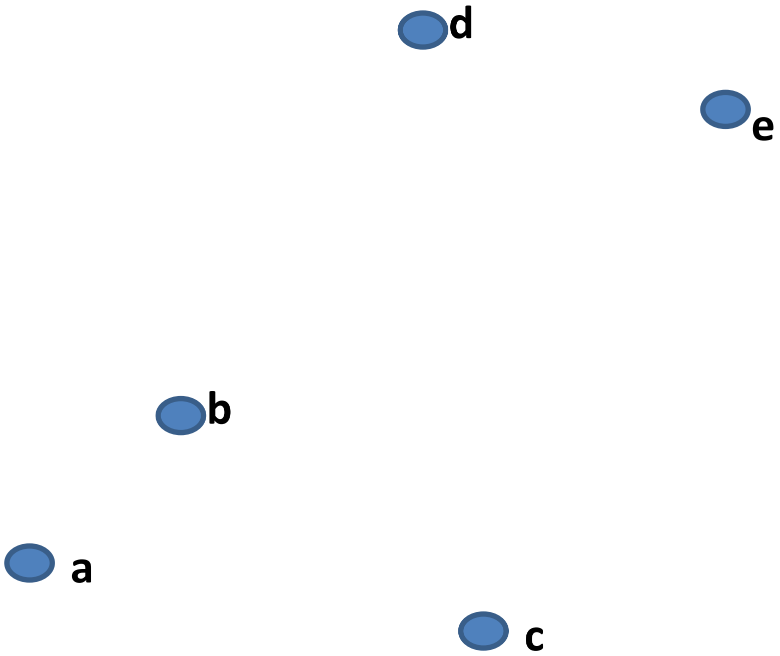
1. Randomly assign a number, from 1 to K, to each of the observations.
2. **Iterate** until the cluster assignments stop changing:
   a. For each of the K clusters, compute the cluster ***centroid***: the vector of the *p* features **means** for the observations in the k-th cluster
   b. **Assign** each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

**K-Means in a nutshell :**

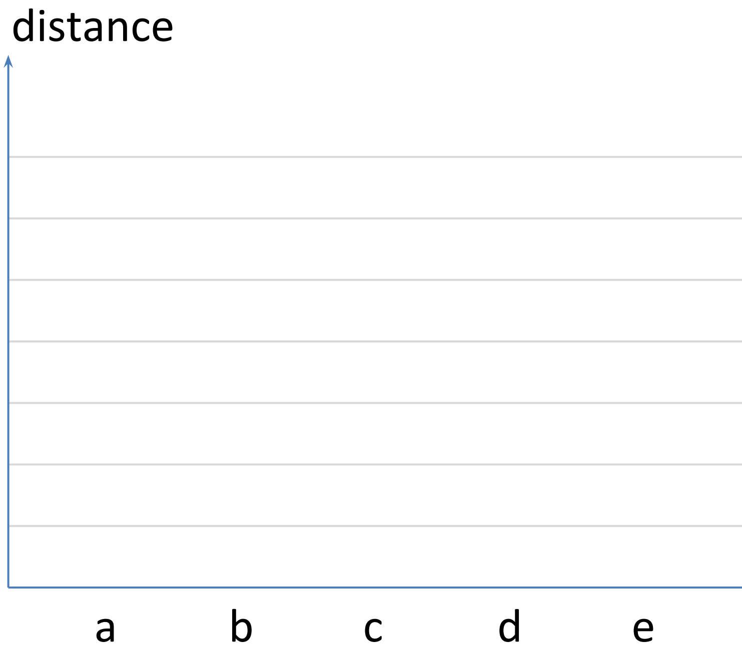
- **Computing distances**
- **Computing means**

# Hierarchical Clustering (step by step)

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

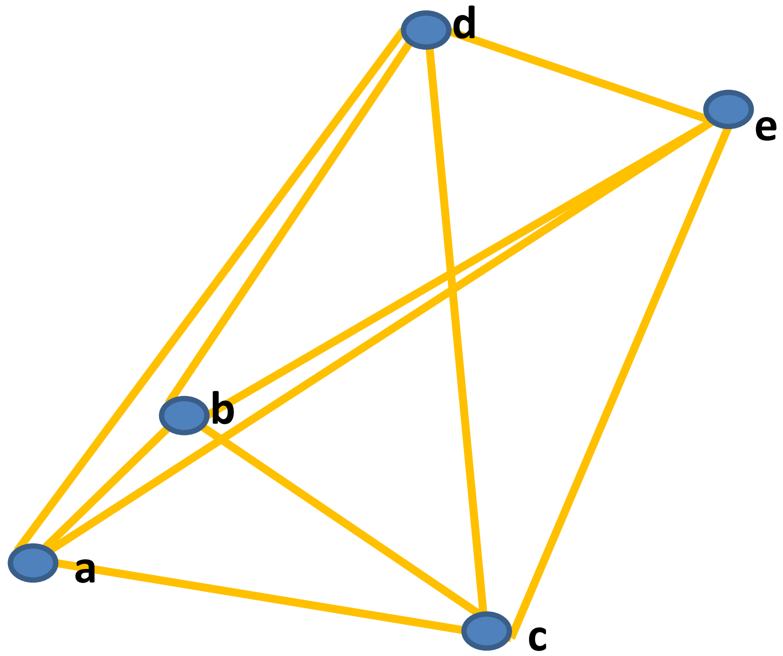



Observations

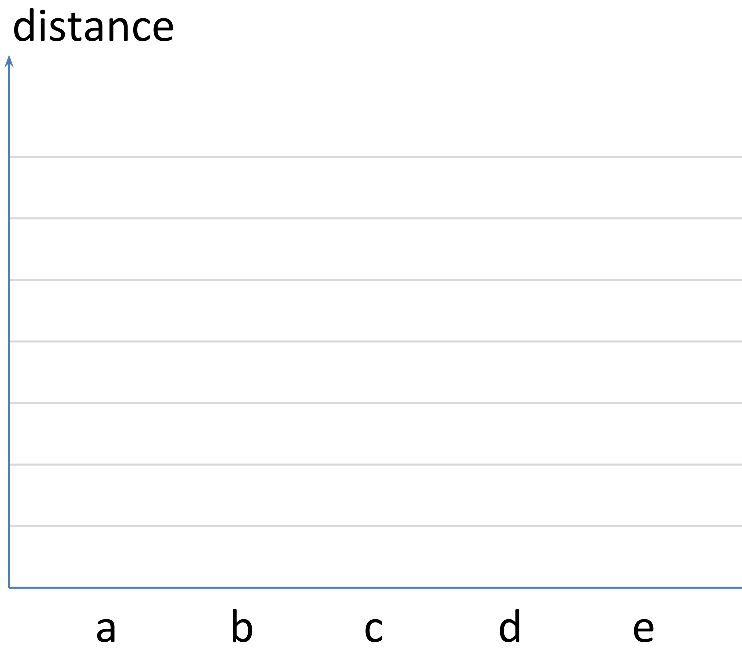



Dendrogram

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

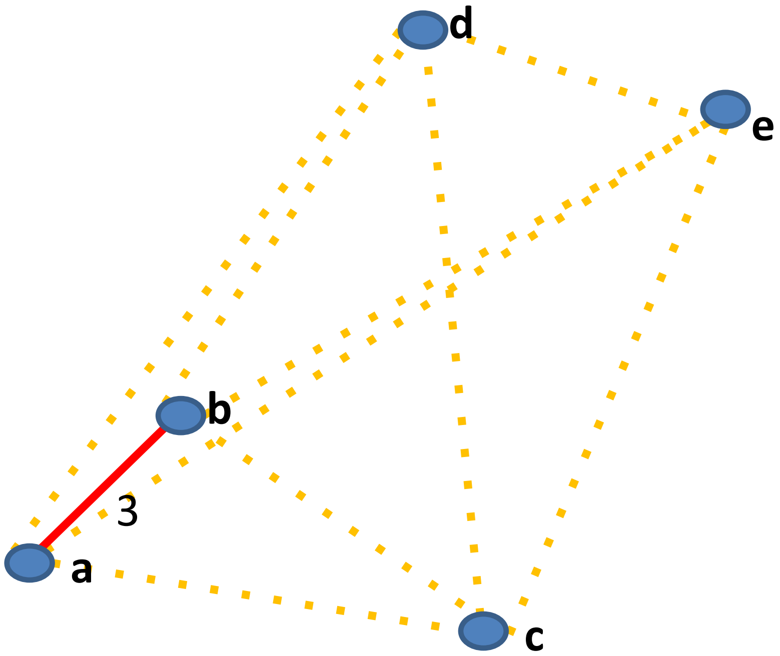



Observations

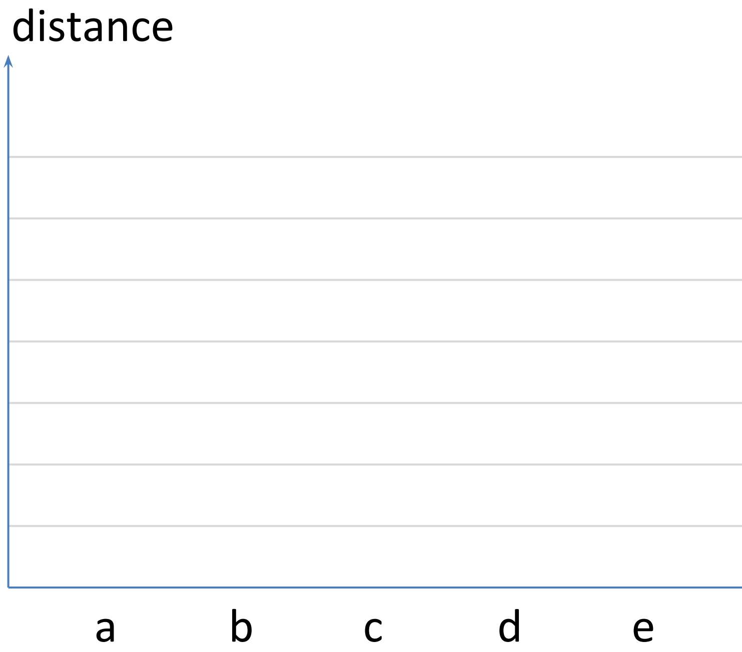



Dendrogram

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

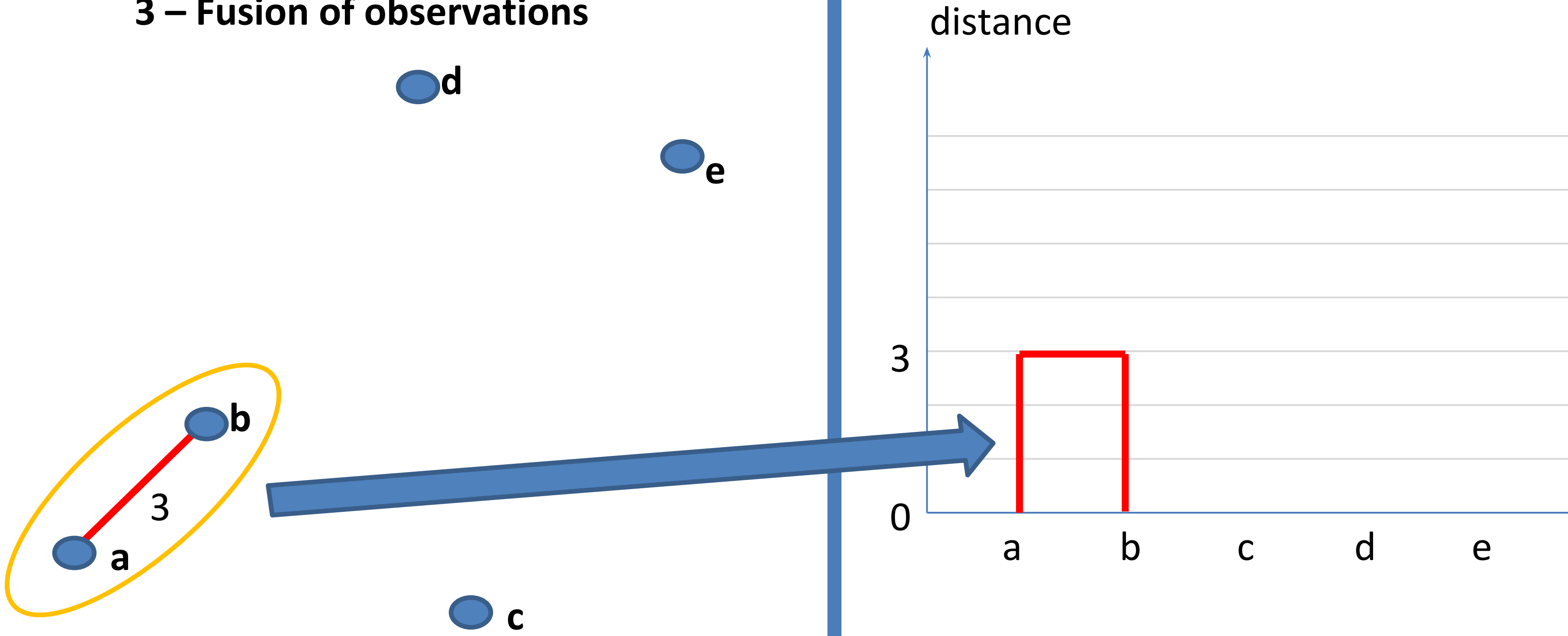



Observations




Dendrogram

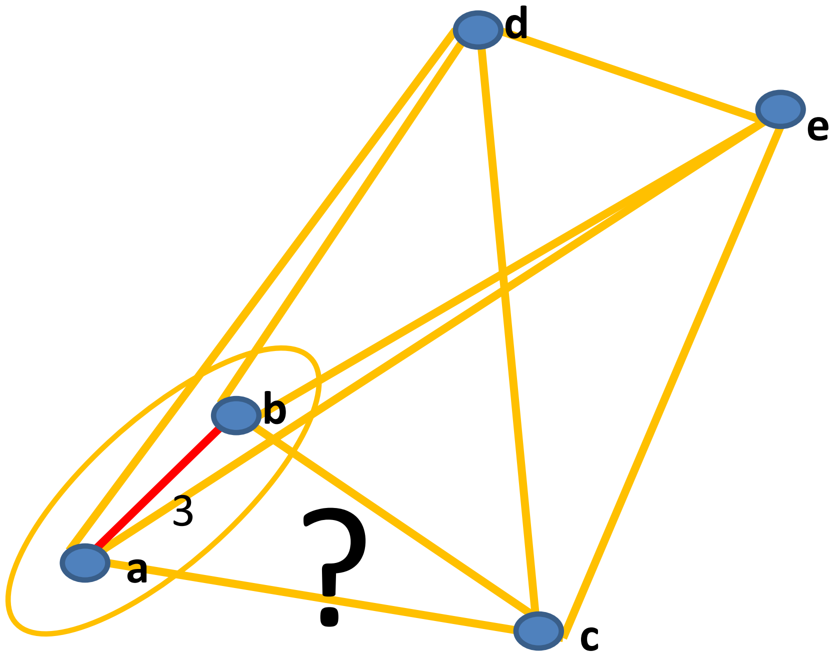
1 - Computing distances between observations
2 – Identification / choose a minimum
**3 – Fusion of observations**



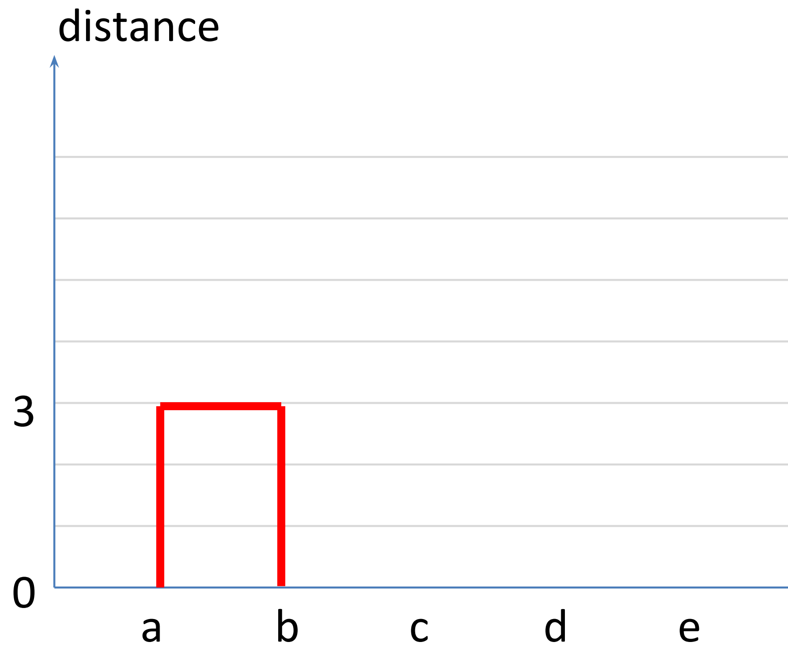

Observations

Dendrogram

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

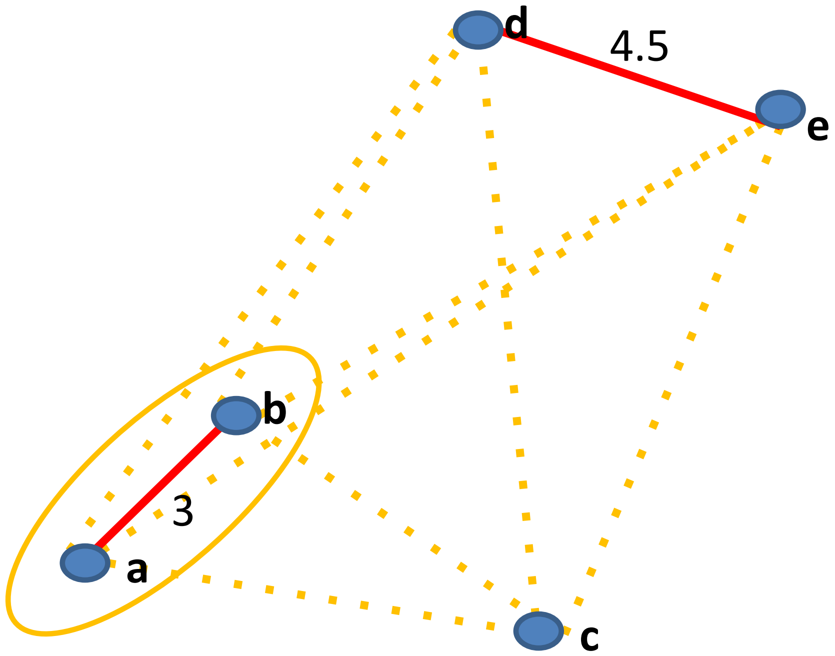



Observations

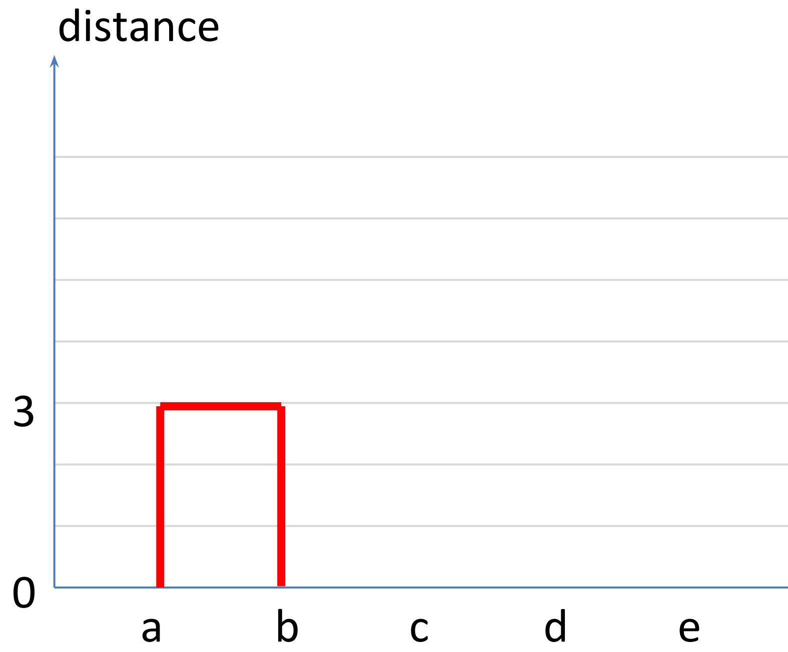



Dendrogram

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

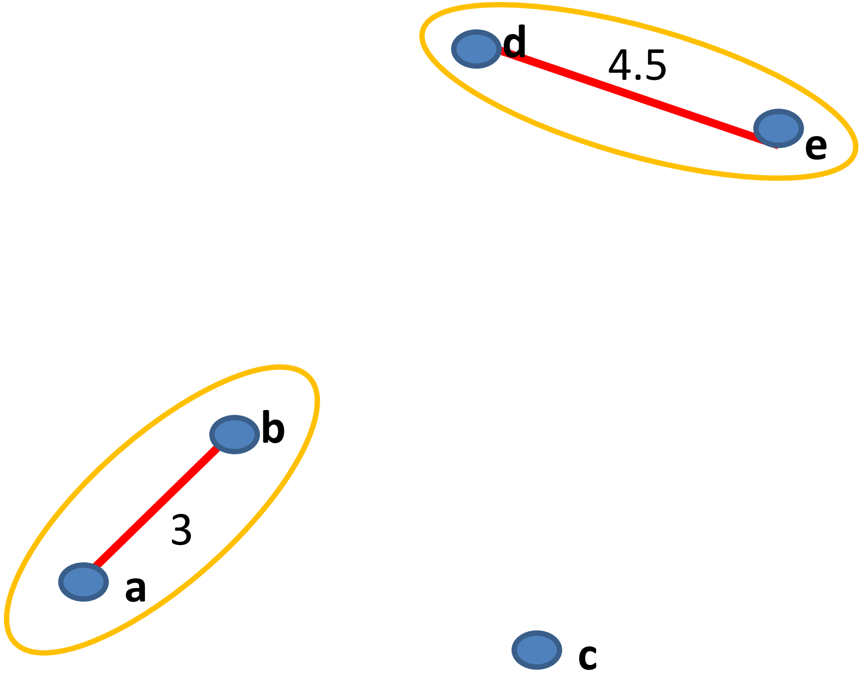



# Observations

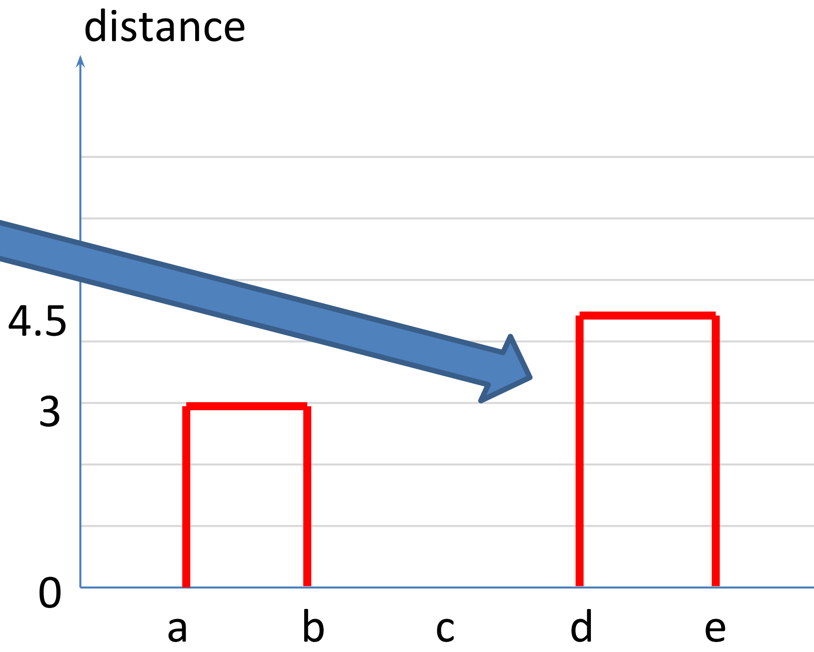



# Dendrogram

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

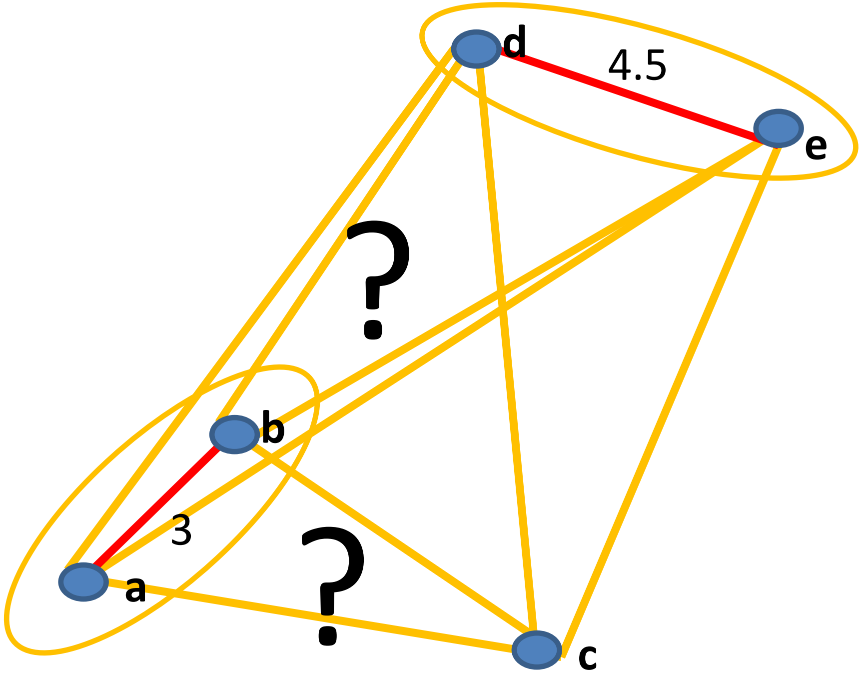



Observations

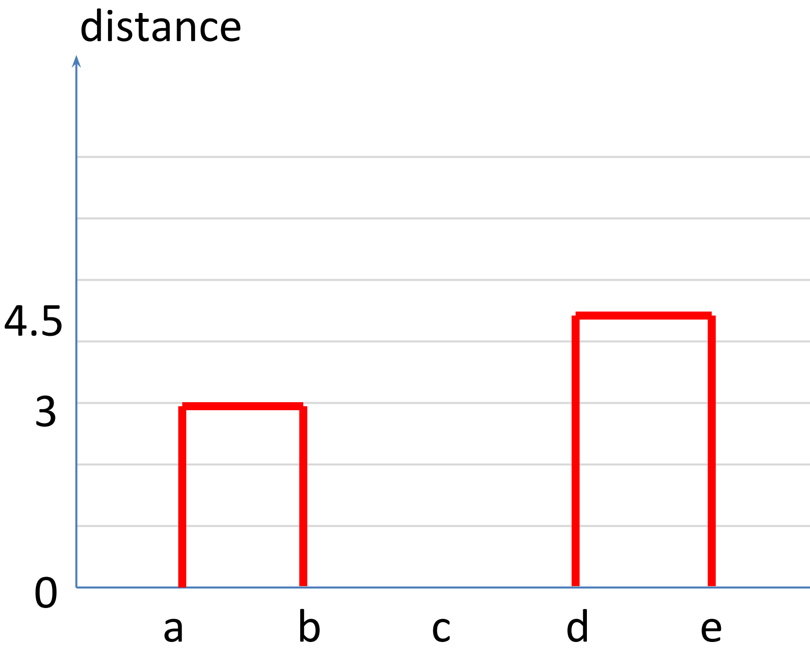



Dendrogram

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

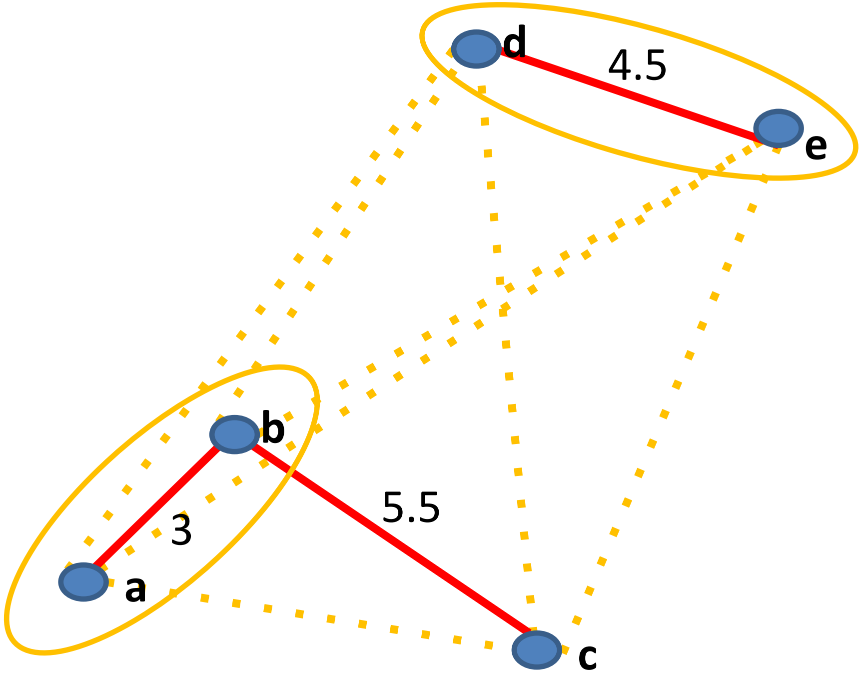



Observations

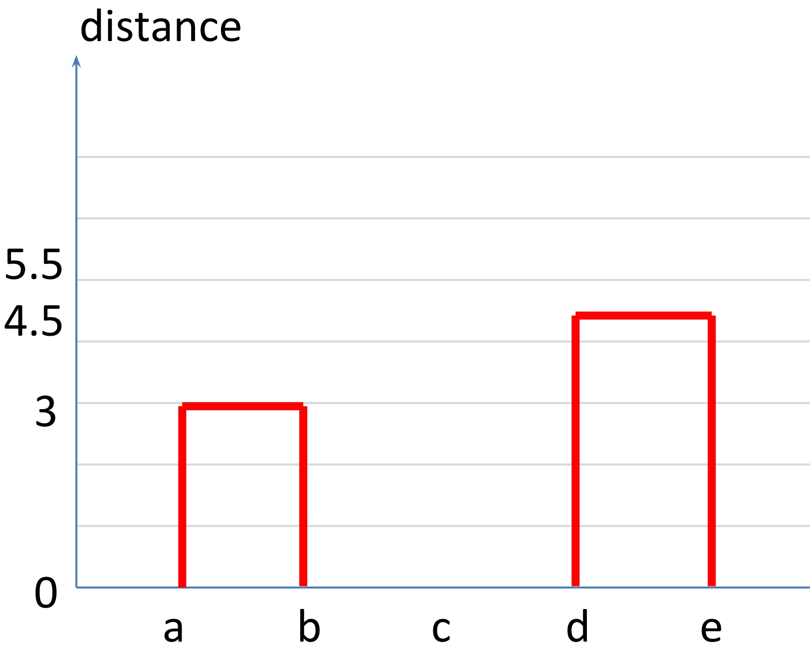



Dendrogram

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

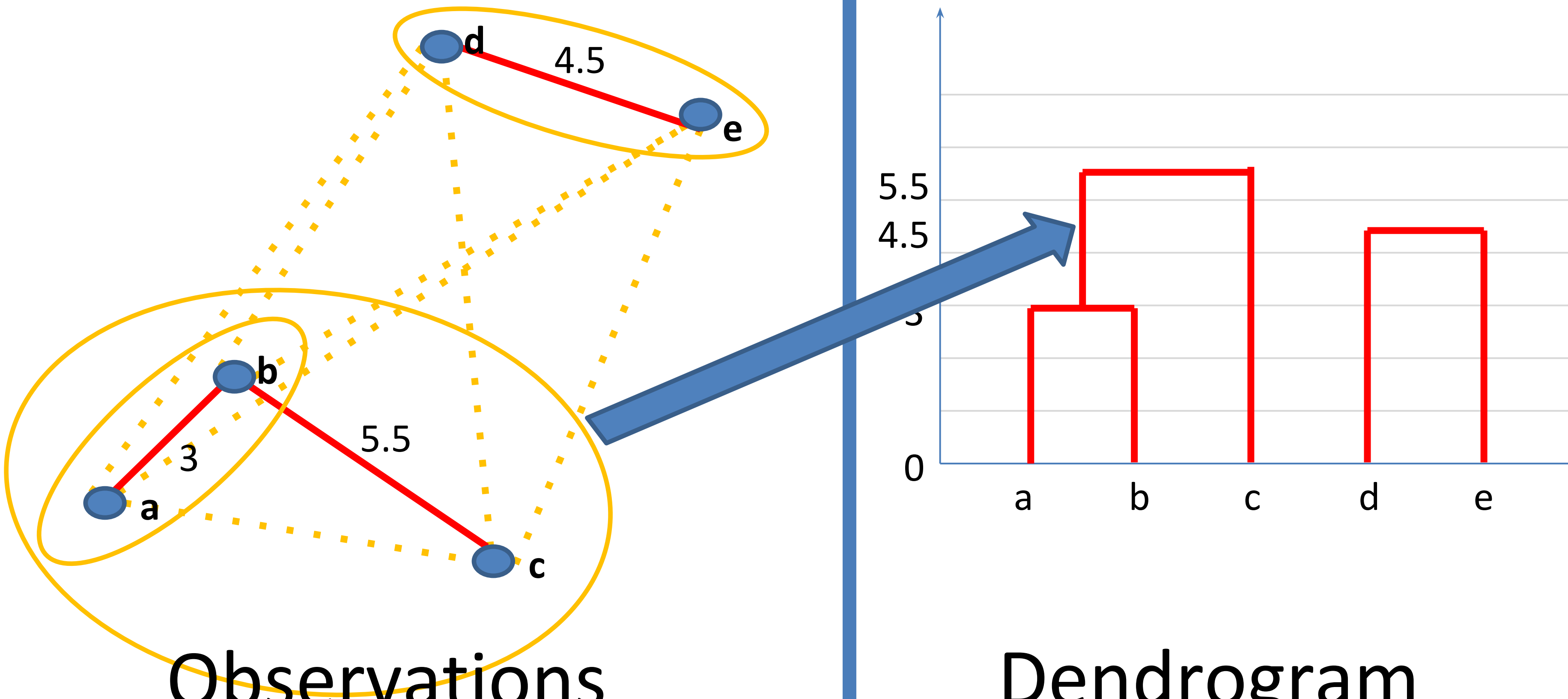



Observations




Dendrogram

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



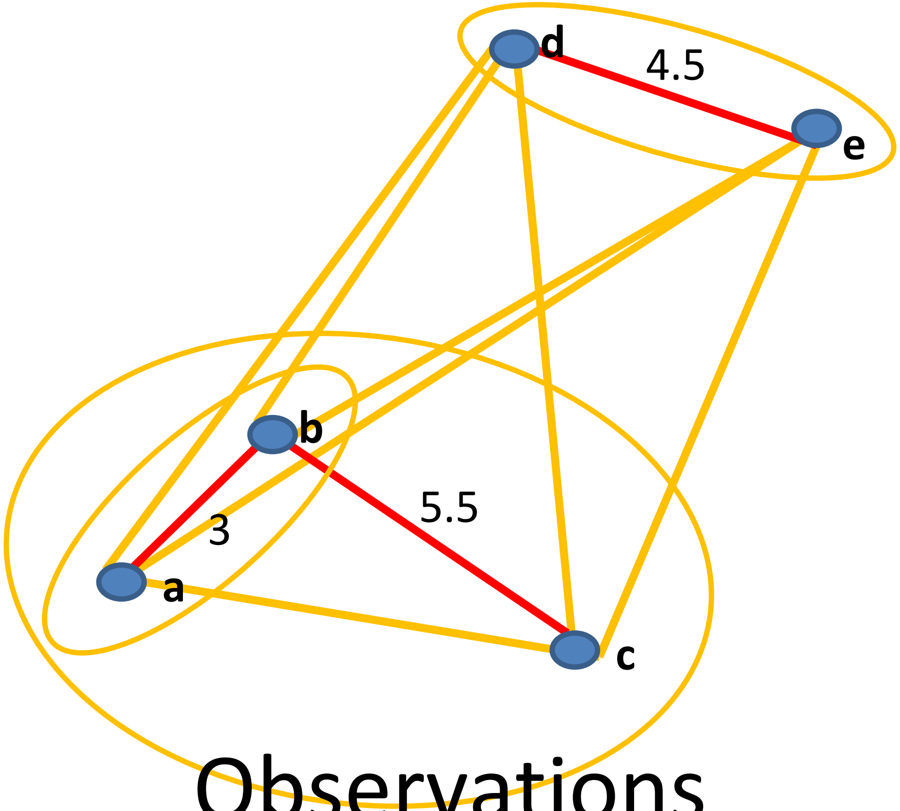

Observations

Dendrogram

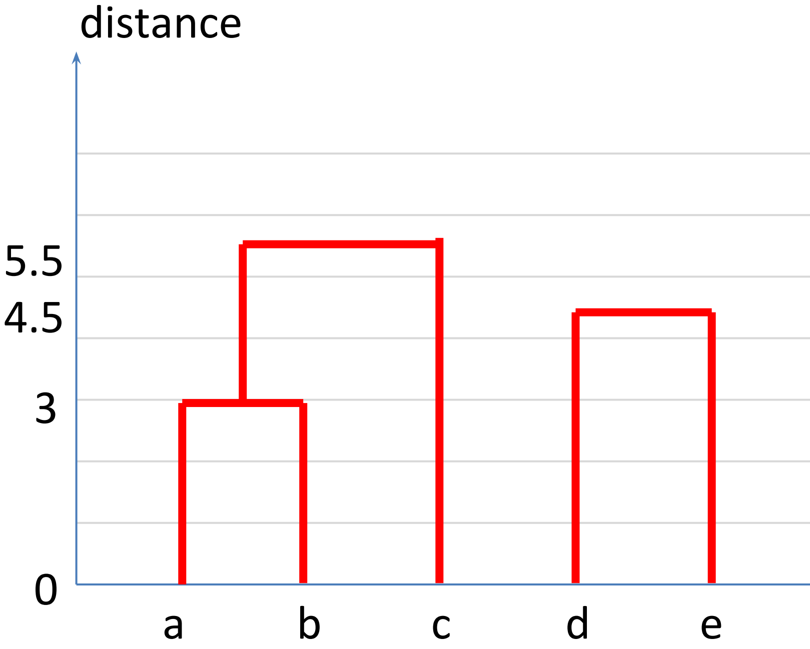
**1 - Computing distances between observations**

2 – Identification / choose a minimum

3 – Fusion of observations




Observations

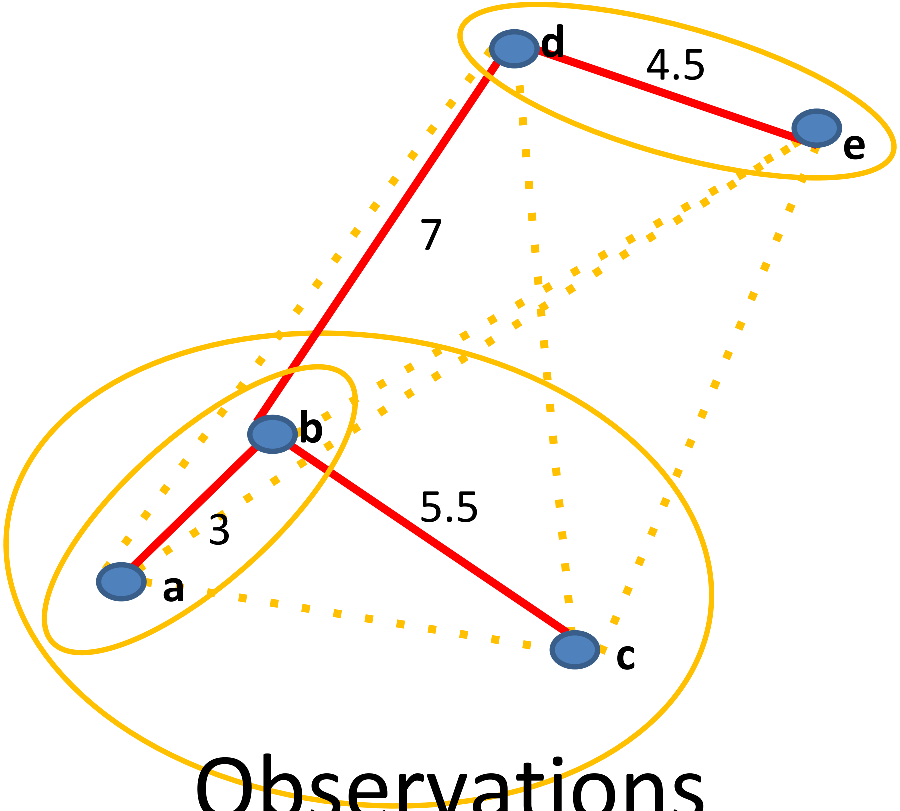



Dendrogram

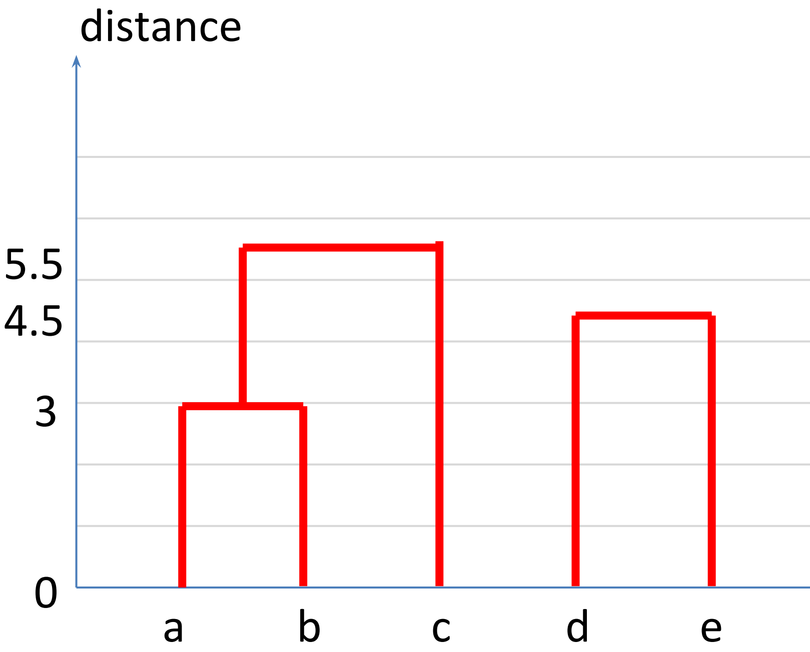
1 - Computing distances between observations

**2 – Identification / choose a minimum**

3 – Fusion of observations




Observations

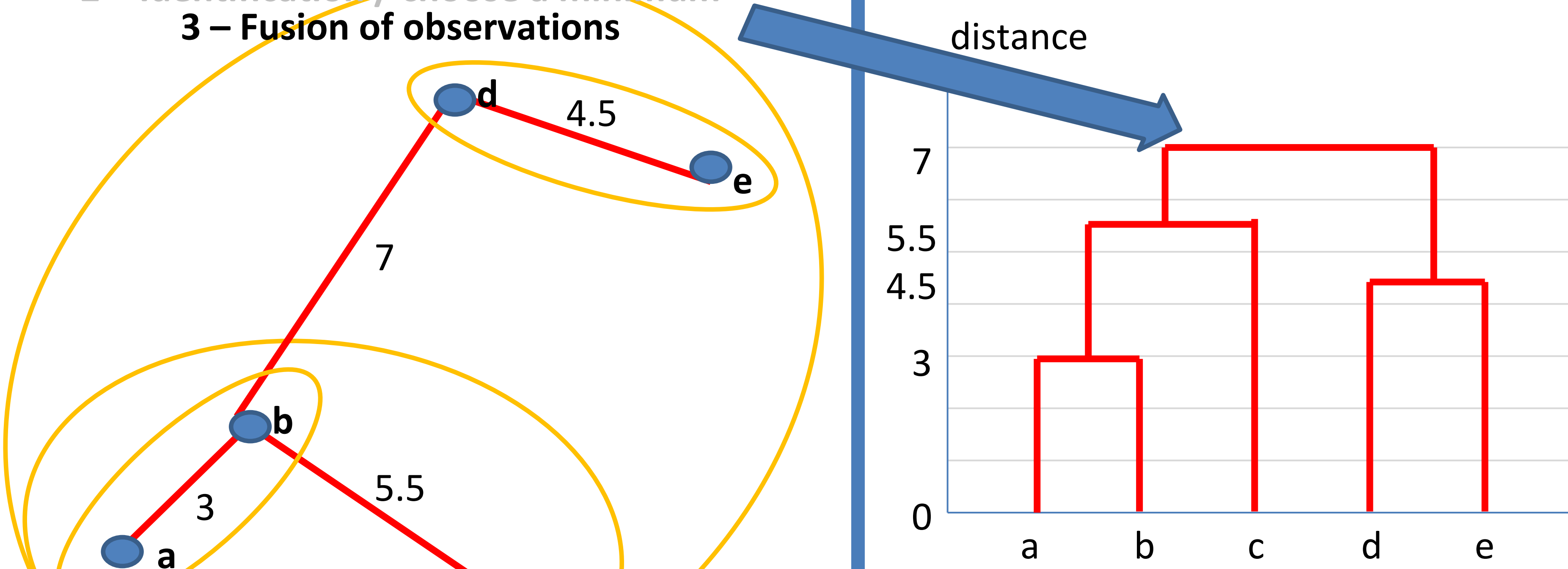



Dendrogram

1 - Computing distances between observations

2 – Identification / choose a minimum

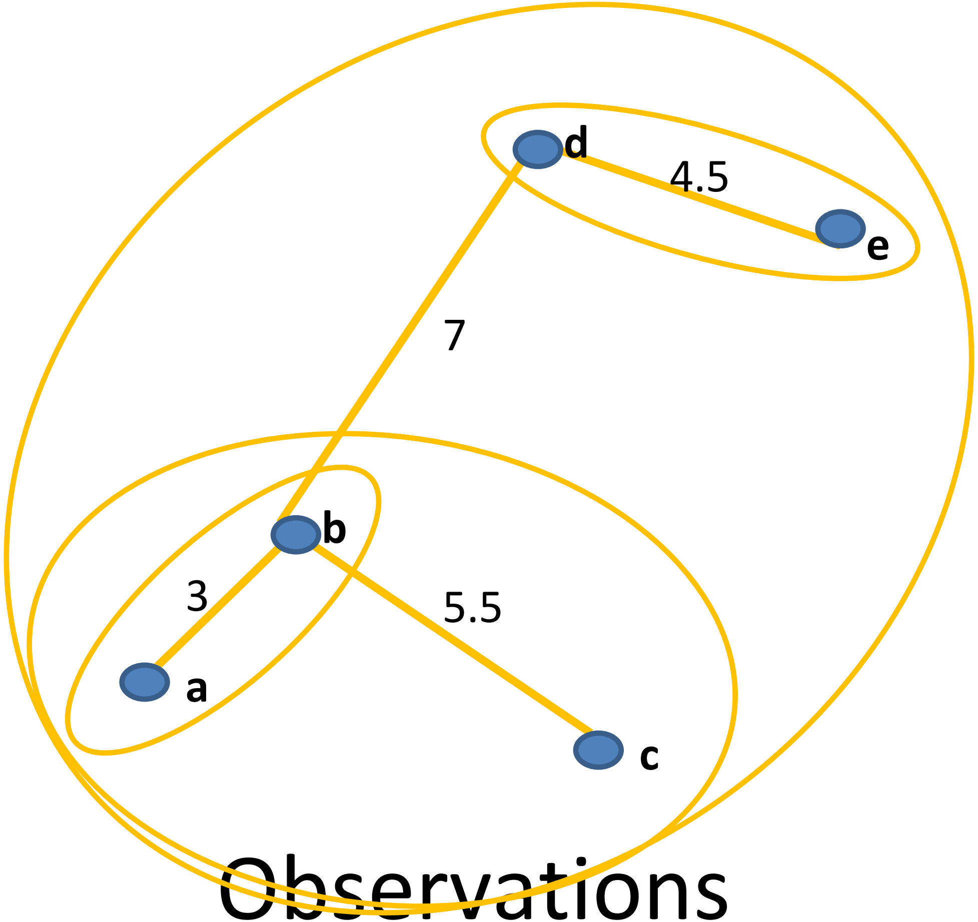
**3 – Fusion of observations**



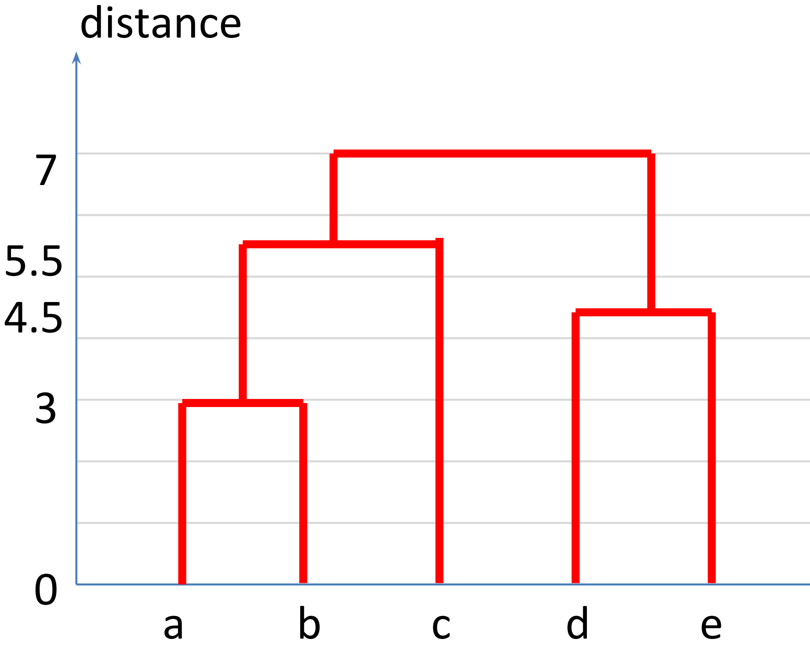

**STOP !**

Observations

Dendrogram




Observations



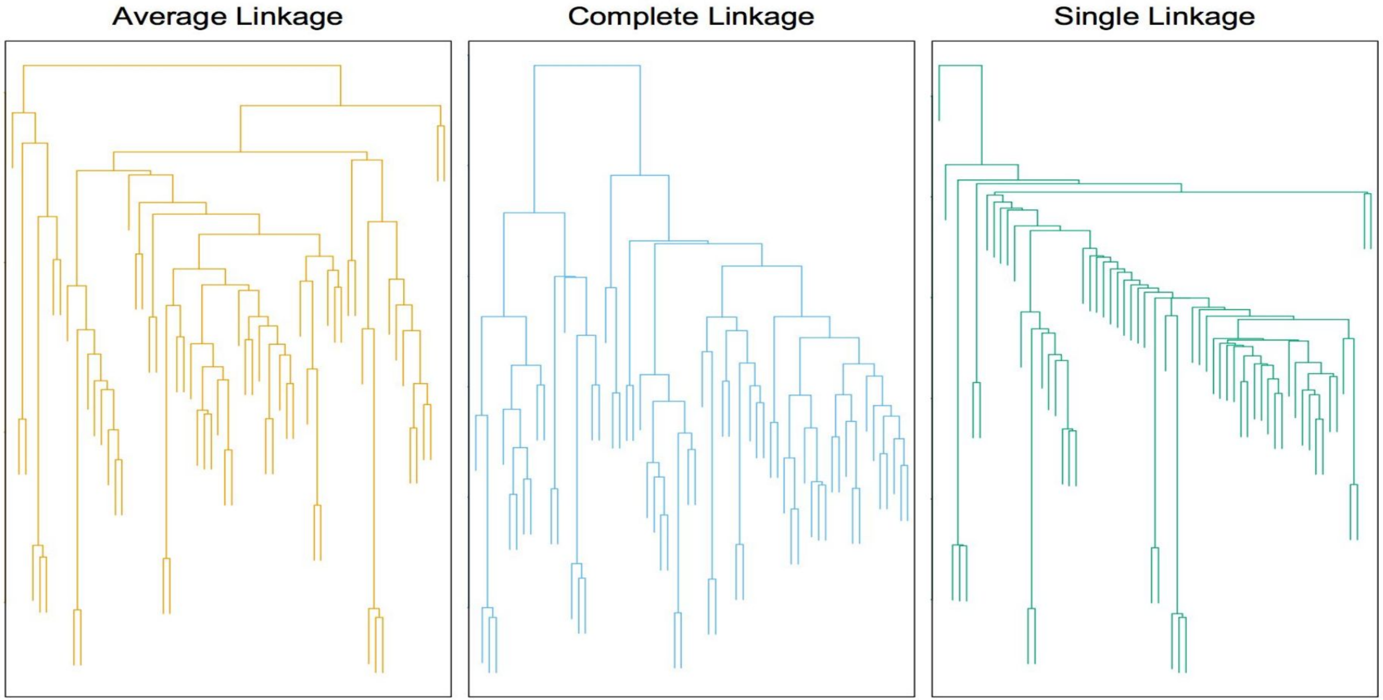

Dendrogram

# 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

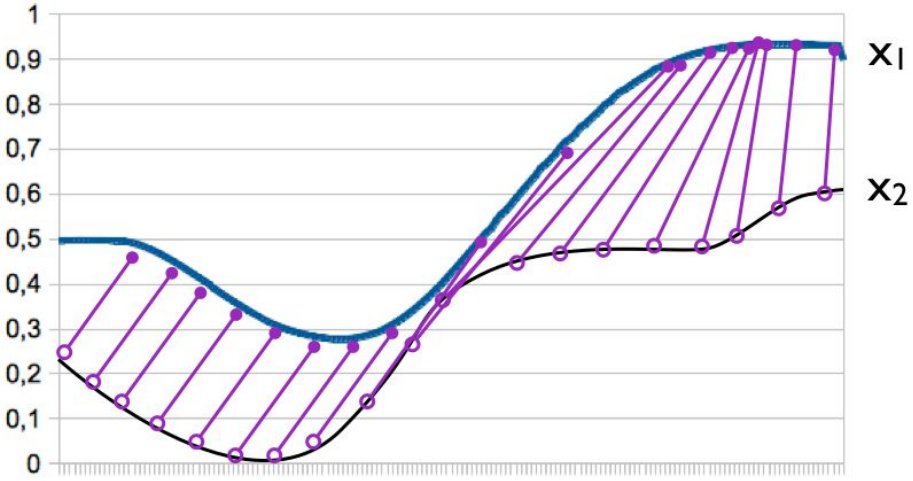
$$S(X,Y) = \frac{|X \cap Y|}{|X \cap Y| + \alpha|X - Y| + \beta|Y - X|}$$

- 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



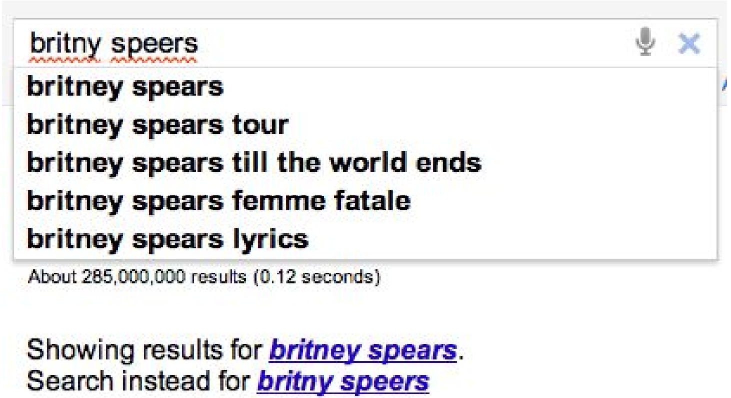

[source]

# 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]

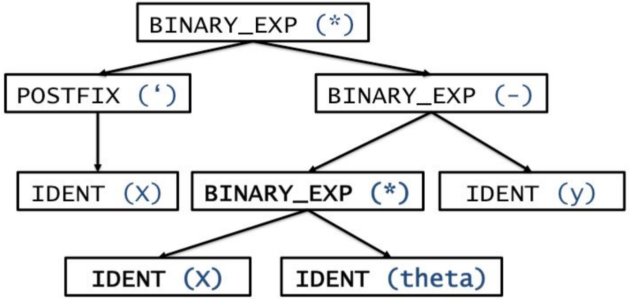



[source]

**=> 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




x' * (x * theta - y)

**{m}**

```
m                     rows (X)        rows (y)
size (X, 1)           length (y)      size (y, 1)
length (x (:, 1))     length (X)      size (X) (1)
```

**{alphaOverM}**

```
alpha / {m}           1 * alpha / {m}        alpha .* 1 / {m}
1 / {m} * alpha       alpha .* (1 / {m})     alpha ./ {m}
alpha * inv ({m})     alpha * pinv ({m})     1 .* alpha ./ {m}
alpha * (1 ./ {m})    alpha * 1 ./ {m}       alpha * (1 / {m})
.01 / {m}             alpha .* (1 ./ {m})    alpha * {m} ^ -1
```

**{hypothesis}**

```
(X * theta)
(theta' * X')'
[X] * theta
(X * theta (:))
theta(1) + theta (2) * X (:, 2)
        ⋮
sum(X.*repmat(theta',{m},1), 2)
```

**{residual}**

```
(X * theta - y)
(theta' * X' - y')'
({hypothesis} - y)
({hypothesis}' - y')'
[{hypothesis} - y]
        ⋮
sum({hypothesis} - y, 2)
```

[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