Aggregation Criteria

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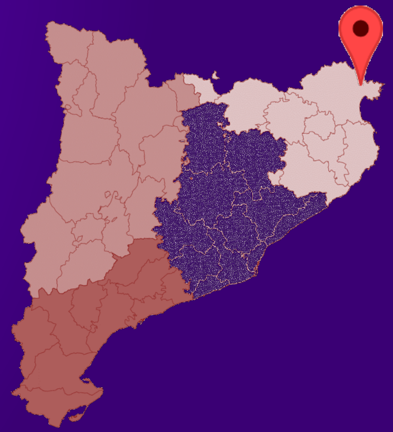
Figuerenca



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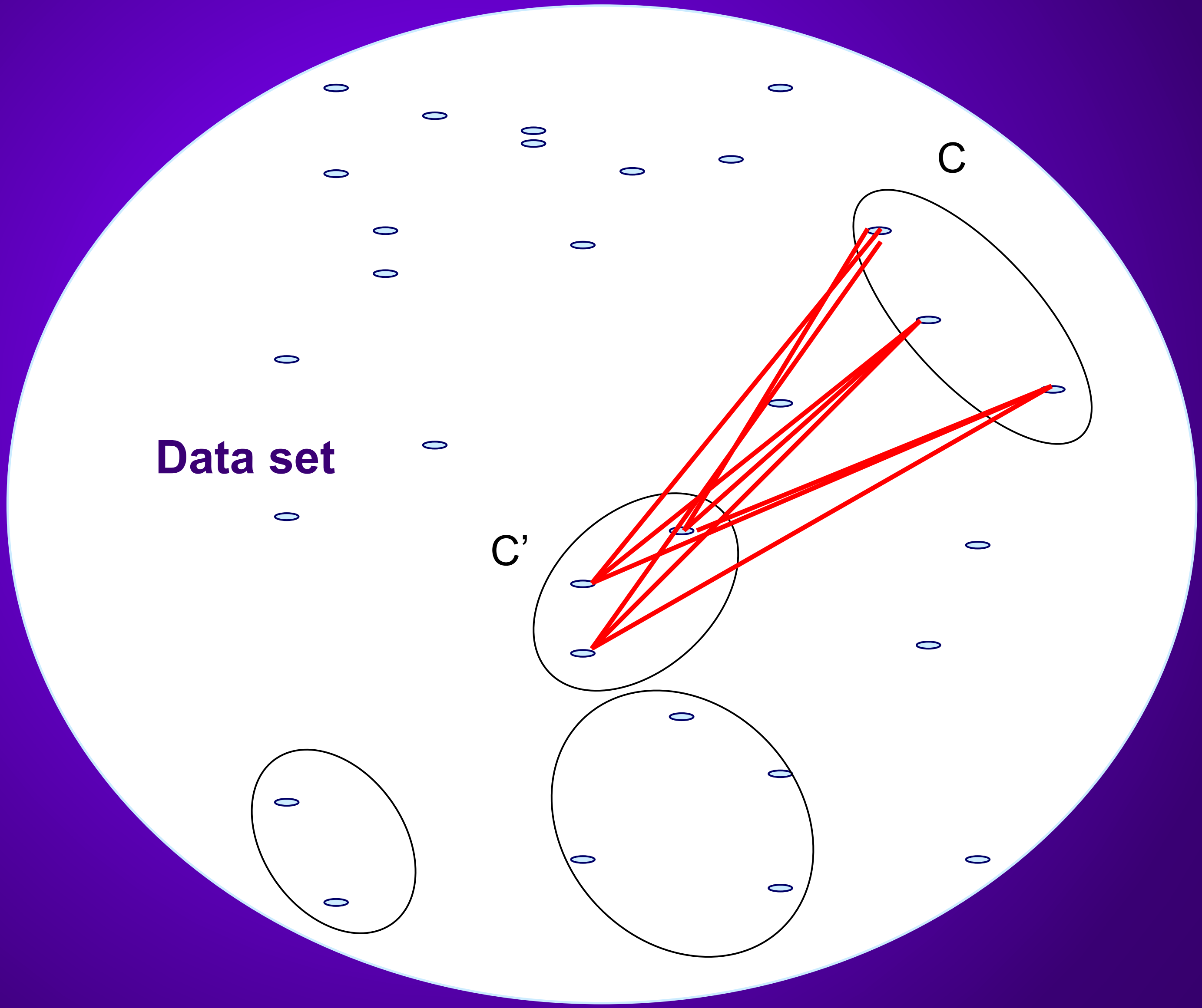
Ascendant hierarchical clustering

Hot points :

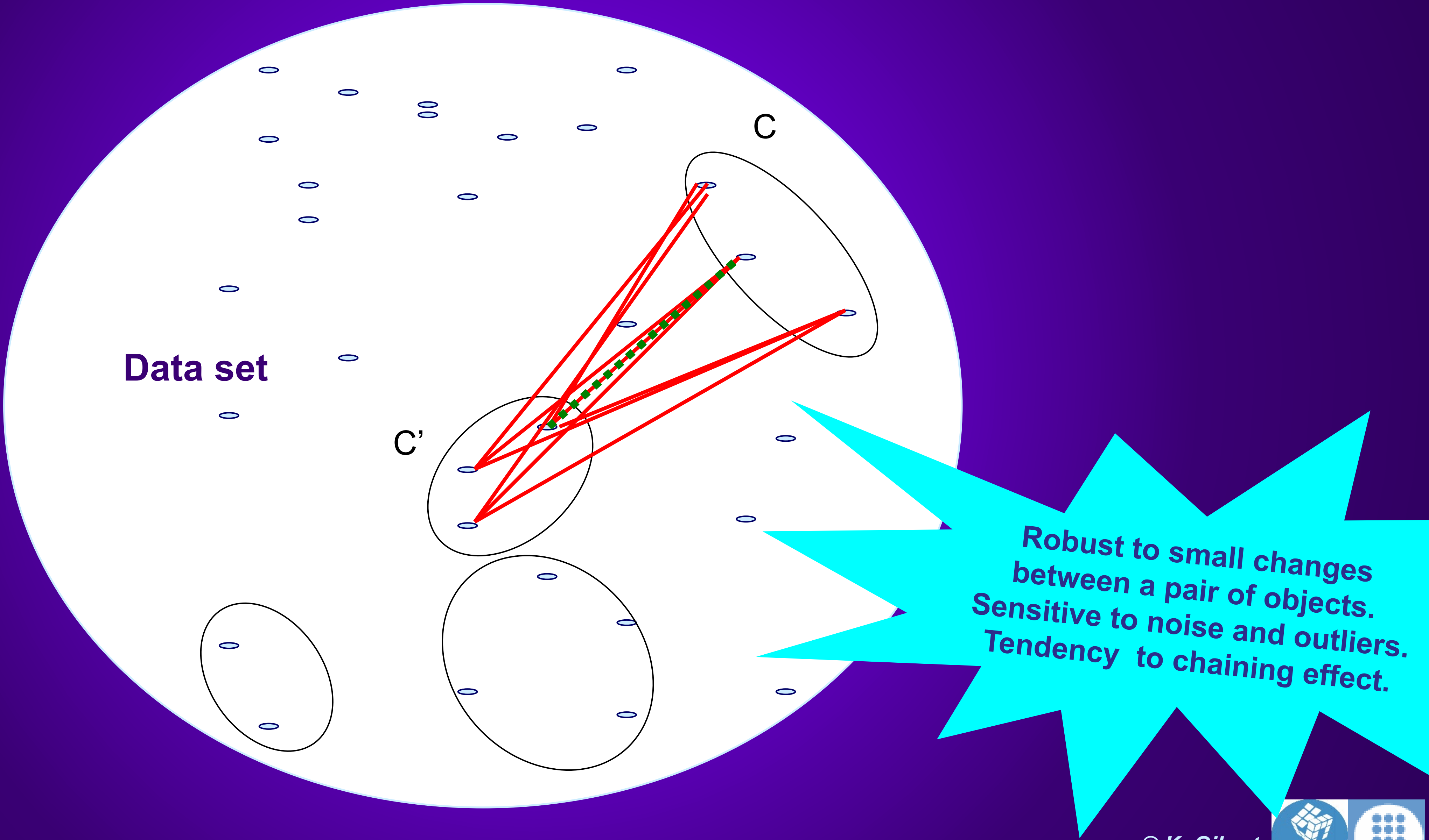
- Agregation criteria
  - Centroid criterion
  - Ward's criterion
- Distance between individuals
  - Only quantitative variables → Euclidean, Correlations
  - Only qualitative variables → χ^2 (Benzécri 80)
  - Heterogenous variables (compatibility measures) → Gower (71)
    Gowda i Diday (91)
    Gibert's Mixed (91)
    Ichino i Yaguchi (94)
    Ralambondrainy (95)
    Generalized Gibert's Mixed (13)

Aggregation Criteria

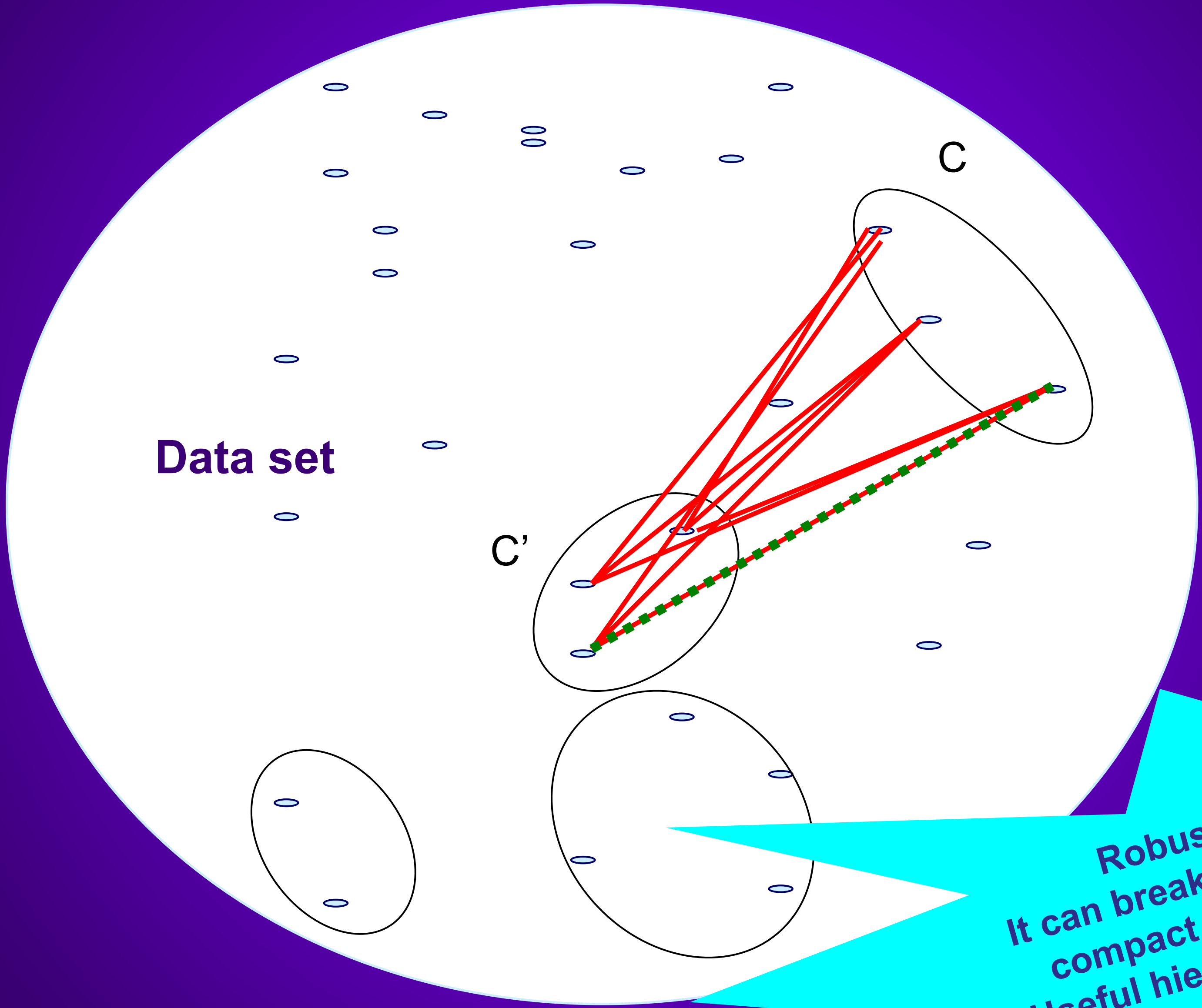
$d(C,C') = f(d(i,i')),\ i \in C,\ i' \in C'$



Single linkage (Sneath 1957) $d(C,C') = \min(d(i,i')),\ i \in C,\ i' \in C'$



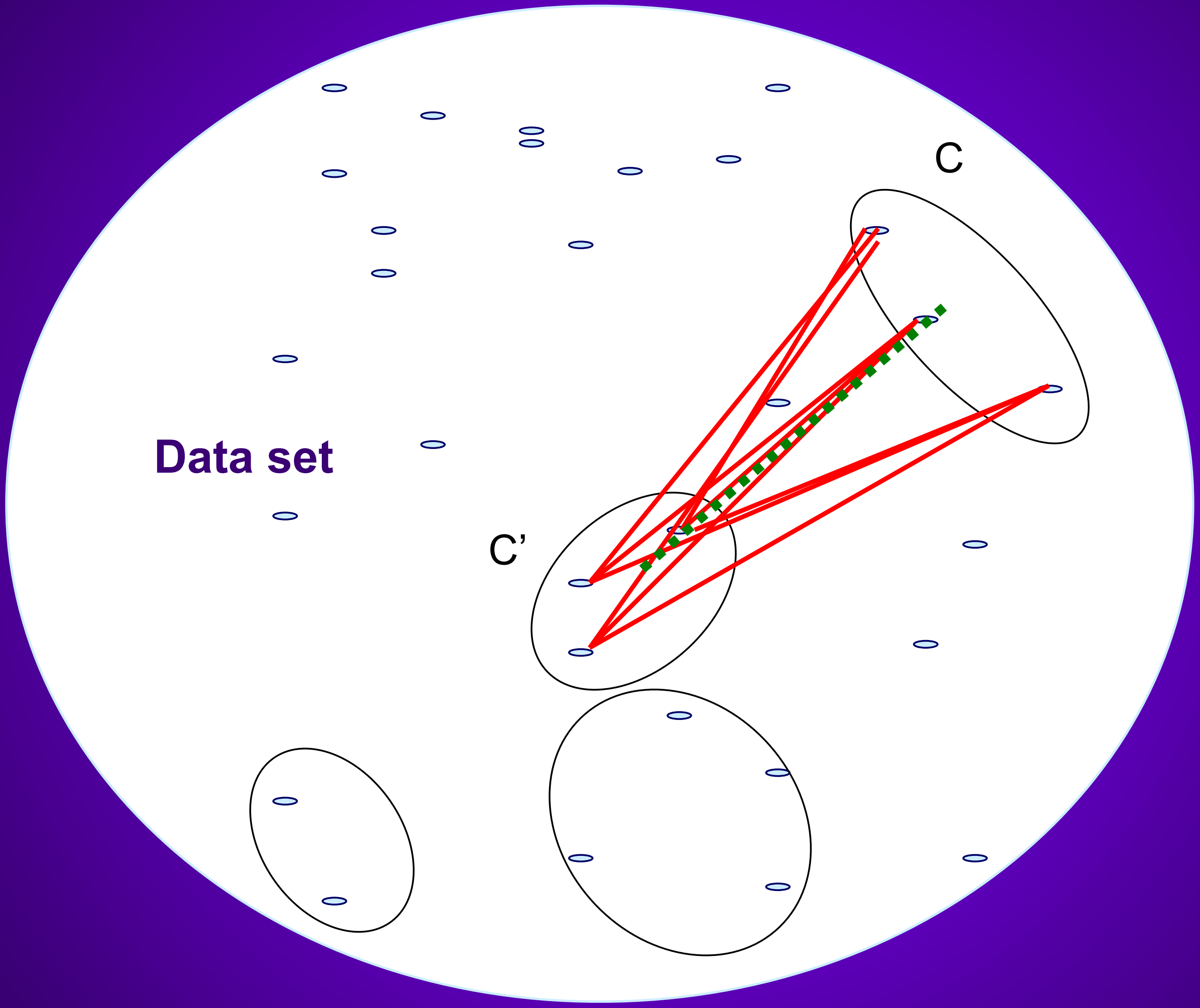
Complete linkage (Sorensen 1948) $d(C,C') = \max(d(i,i')), i \in C, i' \in C'$



Robust to outliers and noise.
It can break large clusters Conservative, compact clusters (Baeza-Yates 1992).
Useful hierarchies (Jain and Dubes 1998)

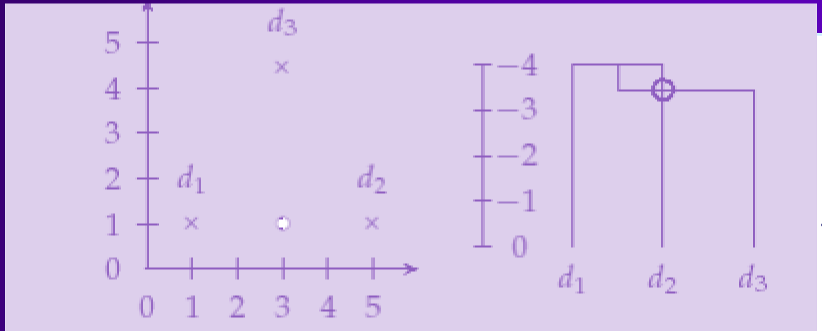
Average linkage

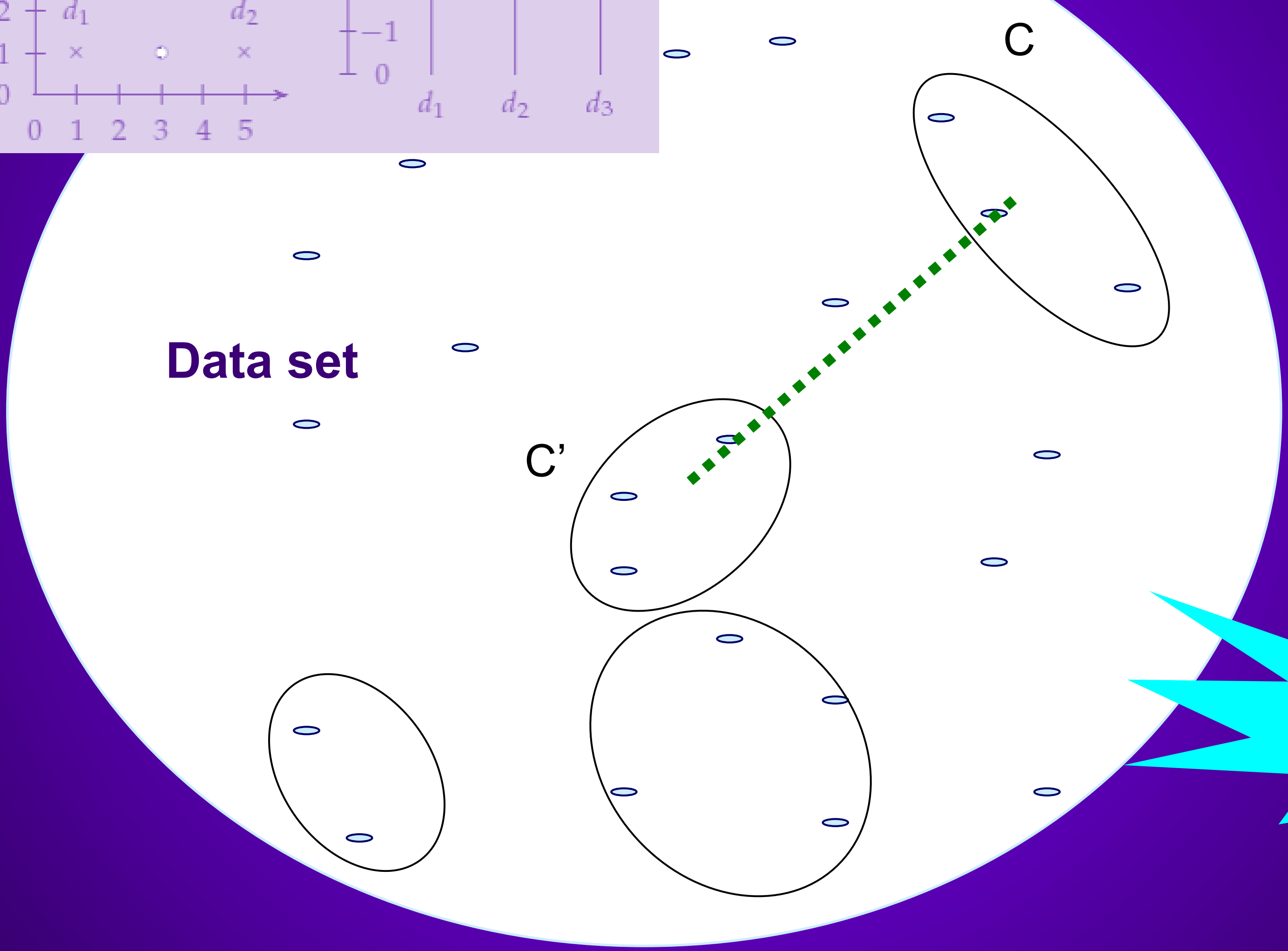
$d(C,C') = \text{mean}(d(i,i')),\ i \in C,\ i' \in C'$



Centroid

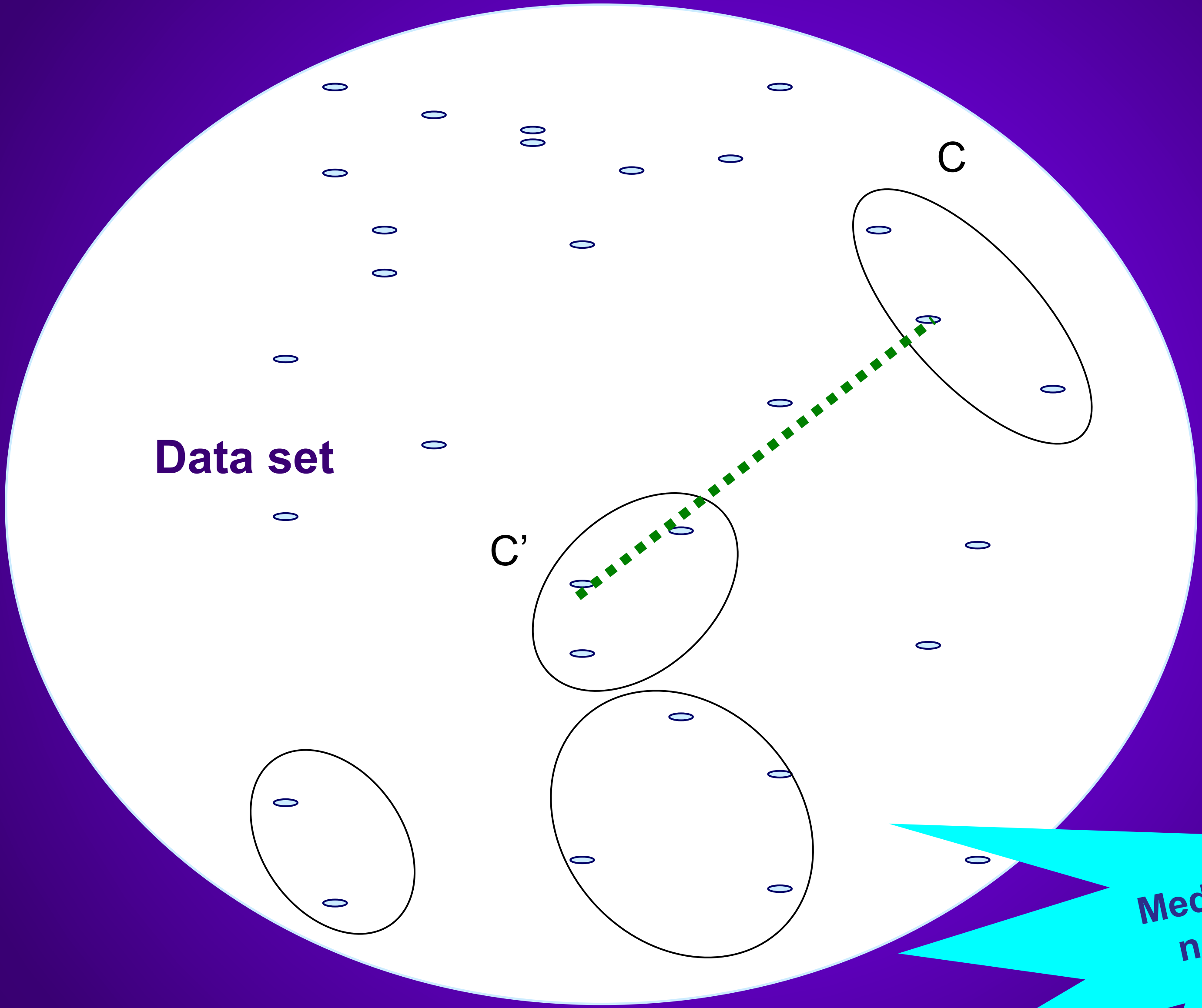
d(C,C’) = d(c,c’), c,c’ centroids





Produce inversions in the dendrogram

Median linkage (Gower 1967) d(C,C’) = d(c,c’)), c,c’ medoids



Median representativeness do not depend on cluster size

Ward's method (Ward 1963)

- Ascendant hierarchical method
- Group the two classes giving minimal inter-class inertia loss
- Inertia (physical concept)

$$M^2(\mathcal{I}/\bar{\imath}) = \sum_{i\in\mathcal{I}} m_i\, d^2(i,\bar{\imath})$$

- Huygens theorem

$$M^2(\mathcal{I}/\bar{\imath}) = Mi^2_{\mathcal{P}}(\mathcal{I}/\bar{\imath}) + Me^2_{\mathcal{P}}(\mathcal{I}/\bar{\imath}),$$

$$Mi^2_{\mathcal{P}}(\mathcal{I}/\bar{\imath}) = \sum_{\mathcal{C}\in\mathcal{P}} M^2(\mathcal{C}/\bar{\imath}_{\mathcal{C}}) = \sum_{\mathcal{C}\in\mathcal{P}}\sum_{i\in\mathcal{C}} m_i\, d^2(i,\bar{\imath}_{\mathcal{C}})$$

$$Me^2_{\mathcal{P}}(\mathcal{I}/\bar{\imath}) = \sum_{\mathcal{C}\in\mathcal{P}} m_{\mathcal{C}}\, d^2(\bar{\imath}_{\mathcal{C}},\bar{\imath})$$

- Every aggregation increases intra-class inertia with

$$\Delta_\xi = Mi^2_{\mathcal{P}_{\xi+1}}(\mathcal{I}/\bar{\imath}) - Mi^2_{\mathcal{P}_\xi}(\mathcal{I}/\bar{\imath}) = m_{\mathcal{C}_e} d^2(\mathcal{C}_e,\bar{\imath}_{\mathcal{C}}) + m_{\mathcal{C}_d} d^2(\mathcal{C}_d,\bar{\imath}_{\mathcal{C}})$$

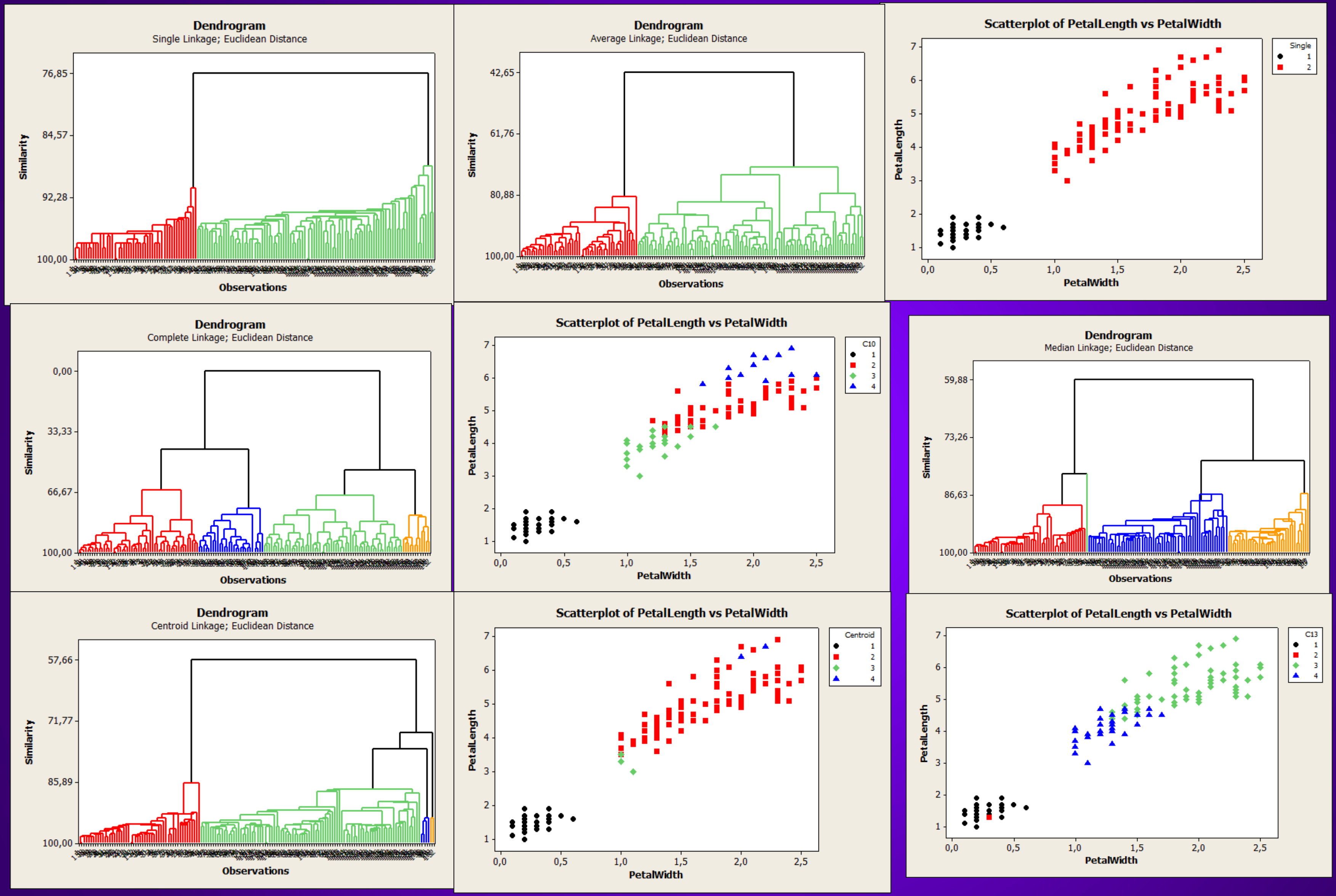
Minimize

- Inertia: related with quantity of information *(Thm Benzecri 1973)*
  - The more informative, more inertia
- Also with variability
  - The more variable, more inertia
- Quite popular

Interpretable classes

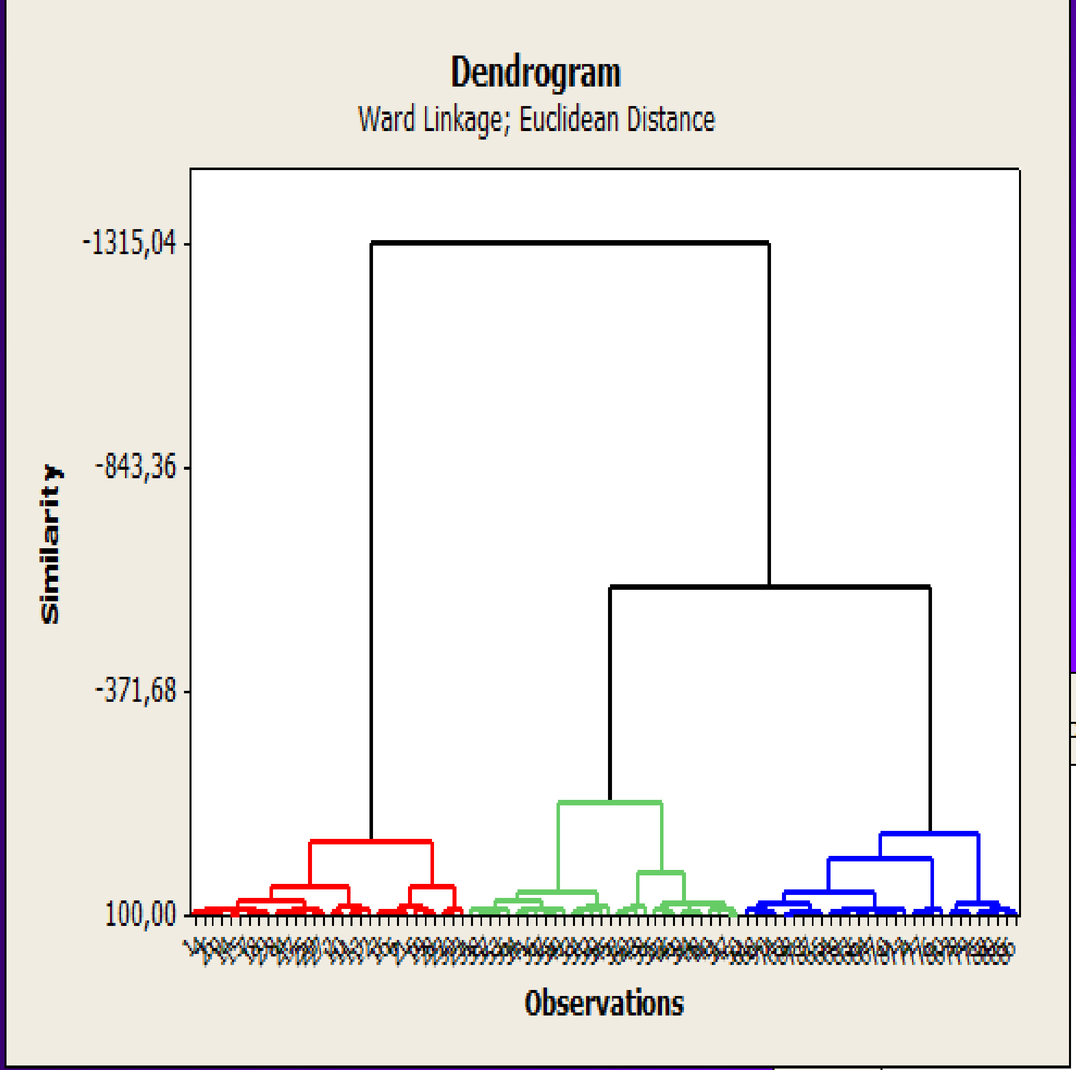
Can exagerate number of Exception-classes

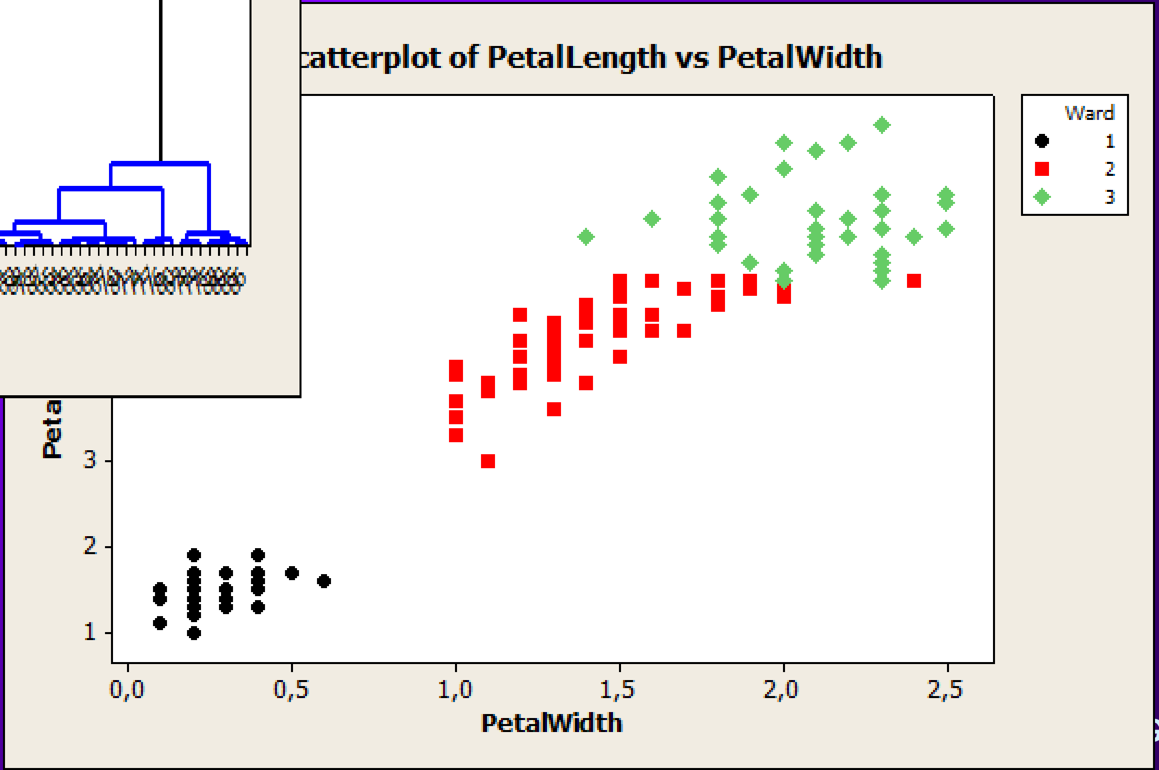
Iris Flowers dataset



Iris Flower Dataset

Ward's method





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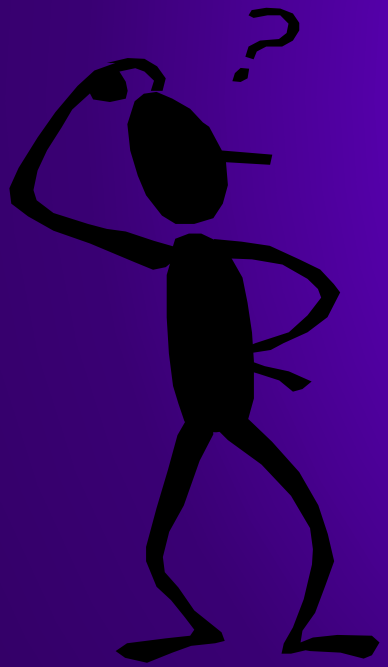

Are there any questions?...