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Hierarchical Clustering and Expectation-Maximization

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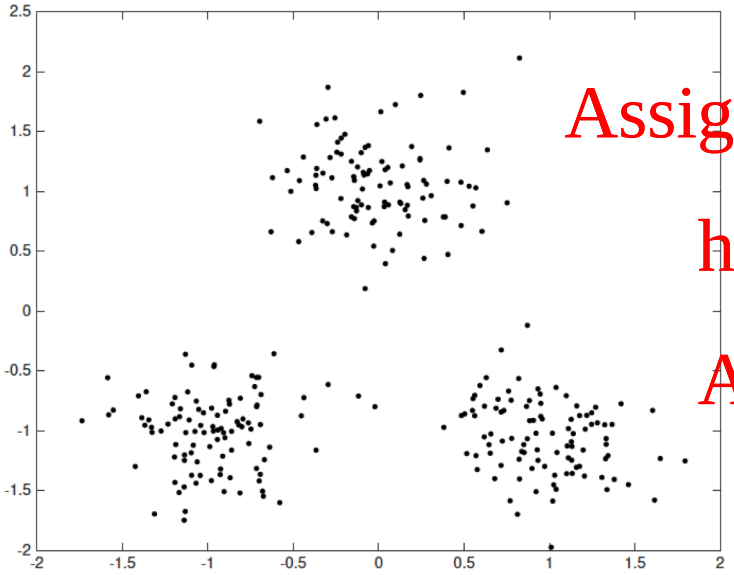
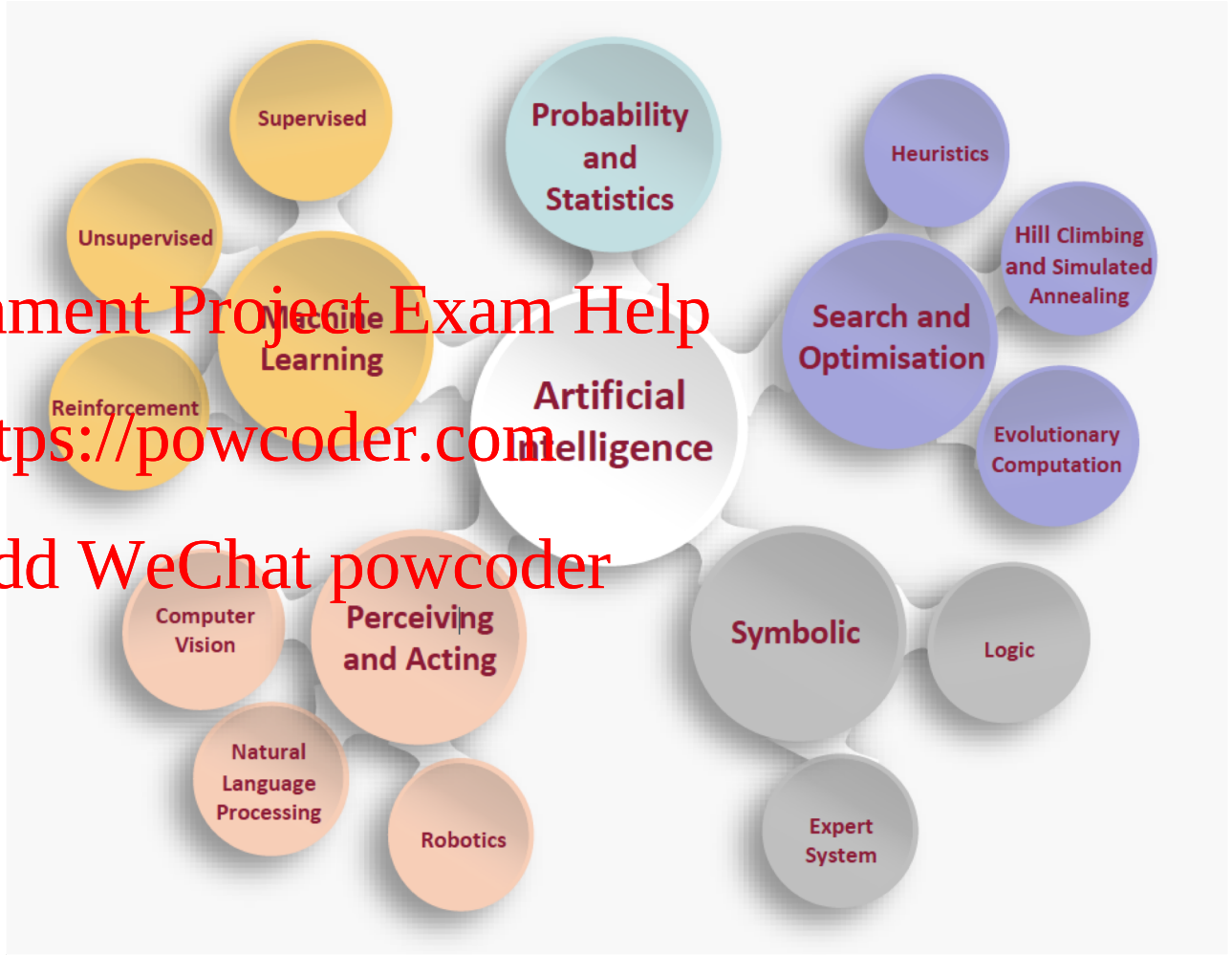
AI Taxonomy





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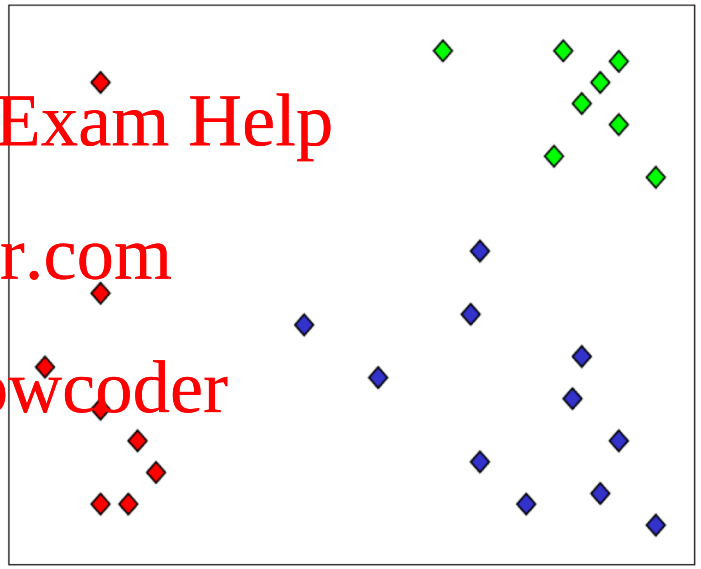
Outline

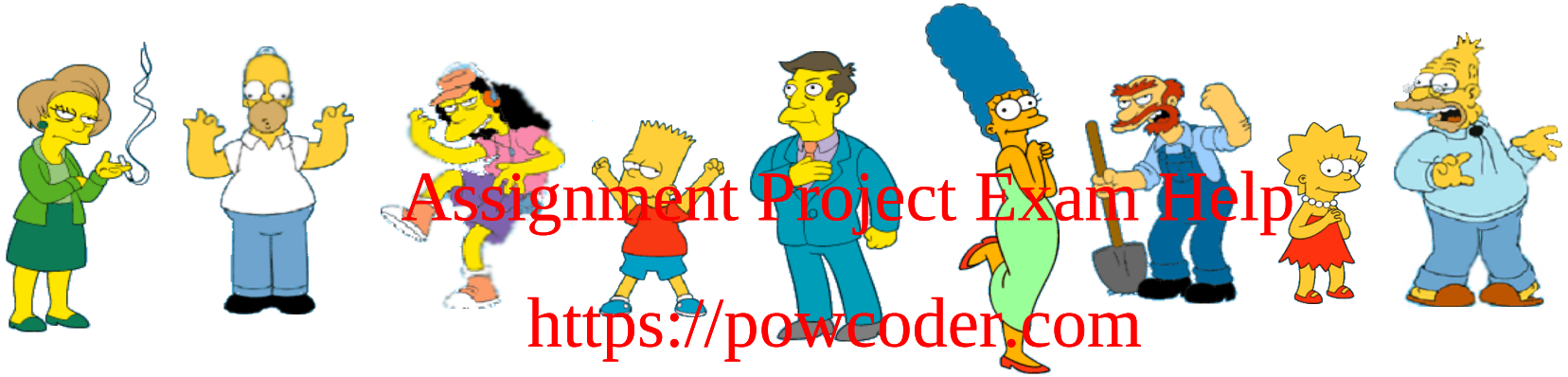
- Clustering concepts
- Hierarchical clustering
- Gaussian mixture models using EM

Clustering

- Segment data into clusters, such that there is
  - high intra-cluster similarity
  - low inter-cluster similarity
- Informally, finding natural groupings among objects.



What is the natural grouping of these objects?



Picture from CMU

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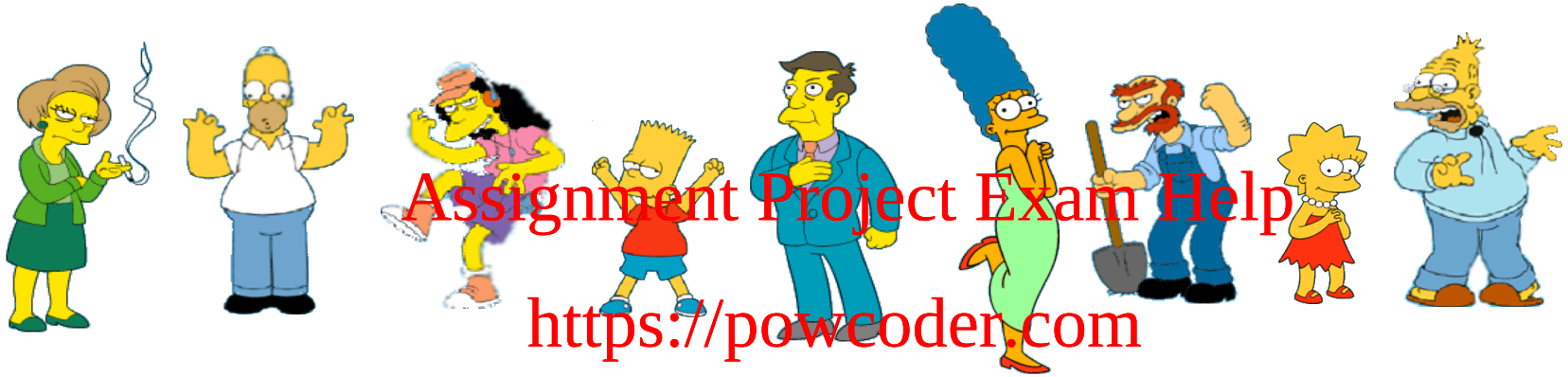
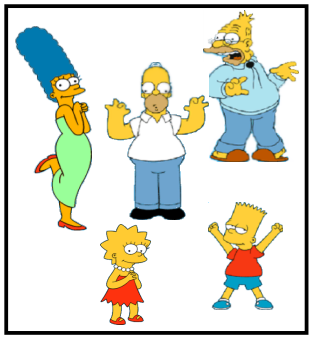
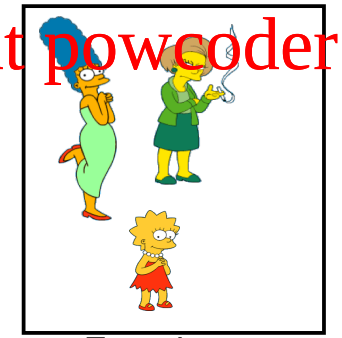




Simpson's family

School employees



Females

Males

Picture from CMU

Clustering set-up

- Our data are: $D = \{x_1, \ldots, x_N\}$.
- Each data point is m-dimensional, i.e. $x_i = \langle x_{i,1}, \ldots, x_{i,m} \rangle$
- Define a *distance function (i.e. similarity measures)* between data, $d(x_i, x_j)$
- Goal: segment x_n into k groups $\{z_1, \ldots, z_N\}$ where $z_i \in \{1, \ldots, K\}$

Similarity Measures

- Between any two data samples p and q, we can calculate their distance d(p,q) using a number of measurements:

Euclidean

$$d(\mathbf{p},\mathbf{q}) = d(\mathbf{q},\mathbf{p}) = \sqrt{(q_1 - p_1)^2 + (q_2 - p_2)^2 + \cdots + (q_n - p_n)^2}$$

Manhattan

$$d(\mathbf{p},\mathbf{q}) = \sum_{i=1}^{n} |p_i - q_i|$$

Chebyshev

$$d_{\text{Chebyshev}}(p,q) = \max_i(|p_i - q_i|)$$

Minkowski

$$d(p,q) = \left(\sum_{i=1}^{n} |p_i - q_i|^b\right)^{1/b}$$

Types of Clustering Algorithms

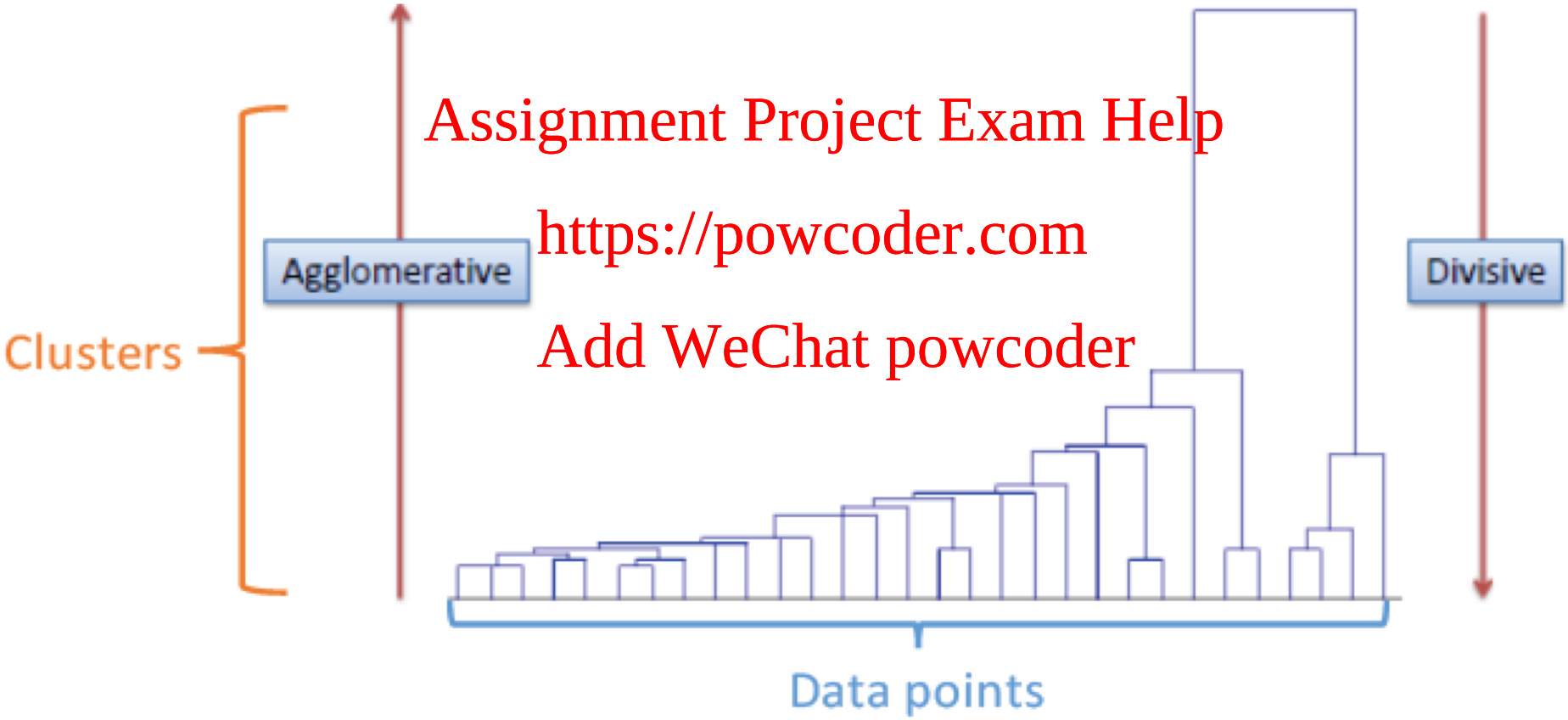
- Partitional clustering, e.g. K-means, K-medoids
- Hierarchical clustering
  - Bottom-up (agglomerative)
  - Top-down
- Density-based clustering, e.g. DBScan
- Mixture density based clustering
- Fuzzy theory based, graph theory based, grid based, etc.

Hierarchical clustering

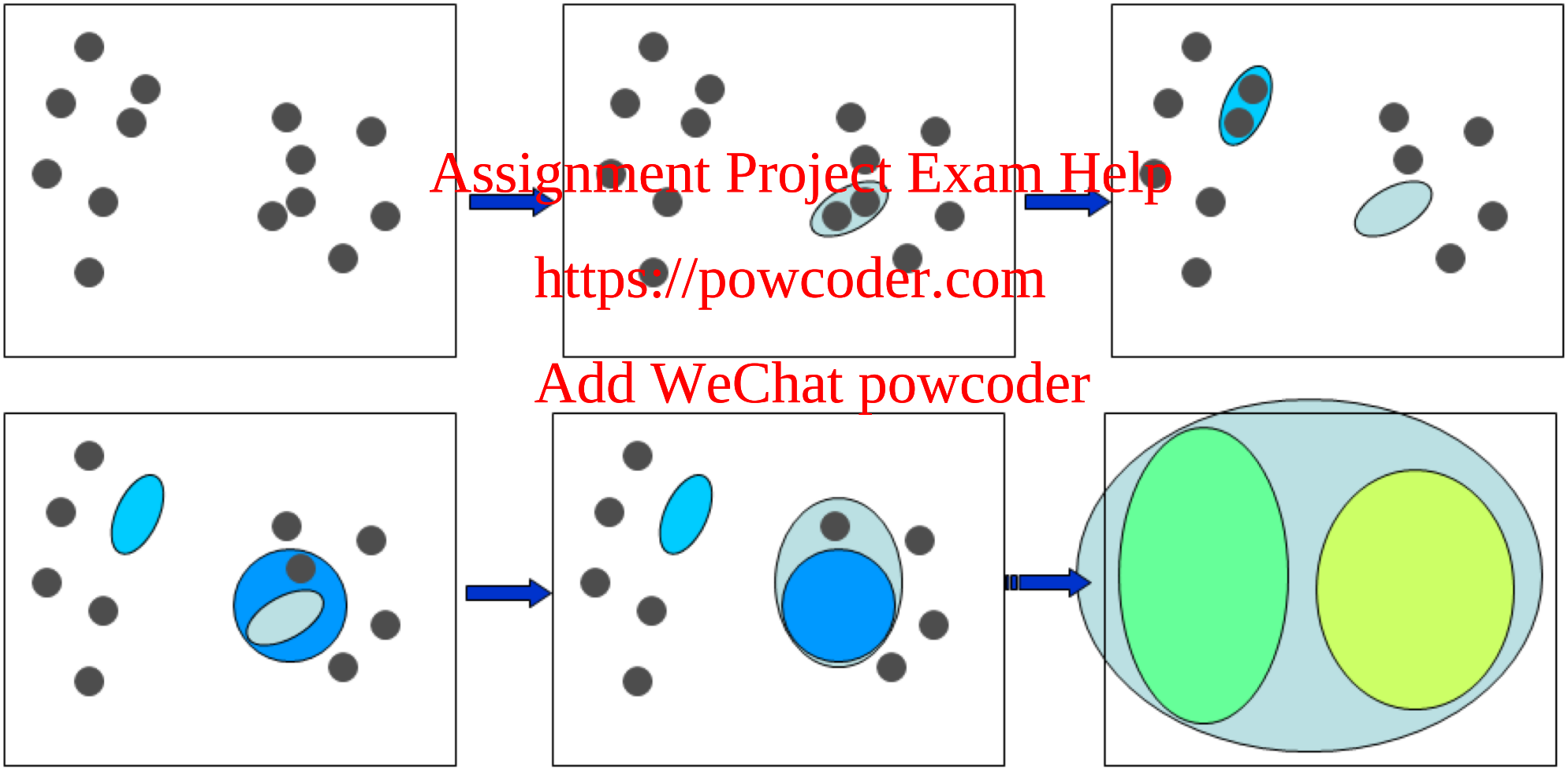
- Create a hierarchical decomposition of the set of objects using some criterion
- Produce a dendrogram

(Bovine, (Spider Monkey, (Gibbon, (Orang, (Gorilla, (Chimp, Human)))));

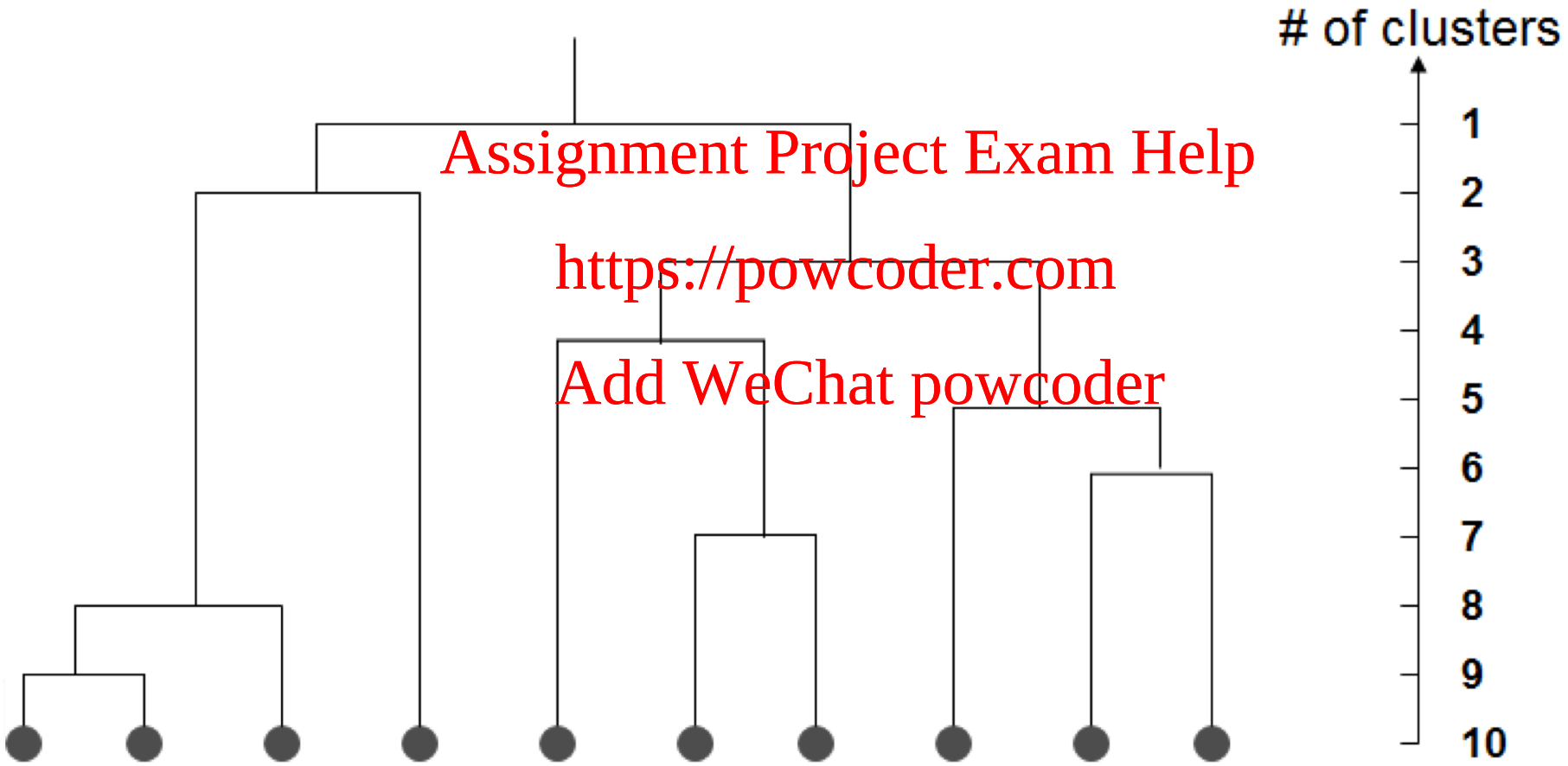
Hierarchical clustering



Agglomerative clustering illustration



Dendrogram: A visual representation of output



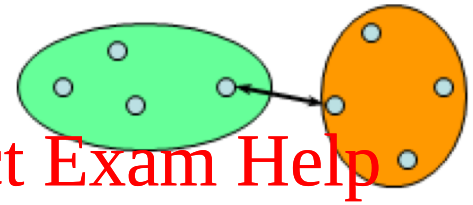
Agglomerative clustering algorithm

1. Place each data point into its own singleton group
2. Repeat: iteratively merge the two closest groups
3. Until: all the data are merged into a single cluster

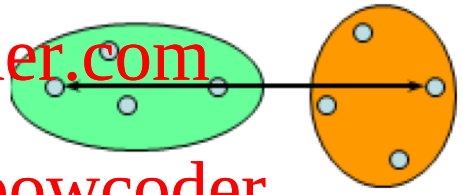
- Output: a dendrogram
- Reply on: a *distance metric* between clusters

Measuring distance between clusters

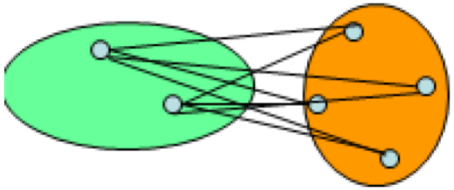
- Single linkage
  - the similarity of the closest pair
- Complete linkage
  - the similarity of the furthest pair
- Group average
  - the average similarity of all pairs
  - more widely used
  - robust against noise



$$d_{SL}(G,H) = \min_{i \in G, j \in H} d_{i,j}$$



$$d_{CL}(G,H) = \max_{i \in G, j \in H} d_{i,j}$$



$$d_{GA} = \frac{1}{N_G N_H} \sum_{i \in G} \sum_{j \in H} d_{i,j}$$

Try your own data here:
http://jydelort.appspot.com/resources/figue/demo.html

Strengths, weaknesses, caveats

- Strengths
  - provides deterministic results
  - no need to specify number of clusters beforehand
  - can create clusters of arbitrary shapes
- Weakness
  - does not scale up for large datasets, time complexity at least O(n^2)
- Caveats
  - Different decisions about group similarities can lead to vastly different dendrograms.
  - The algorithm imposes a hierarchical structure on the data, even data for which such structure is not appropriate.