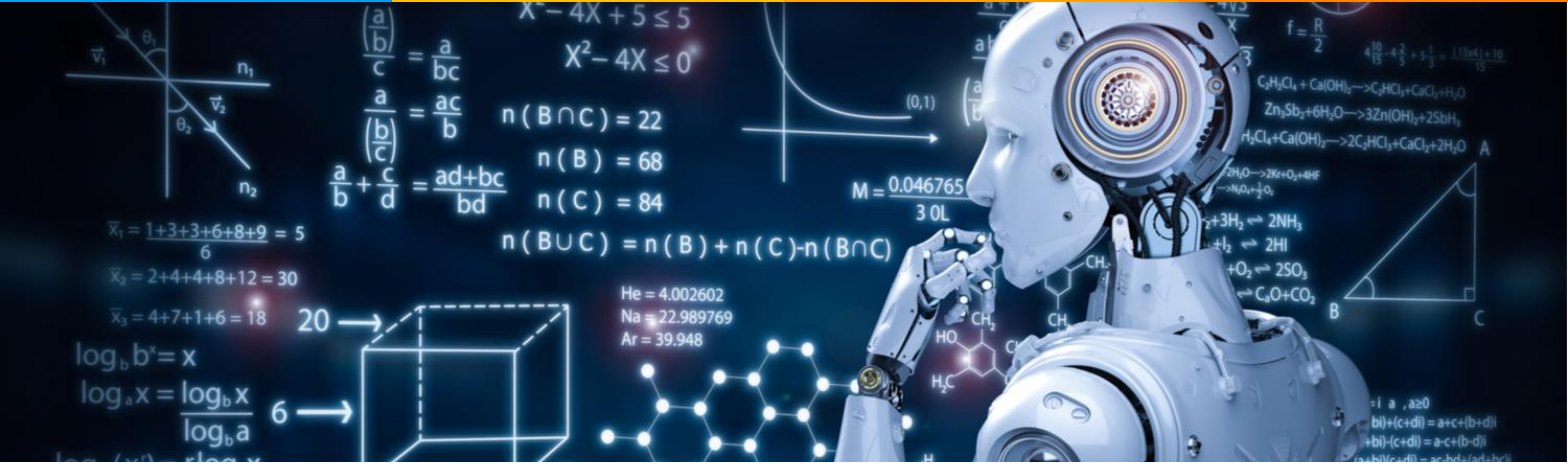
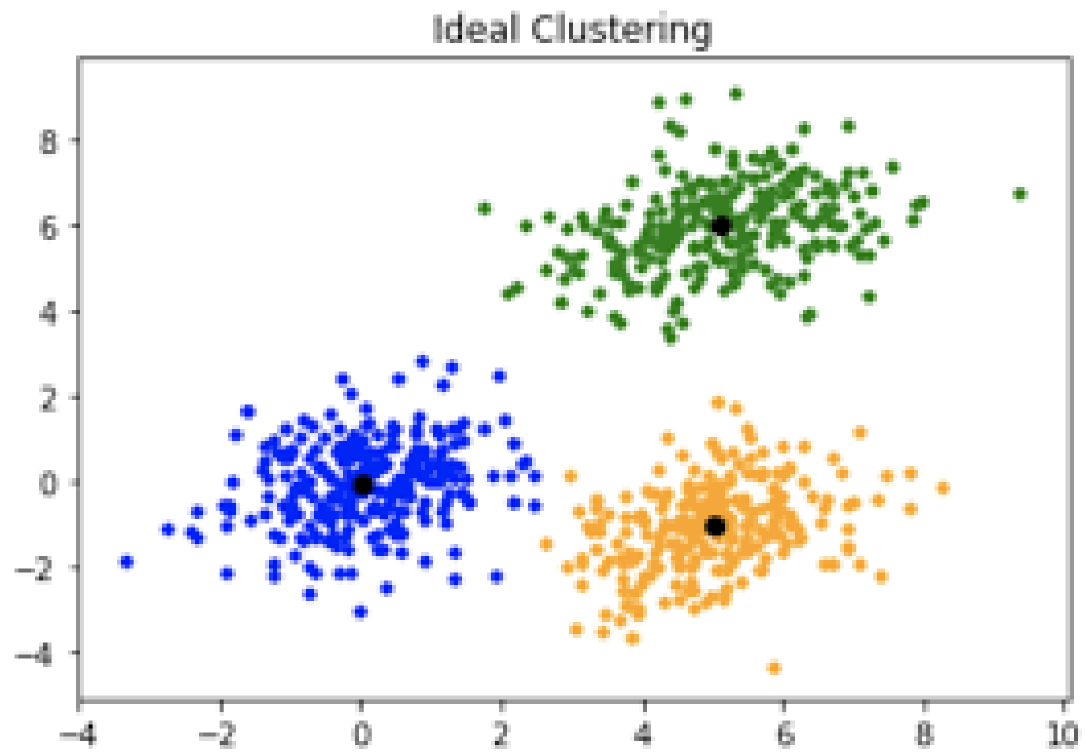
Duration: 60 min | Srikanth Shenoy | AML 5102 | M.E. AI & ML

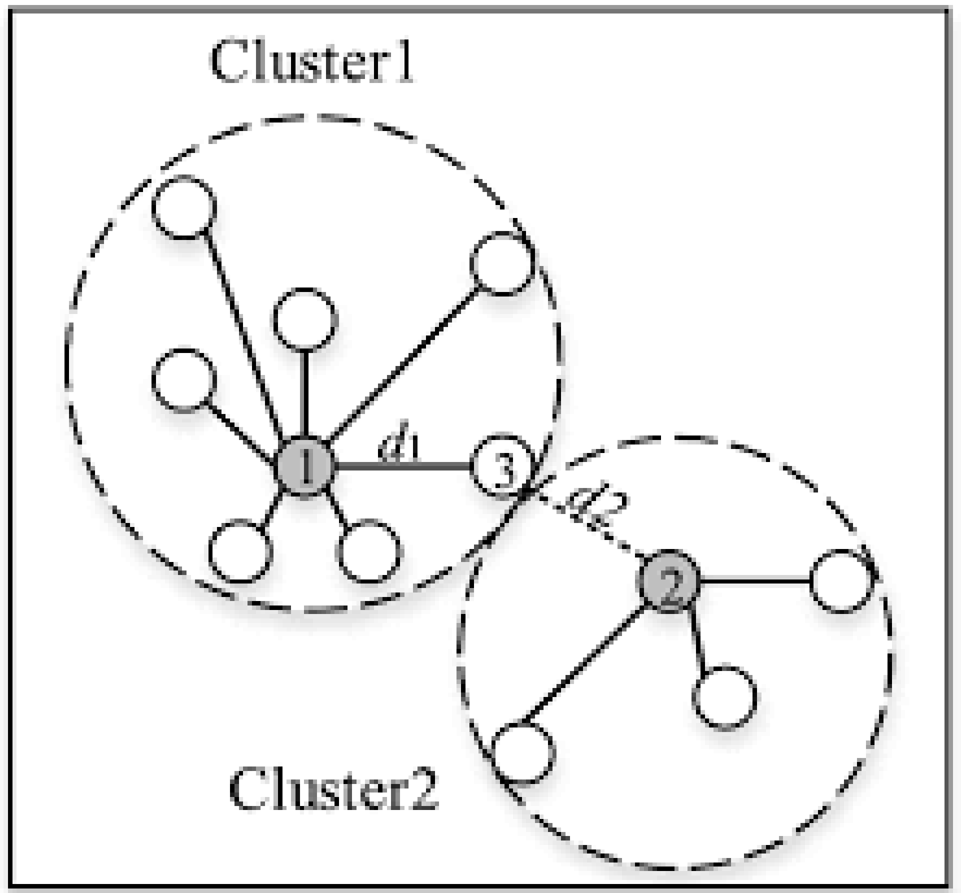


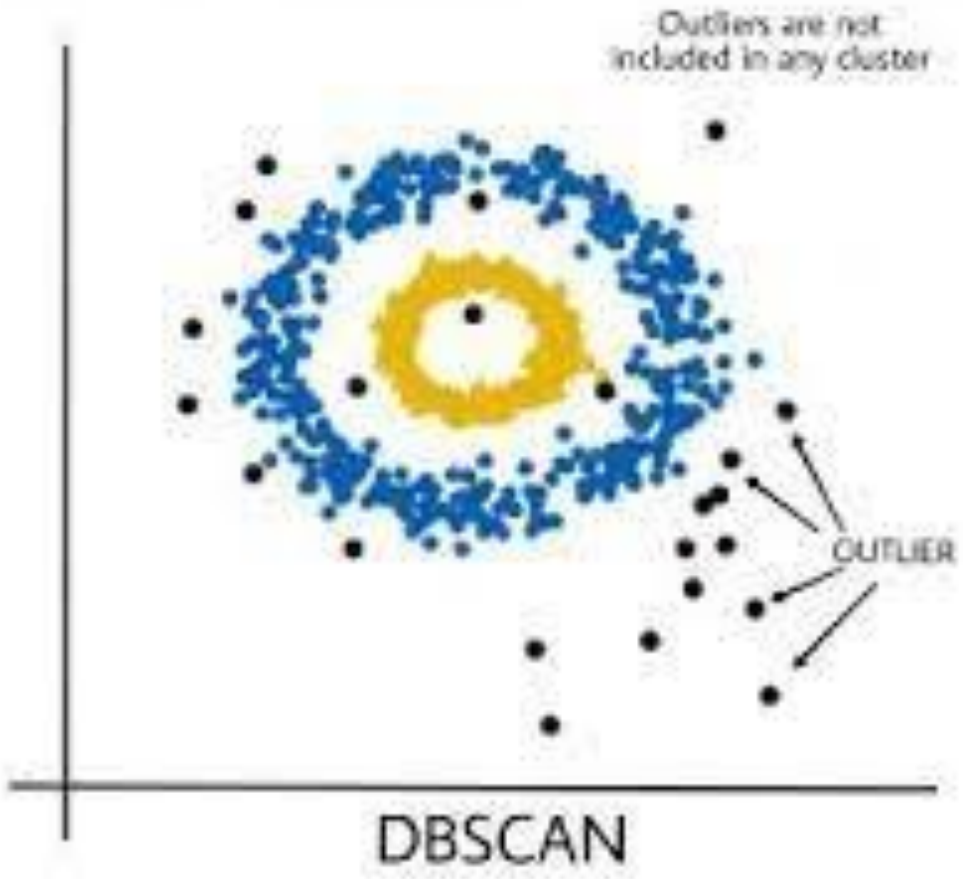
Lecture 16: Hierarchial Clustering

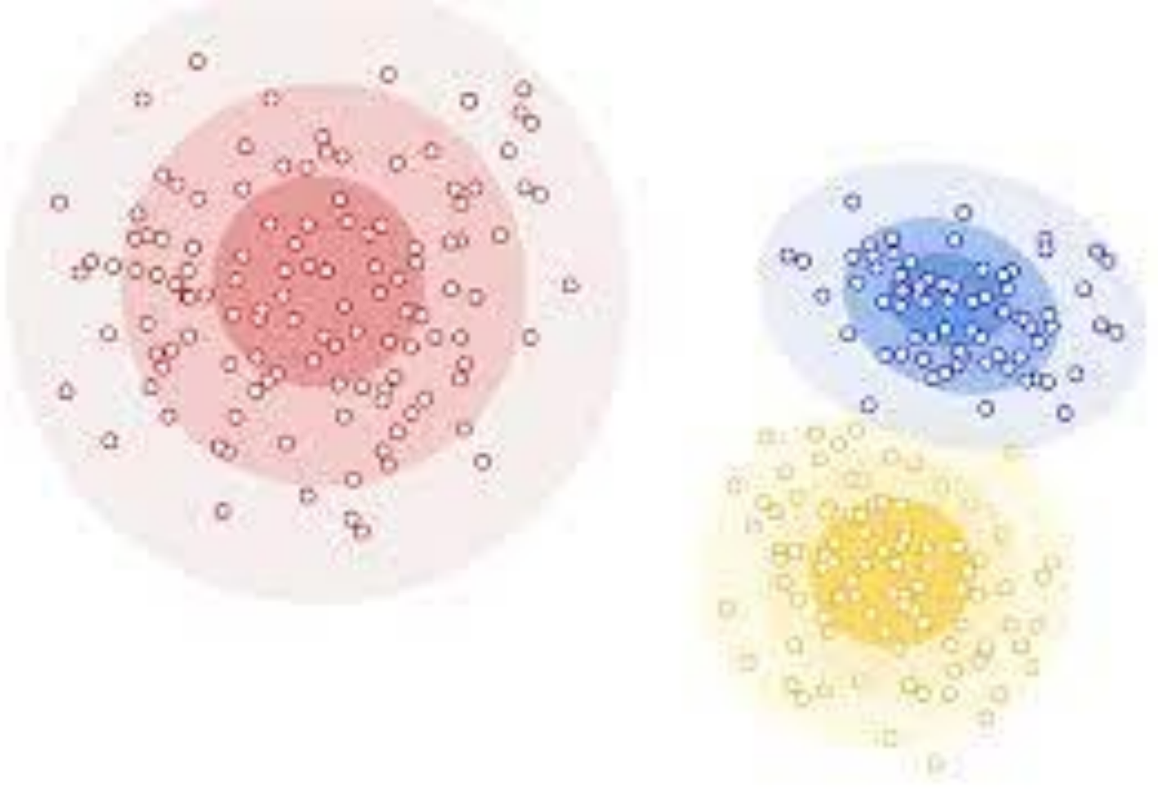
Cluster Analysis - Recap

- Centroid based clustering
- Distribution based clustering
- Density based clustering
- Connectivity based clustering

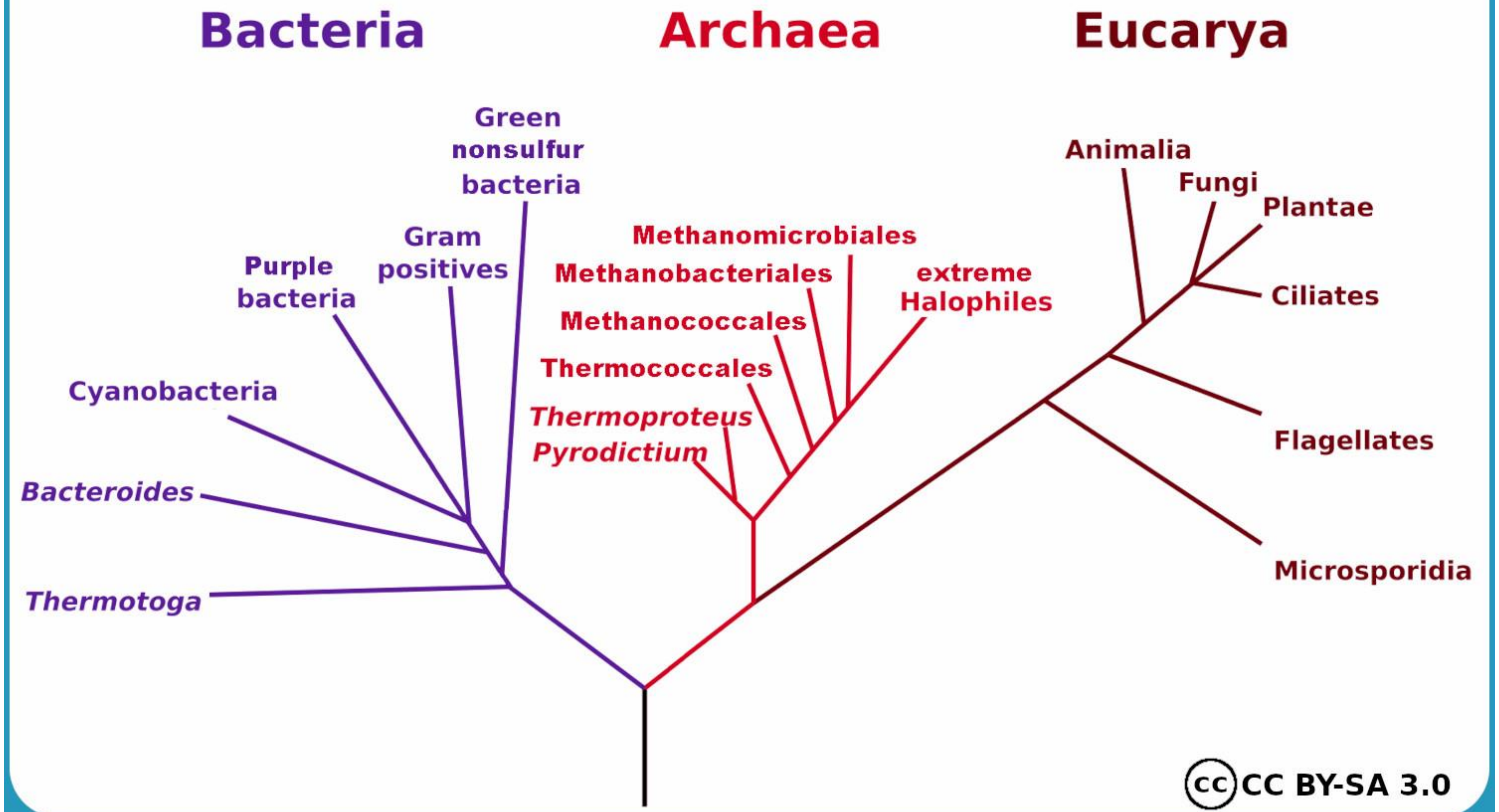




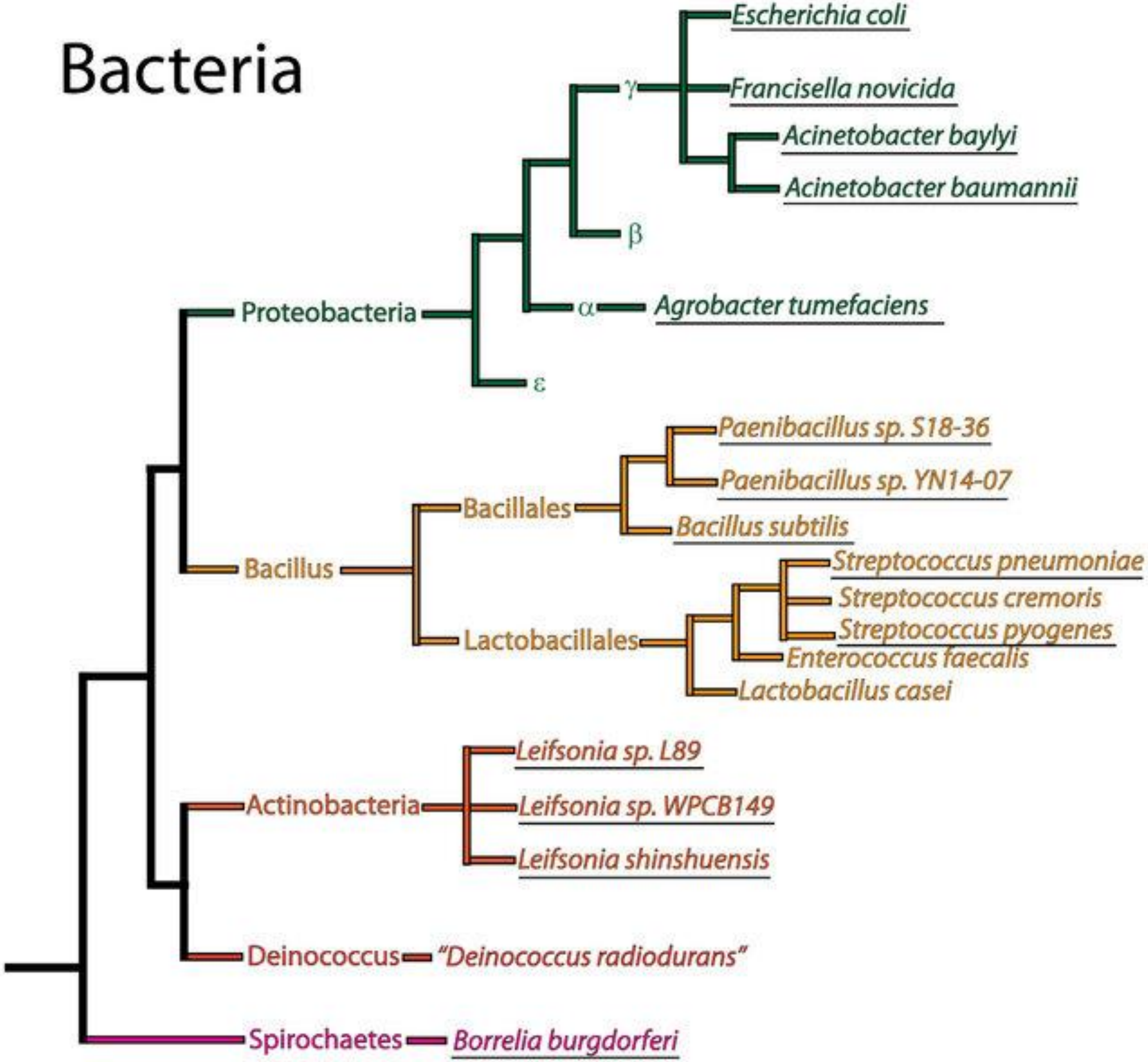




Phylogenetic Tree of Life



Bacteria


Escherichia coli
Francisella novicida
Acinetobacter baylyi
Acinetobacter baumannii
γ
β
Proteobacteria
α
Agrobacter tumefaciens
ε
Paenibacillus sp. S18-36
Paenibacillus sp. YN14-07
Bacillales
Bacillus subtilis
Bacillus
Streptococcus pneumoniae
Streptococcus cremoris
Streptococcus pyogenes
Lactobacillales
Enterococcus faecalis
Lactobacillus casei
Leifsonia sp. L89
Actinobacteria
Leifsonia sp. WPCB149
Leifsonia shinshuensis
Deinococcus
"Deinococcus radiodurans"
Spirochaetes
Borrelia burgdorferi

$n(B \cap C) = 22$
$n(B) = 68$
$n(C) = 84$
$n(B \cup C) = n(B) + n(C) - n(B \cap C)$
$X^2 - 4X \le 0$
$\frac{a}{b} + \frac{c}{d} = \frac{ad+bc}{bd}$
$\bar{x}_1 = \frac{1+3+3+6+8+9}{6} = 5$
$\bar{x}_2 = 2+4+4+8+12 = 30$
$\bar{x}_3 = 4+7+1+6 = 18$
$\log_b b^x = x$
$\log_a x = \frac{\log_b x}{\log_b a}$
20 →
6 →
He = 4.002602
Na = 22.989769
Ar = 39.948
$M = \frac{0.046765}{3\ 0L}$
(0,1)
$f = \frac{R}{2}$
A
B
C

Types of Hierarchial Clustering

Intro to hierarchical clustering

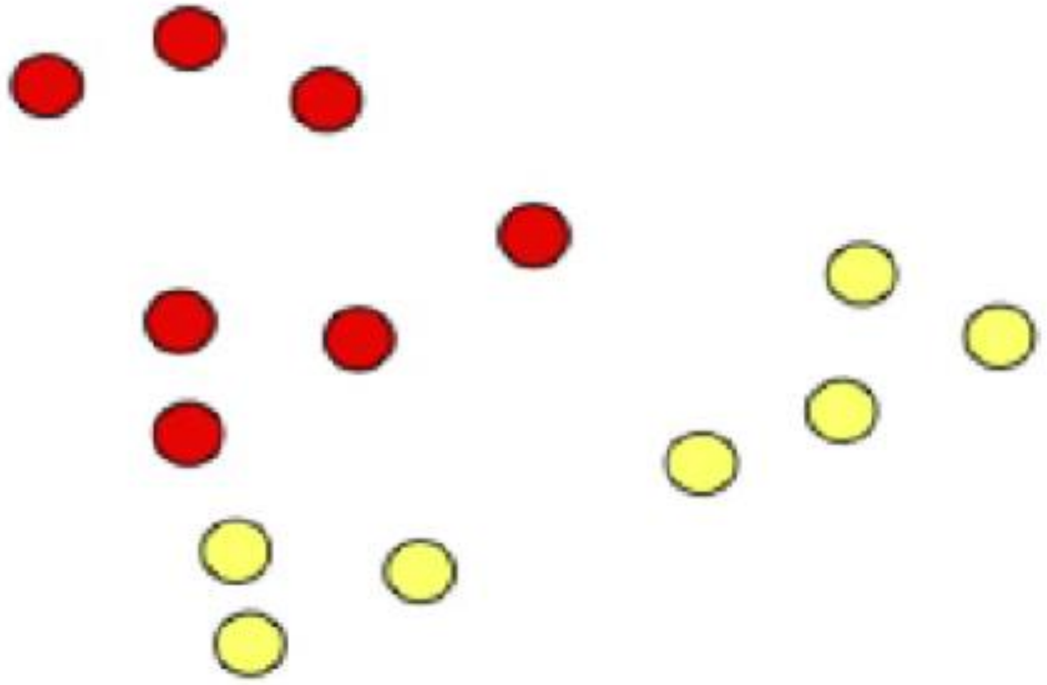
- How many clusters in the data is
  - Technical question
  - Centroid, Distribution & Density answers this question
- Business questions
  - How are clusters related?
  - How to say 2 clusters are different but are also similar?
- We need a hierarchical organization of clusters
  - Based on high level effects / granular sub groupings
- Very natural for some problems
  - Taxonomy

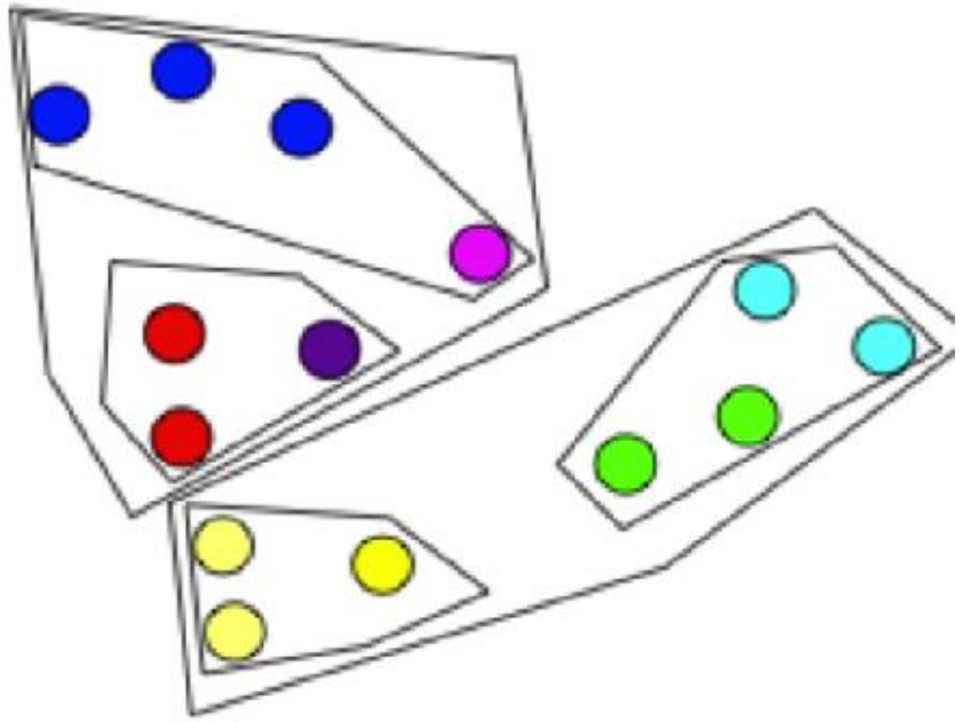
Hierarchical clustering

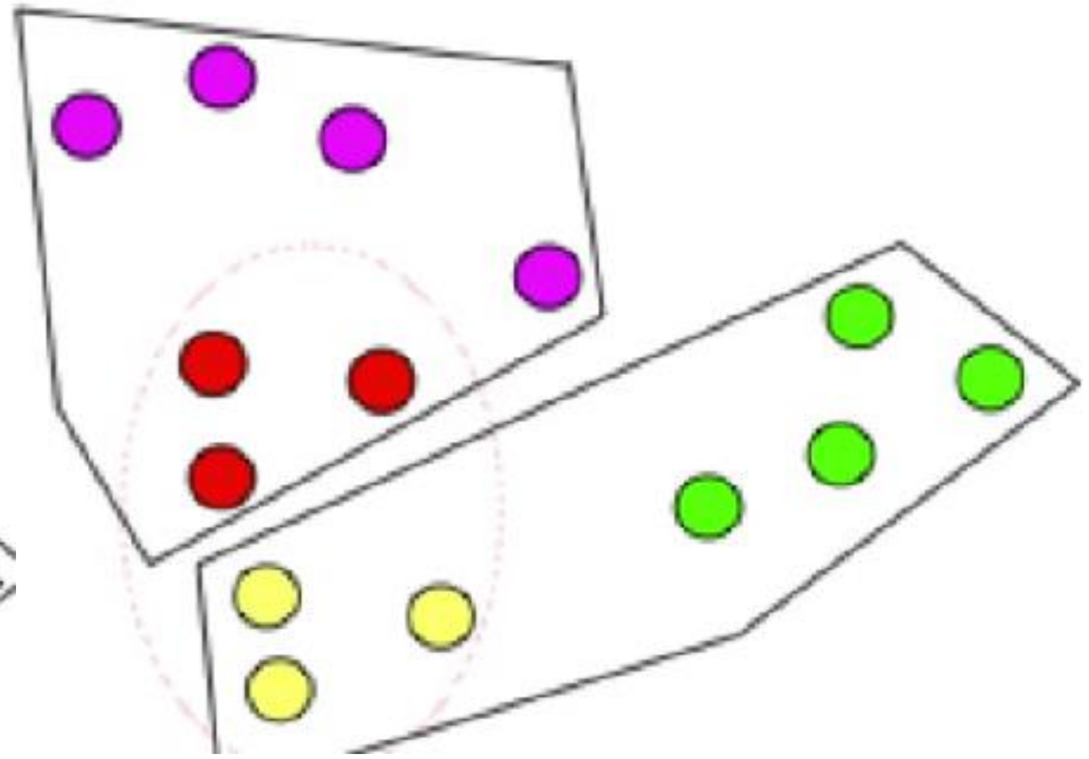
- Top-down
  - Start with one cluster, split recursively
  - Divisive clustering
- Bottom-up
  - Each point is a cluster, merge clusters
  - Agglomerative clustering
- Tree in both cases
  - All data in one cluster at top
  - Each data in its own cluster at bottom

Divisive clustering

- Recursively run K means (say K = 2)
- Partition into two may not be reasonable
- Split into 2. Further split each into 2
- No going back and changing the splits
  - Greedy
  - Sometimes problematic
- Computationally efficient







$X^2 - 4X + 5 \leq 5$
$X^2 - 4X \leq 0$
n(B∩C) = 22
n(B) = 68
n(C) = 84
n(B∪C) = n(B)+n(C)-n(B∩C)
$\frac{a}{b} + \frac{c}{d} = \frac{ad+bc}{bd}$
$\bar{x}_1 = \frac{1+3+3+6+8+9}{6} = 5$
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(0,1)
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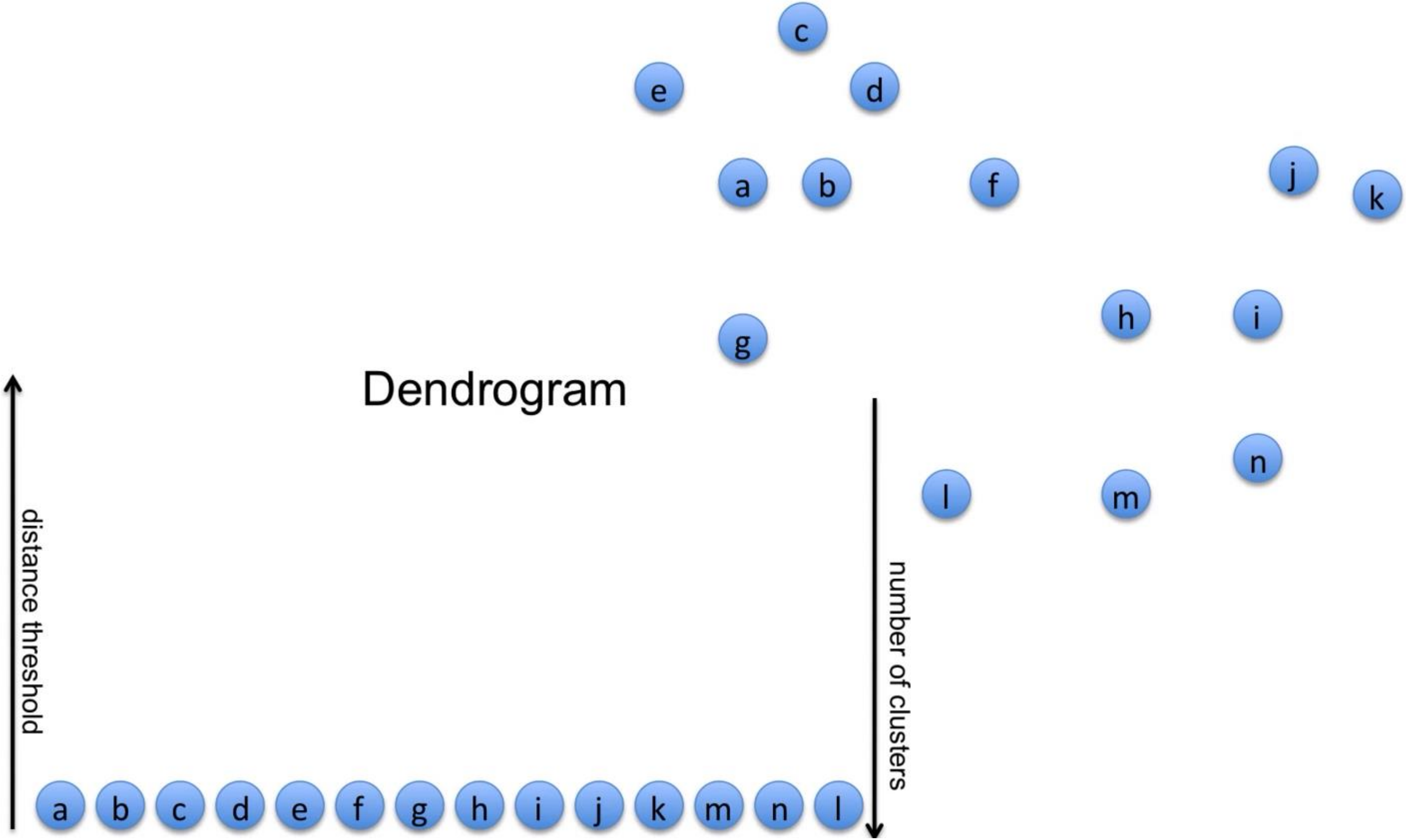
A
B
C

Agglomerative Clustering

Dendrogram


c
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a
b
f
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i
g
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l
m
distance threshold
number of clusters
a
b
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e
f
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h
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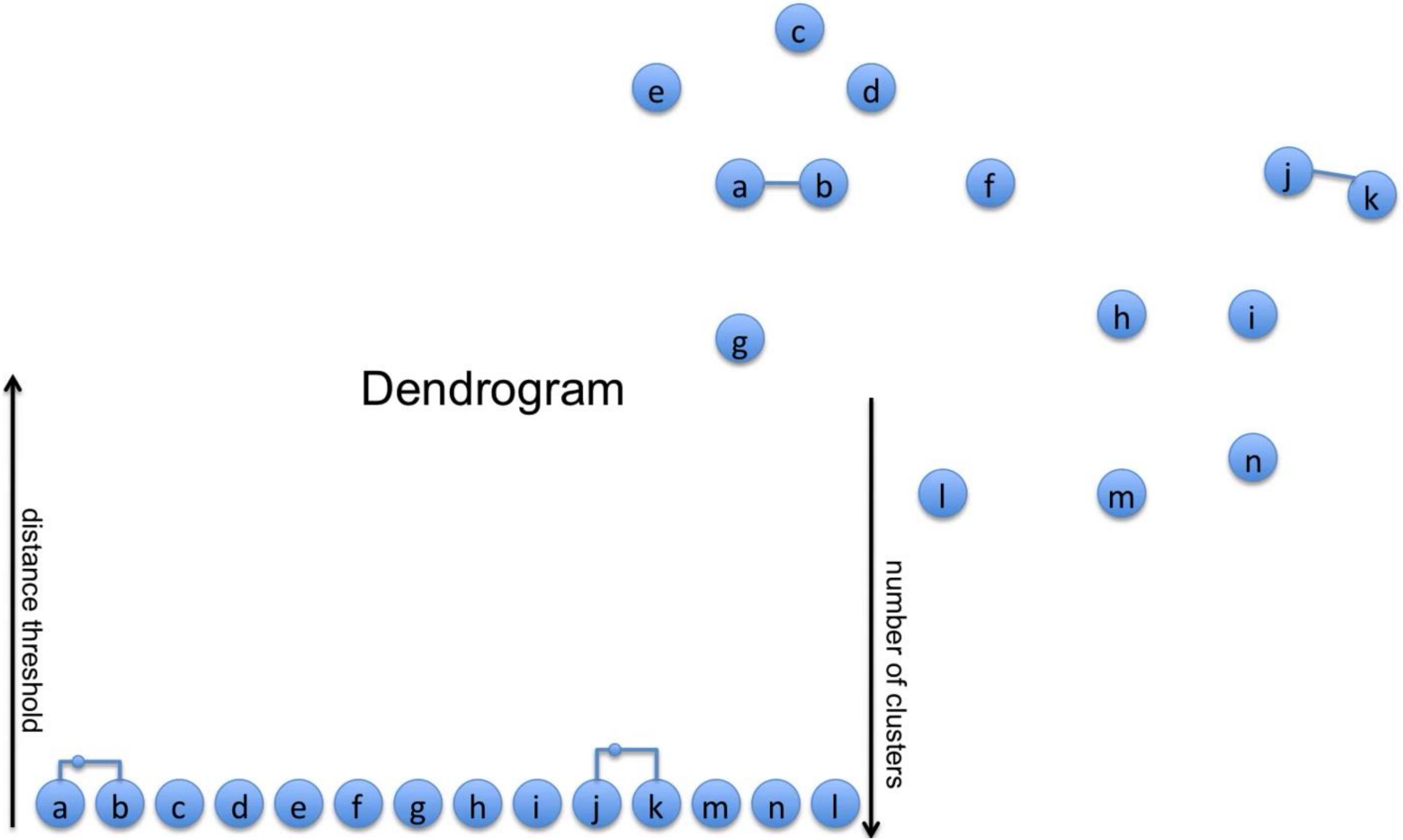
j
k
m
n
l

Dendrogram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distance threshold
number of clusters
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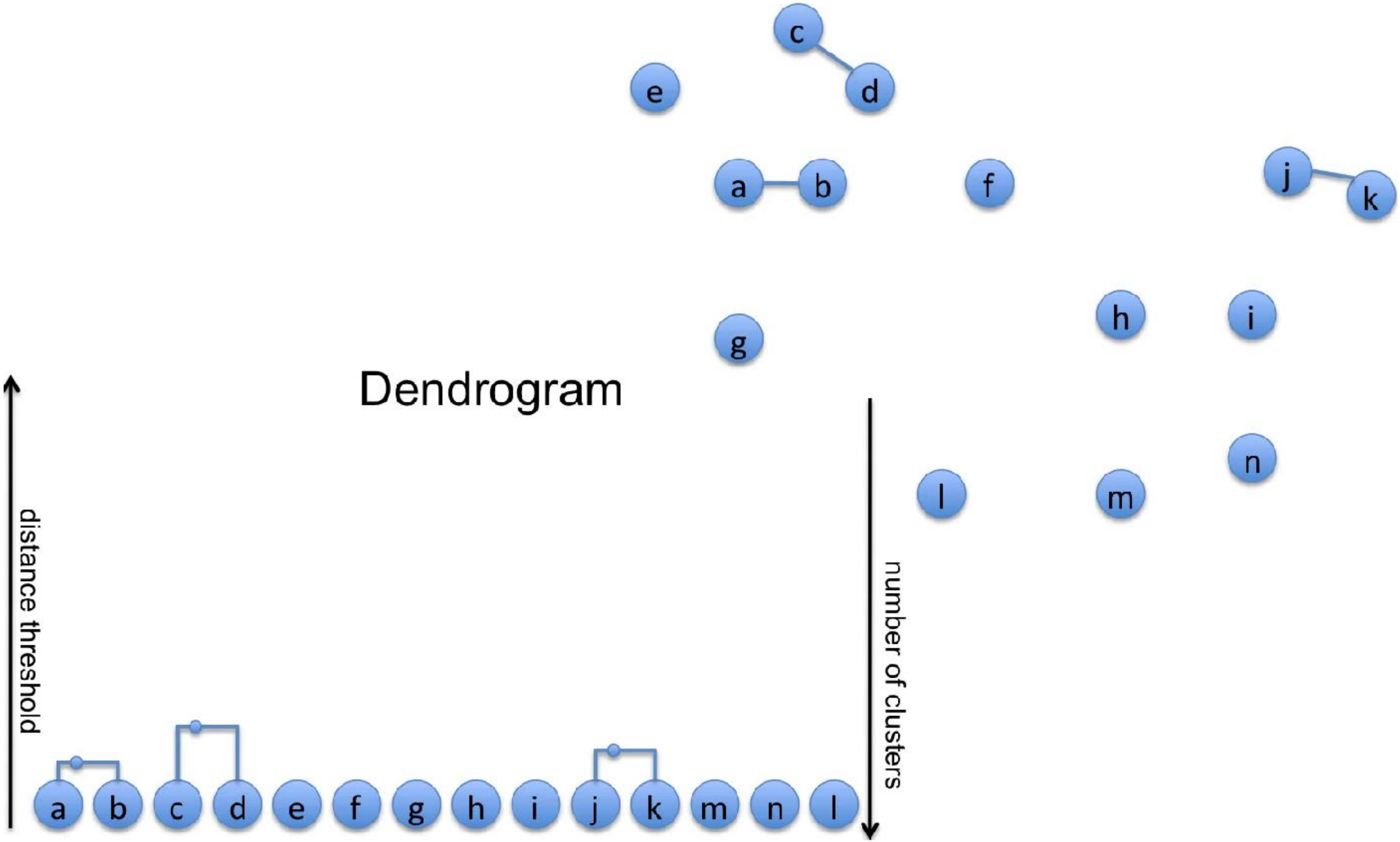
l

Dendrogram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distance threshold
number of clusters
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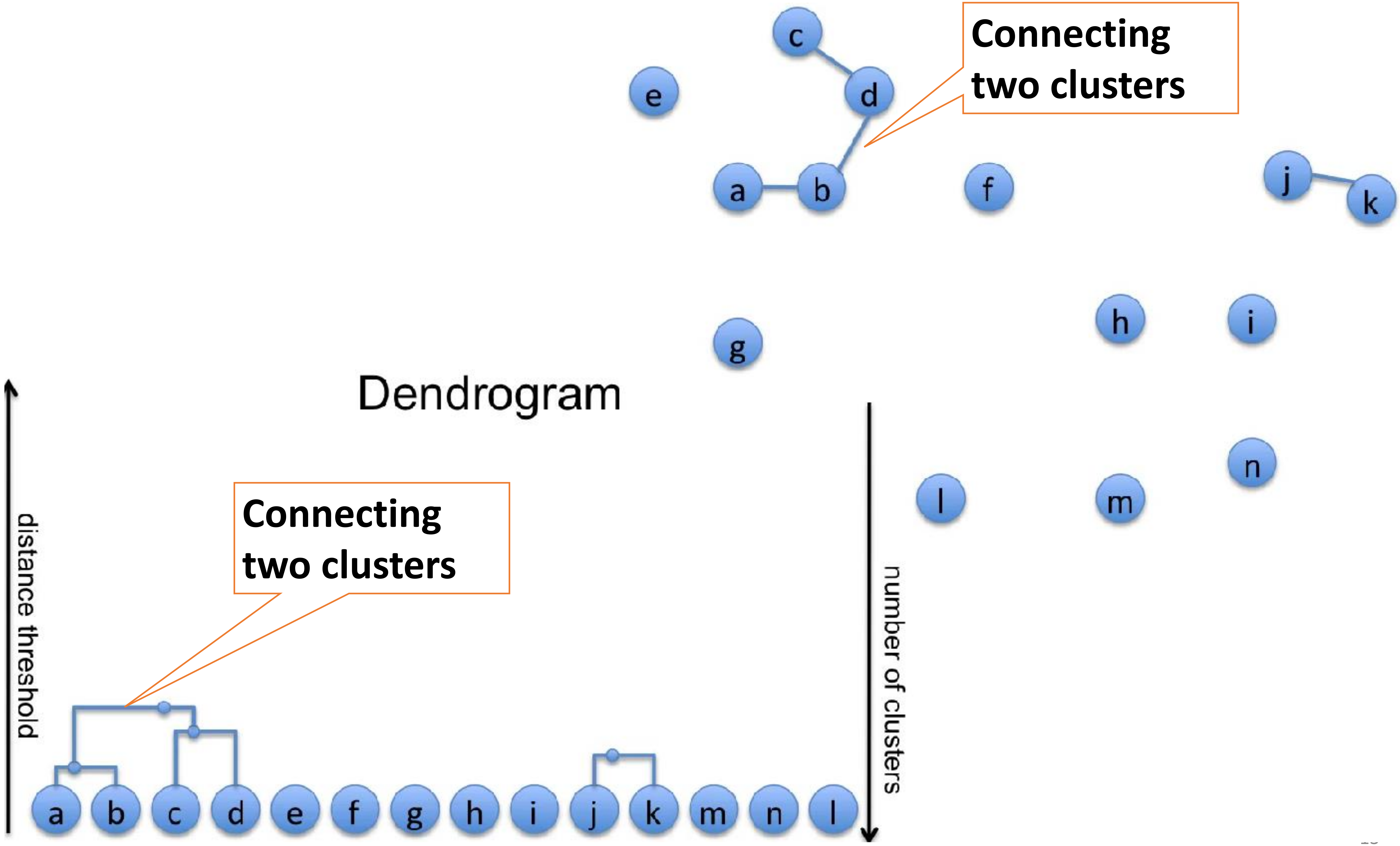
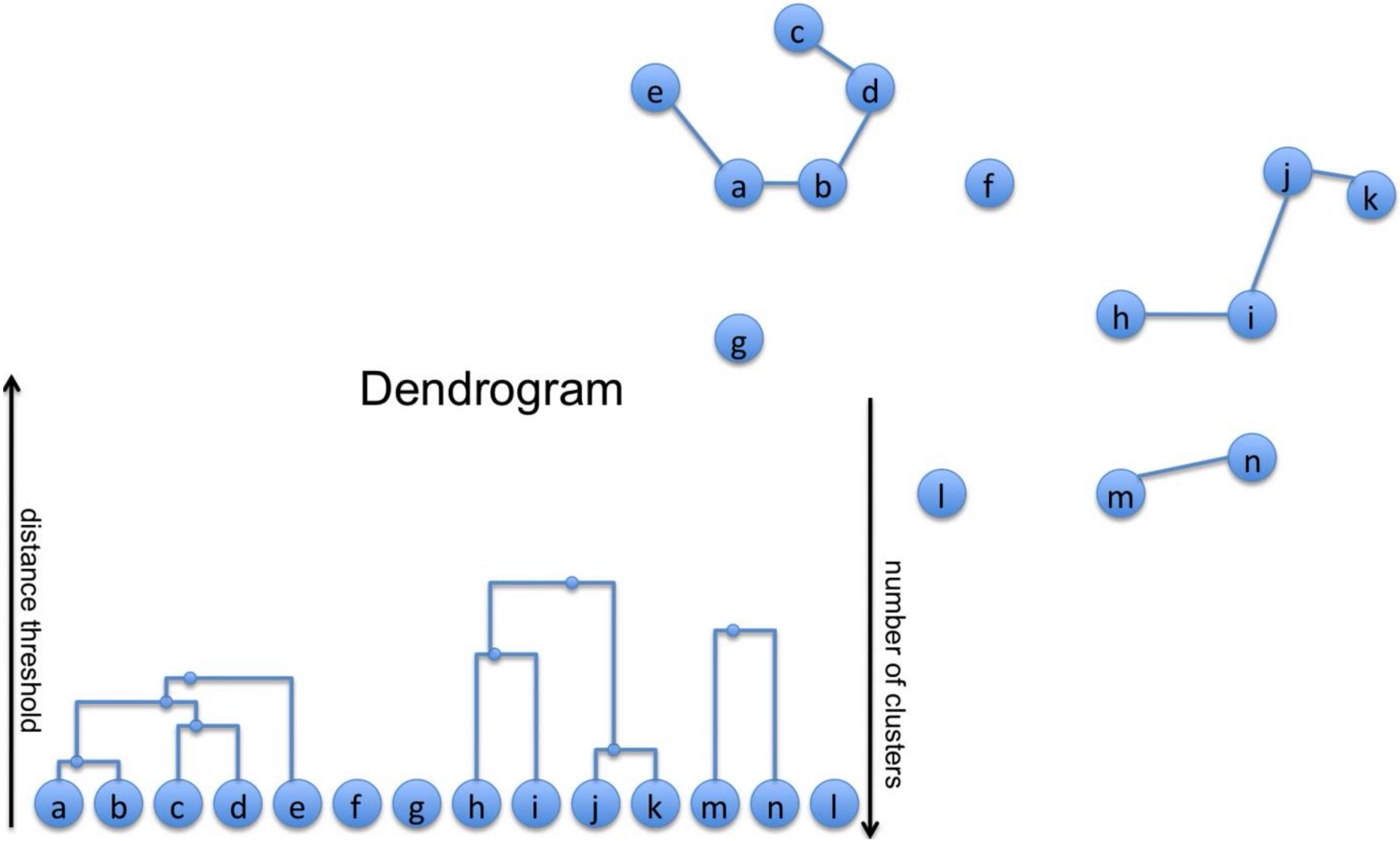


Connecting two clusters

Dendrogram

Connecting two clusters

Dendrogram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distance threshold
number of clusters
a
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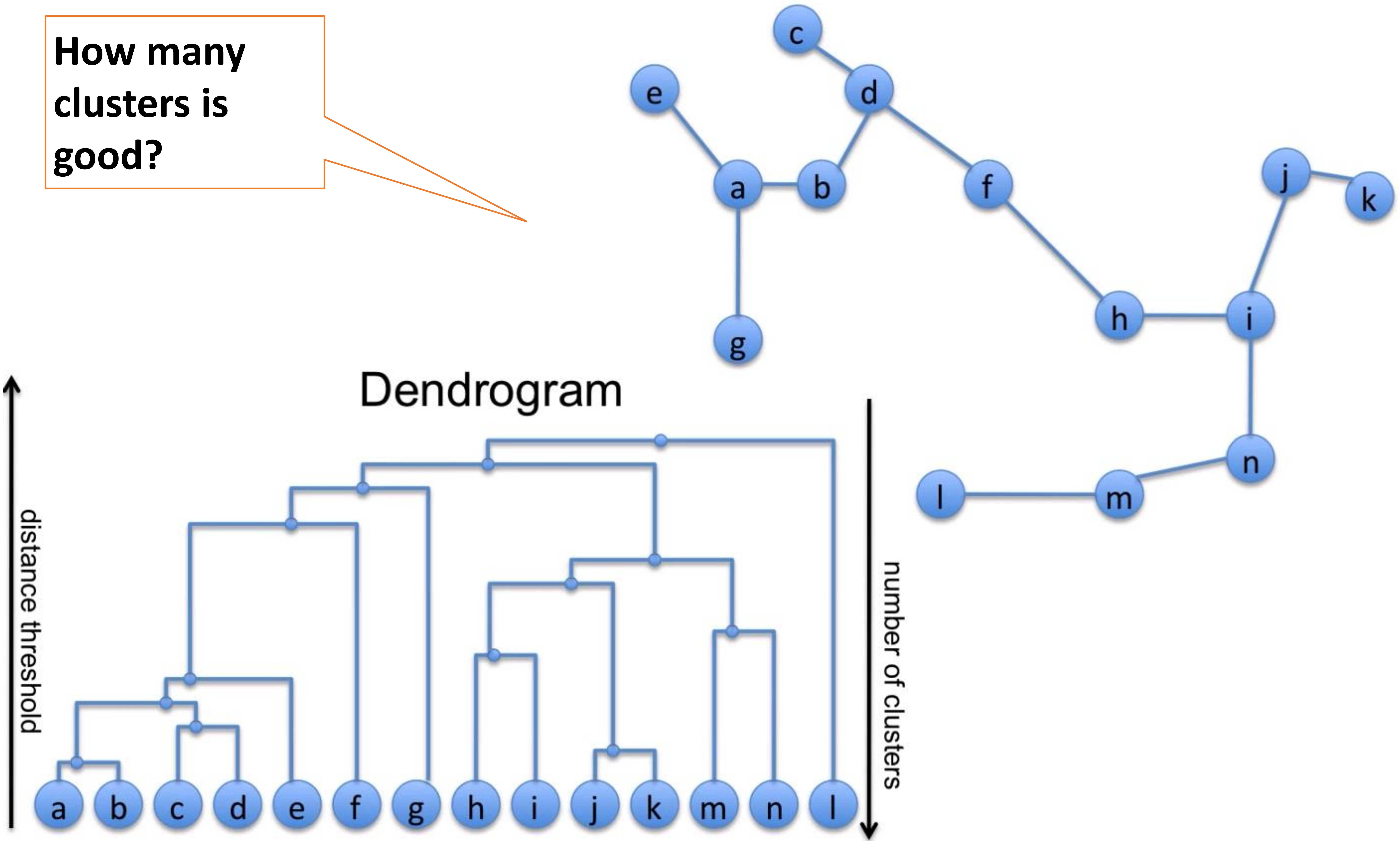
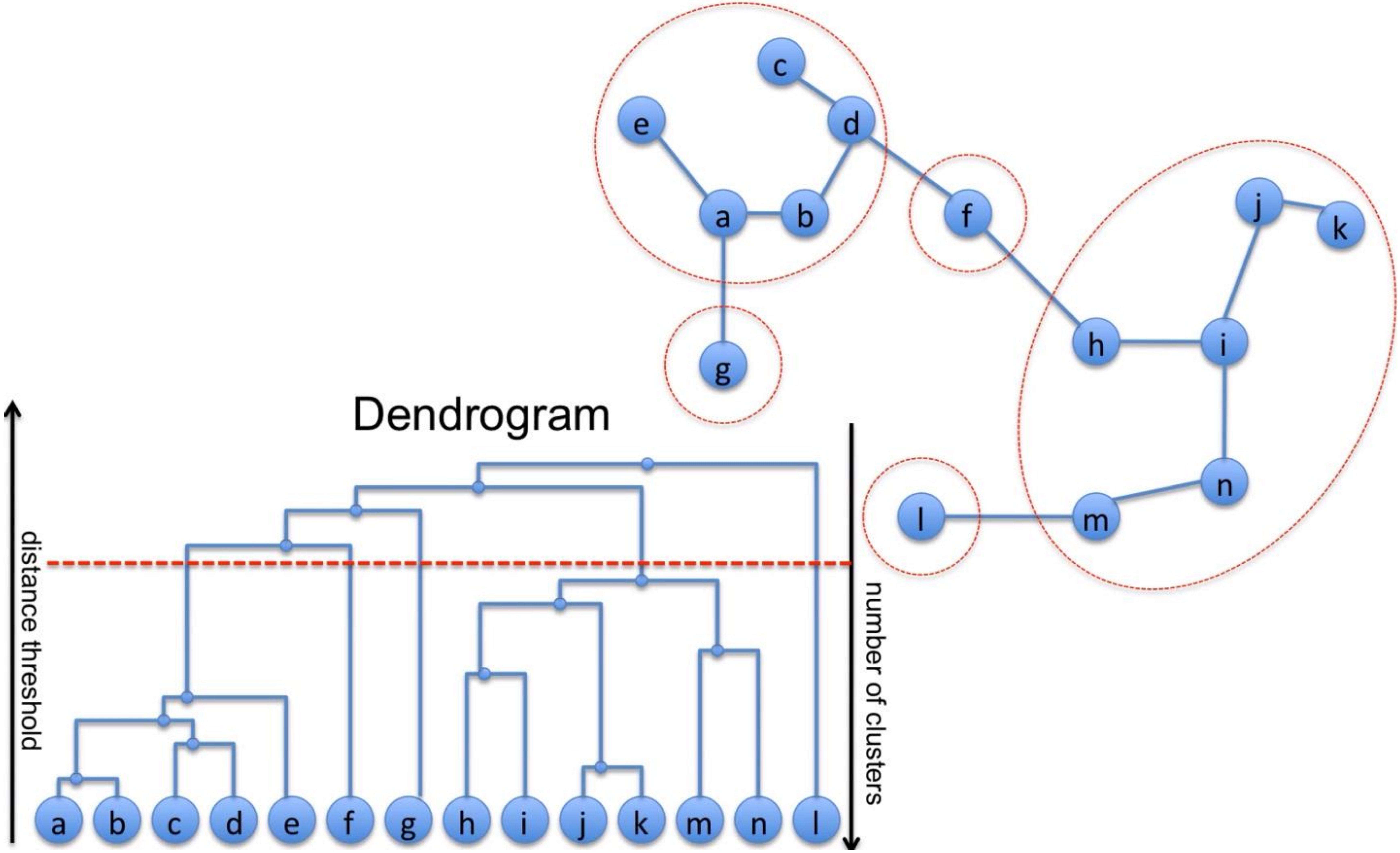


How many clusters is good?

Dendrogram



Dendrogram

c
e
d
a
b
f
g
j
k
h
i
n
l
m
distance threshold
number of clusters
a
b
c
d
e
f
g
h
i
j
k
m
n
l

Agglomerative clustering

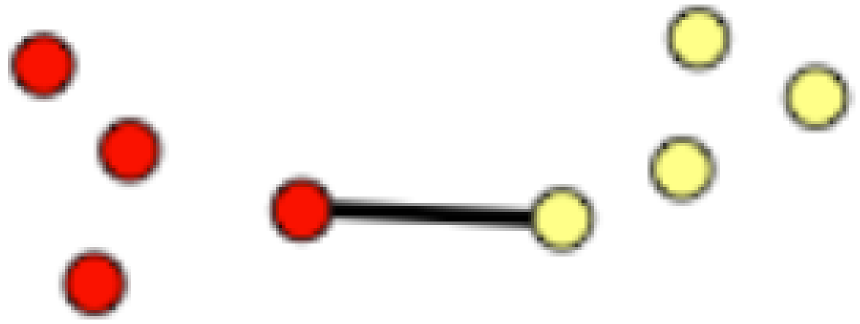
- Idea: Nearby points end up in same cluster
- Algorithm
  - Start with collection C of N singleton clusters
  - cj = {xj}
  - Find another cluster that is closest min ij (ci, cj)
  - Merge ci and cj into new cluster ci+j
  - Remove ci and cj from C. Add ci+j
  - Repeat
- Slower algorithm
- Understand with dendrogram (connectivity tree)

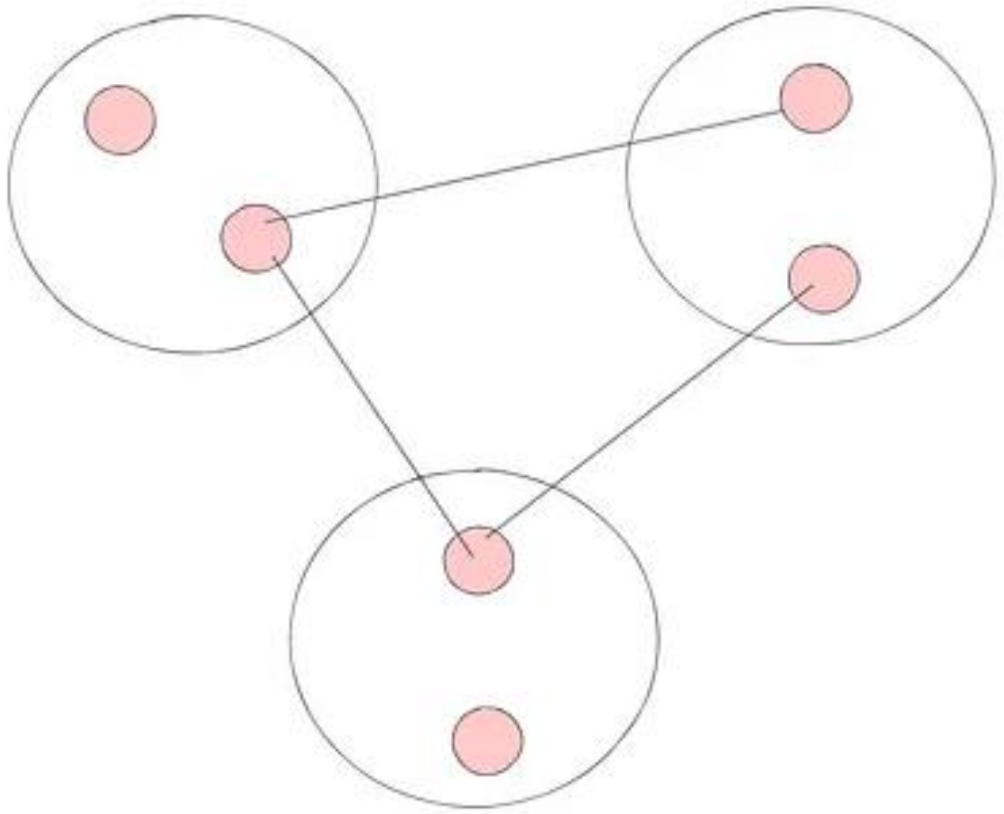
Cluster distance metric for hierarchical clustering

- Distance between clusters
- Not individual points
- Single Link
  - Distance b/w closest elements of clusters

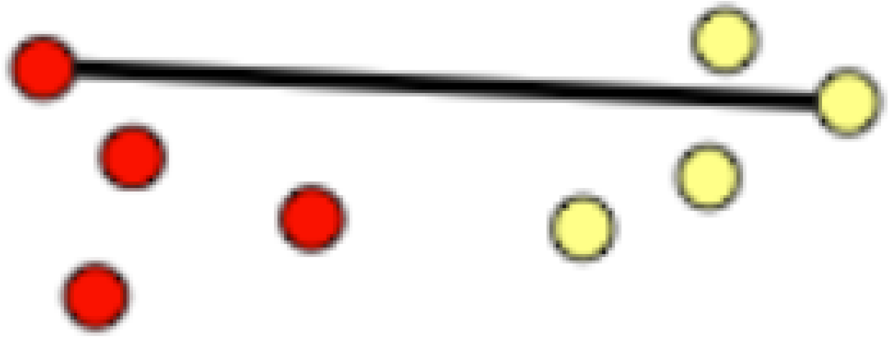
$$\mathcal{D}(c_1, c_2) = \min_{x_1 \in c_1, x_2 \in c_2} \mathcal{D}(x_1, x_2)$$

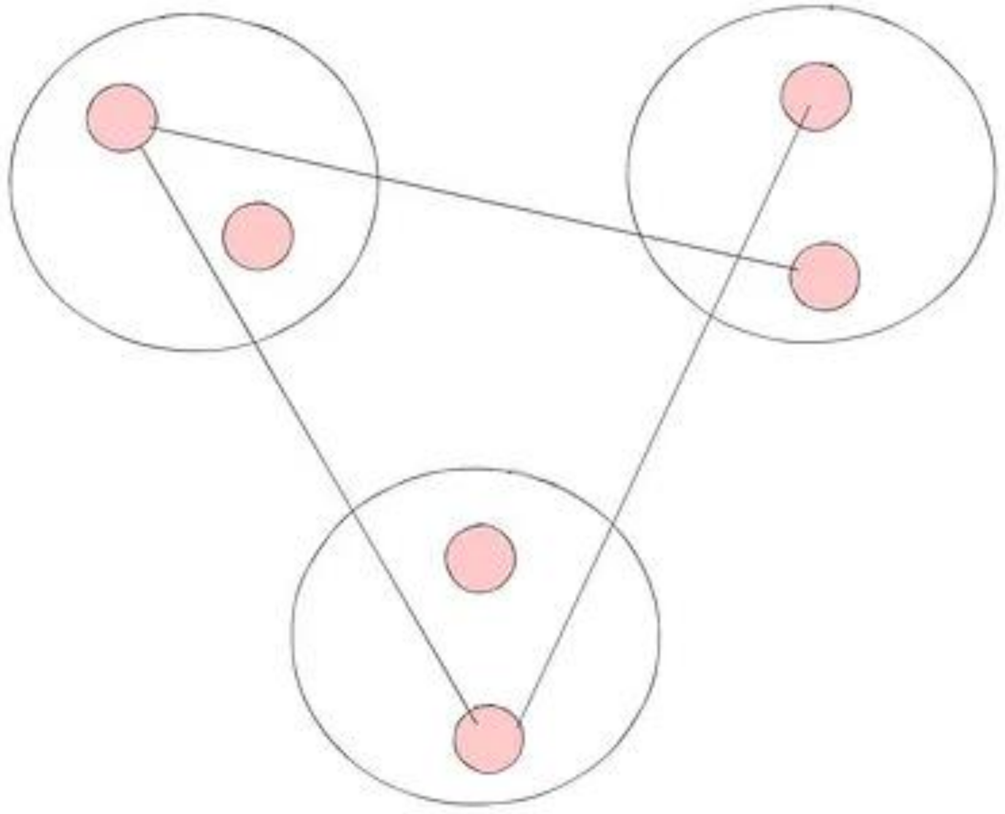
  - Produces long chains





- Complete Link





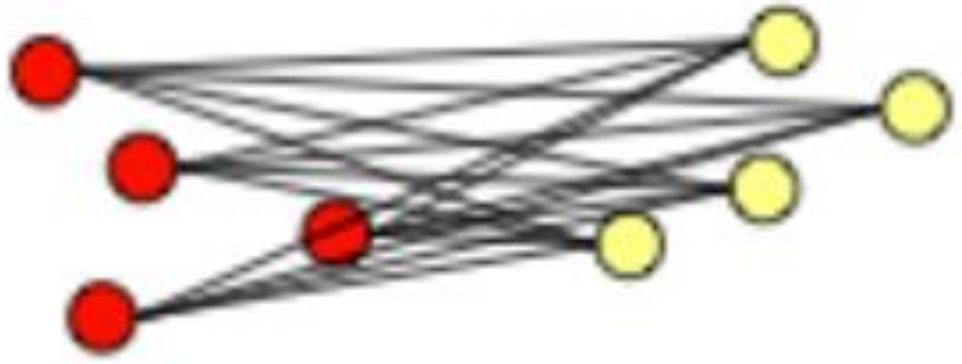
  - Distance b/w farthest elements of clusters

$$\mathcal{D}(c_1, c_2) = \max_{x_1 \in c_1, x_2 \in c_2} \mathcal{D}(x_1, x_2)$$

  - Produces spherical clusters

Cluster distance metric for hierarchical clustering

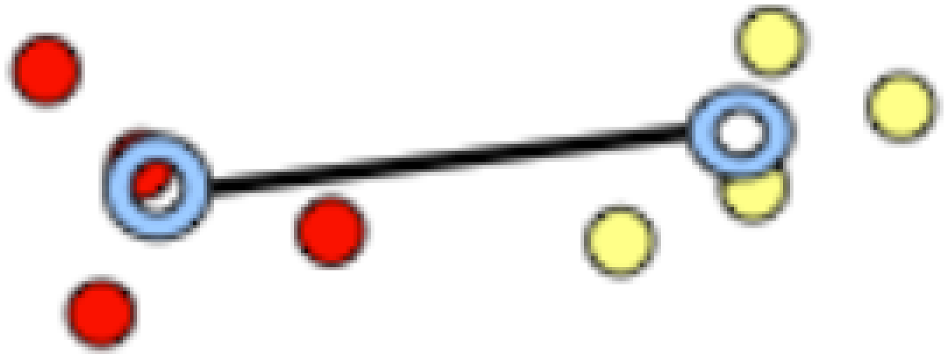
- Average Link



$$\mathcal{D}(c_1, c_2) = \frac{1}{|c_1||c_2|} \sum_{x_1 \in c_1} \sum_{x_2 \in c_2} \mathcal{D}(x_1, x_2)$$

  - Avg of pairwise distance b/w cluster elements
  - Less affected by outliers

- Centroid Link

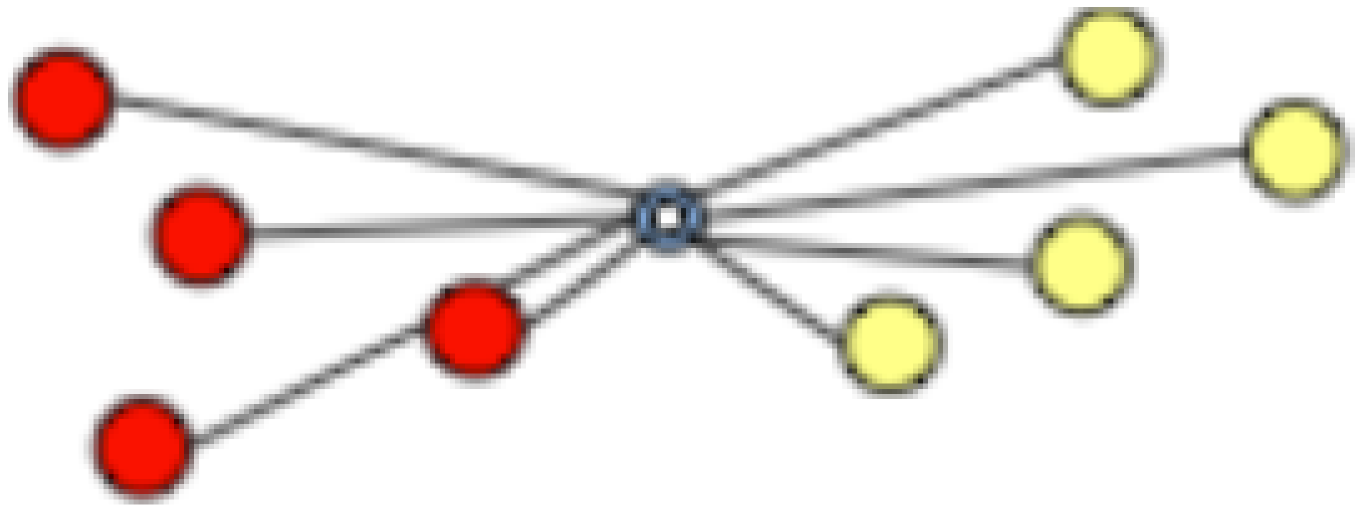


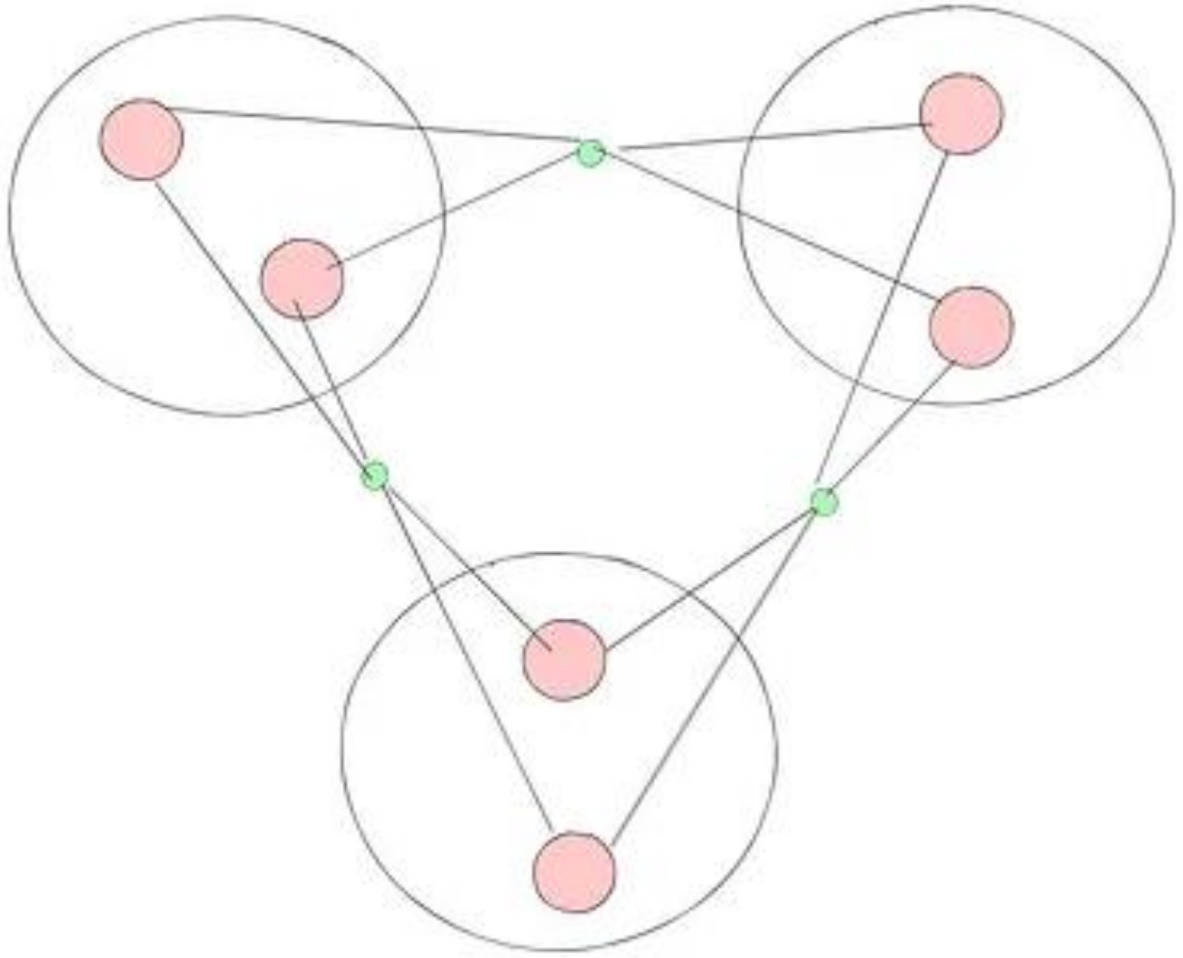
  - Distance b/w cluster centroids

$$\mathcal{D}(c_1, c_2) = \mathcal{D}\left((\frac{1}{|c_1|} \sum_{x_1 \in c_1}) \ , \ (\frac{1}{|c_2|} \sum_{x_2 \in c_2}) \right)$$

Cluster distance metric for hierarchical clustering

- Ward Link
  - If the two clusters were to join
  - What will be their mean and standard deviation?
  - The two clusters with minimum SD will be merged





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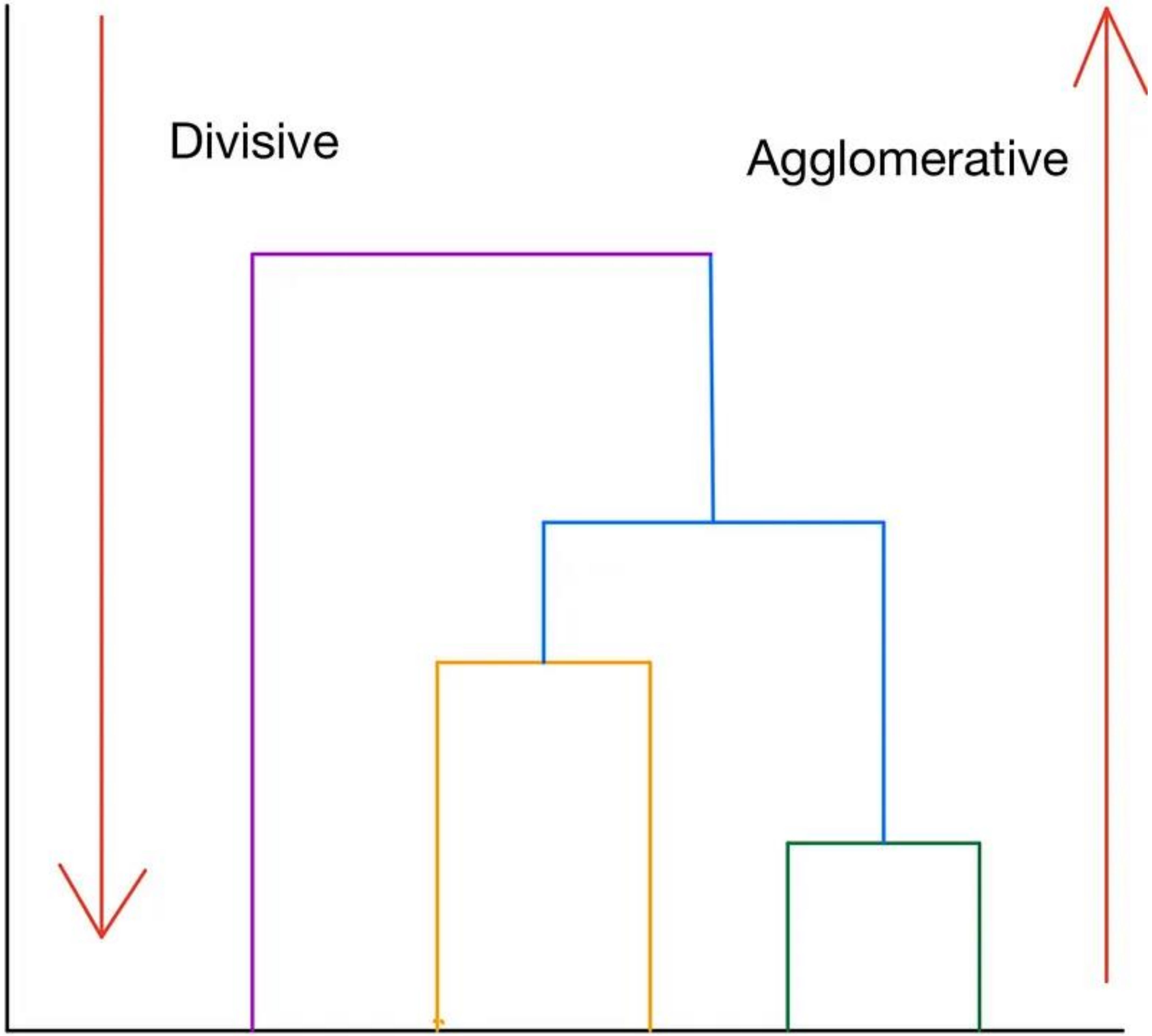
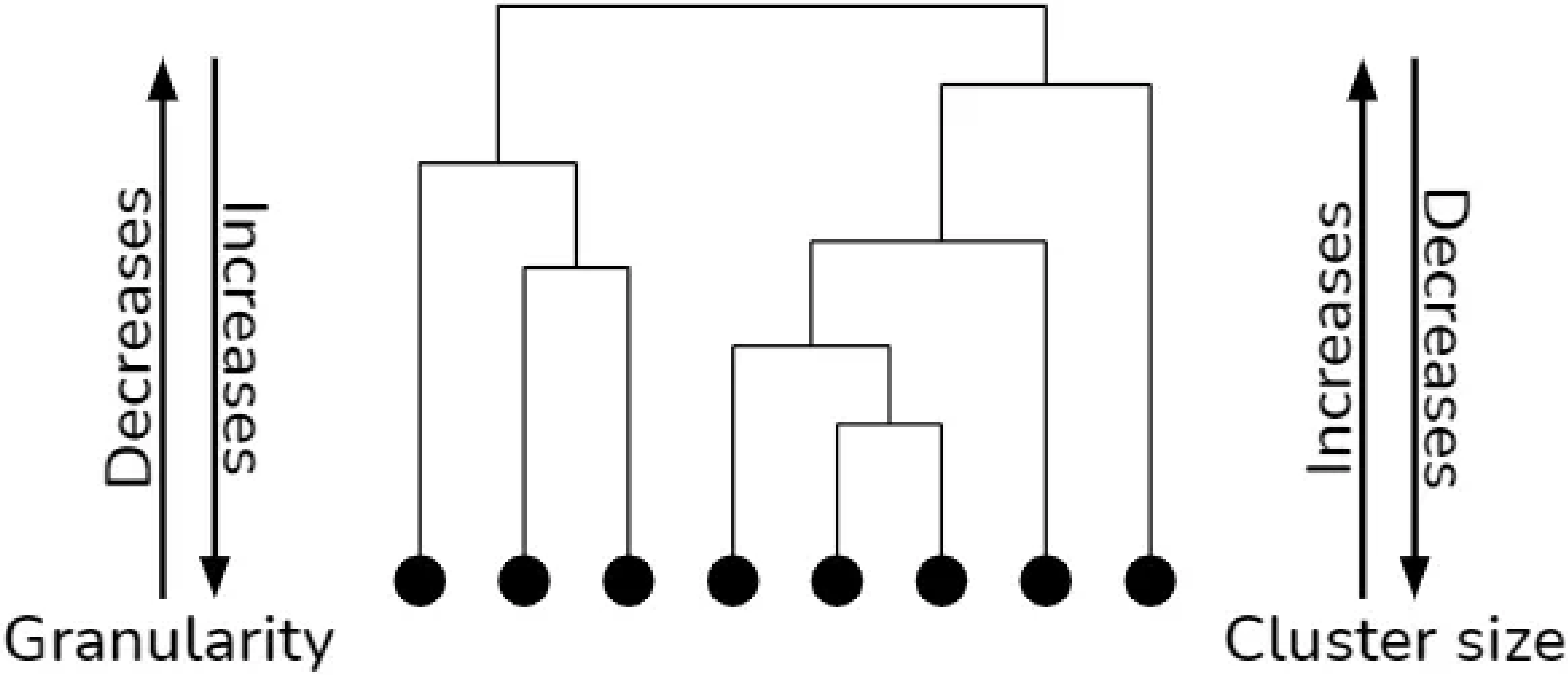
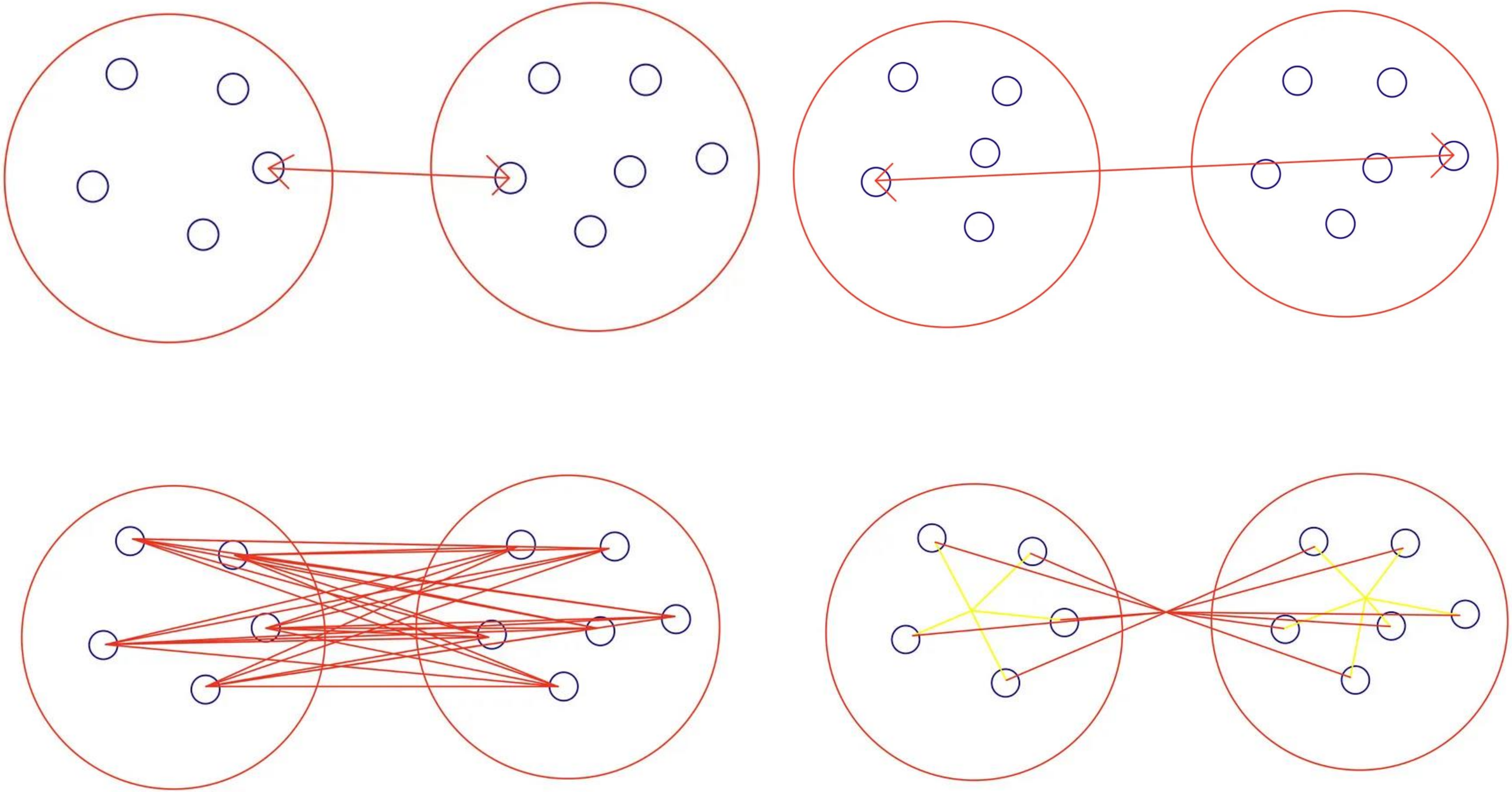
x̄₃ = 4+7+1+6 = 18
log_b b^x = x
log_a x = log_b x / log_b a
a/b + c/d = ad+bc / bd
f = R/2
C₂H₂Cl₄ + Ca(OH)₂ → C₂HCl₃+CaCl₂+H₂O
Zn₃Sb₂+6H₂O → 3Zn(OH)₂+2SbH₃
2NH₃
2HI
2SO₃
C₂O+CO₂
A
B
C
n₁
n₂
θ₁
θ₂
v₁
v₂
CH₃
HO
H₃C
(a+bi)+(c+di) = a+c+(b+d)i
(a+bi)-(c+di) = a-c+(b-d)i

Recap


Divisive
Agglomerative


Decreases
Increases
Granularity
Increases
Decreases
Cluster size



Connectivity v/s other clustering algorithms

- Compactness (Cluster cohesion)
- Separation

$$Index = \frac{(\alpha \times Separation)}{(\beta \times Compactness)}$$

- Density – looks for a point within a epsilon distance
- Connectivity – No upper limit on nearest point distance
  - No good evaluation metric
  - Empirical or distance metric should capture domain knowledge

QUESTIONS