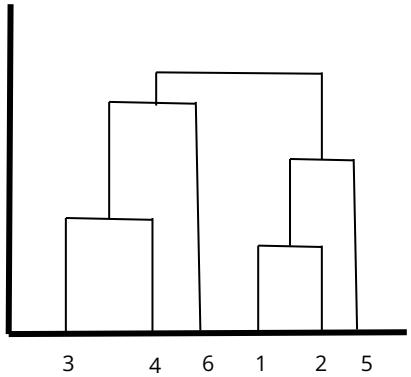
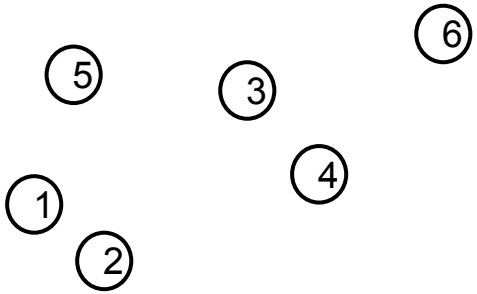
Hierarchical Clustering

Boston University CS 506 - Lance Galletti

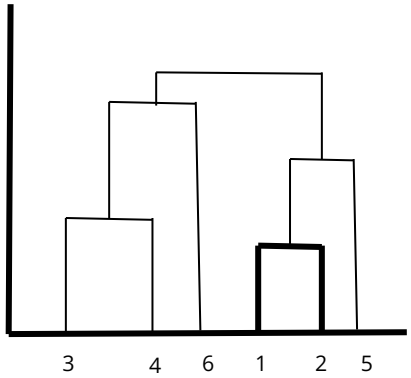
Hierarchical Clustering

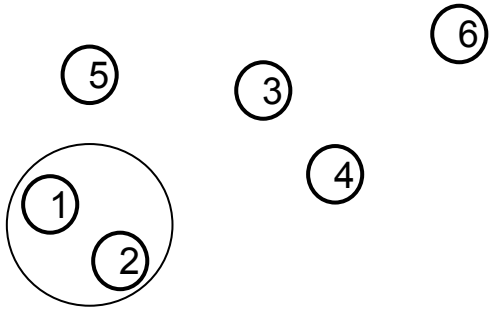




Hierarchical Clustering

At every step, we record which clusters were merged in order to produce a dendrogram:





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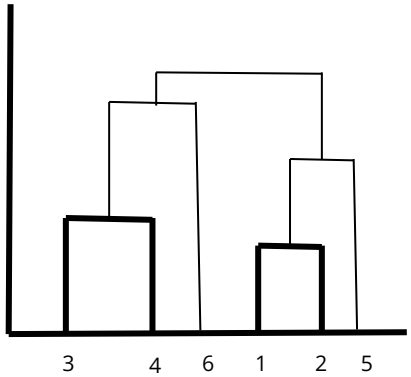

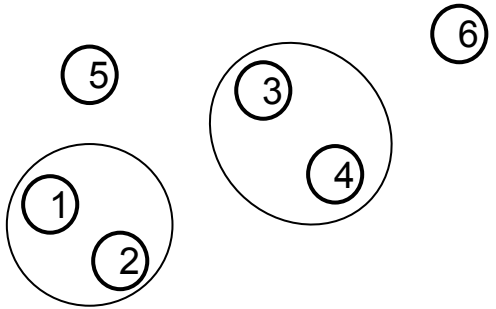

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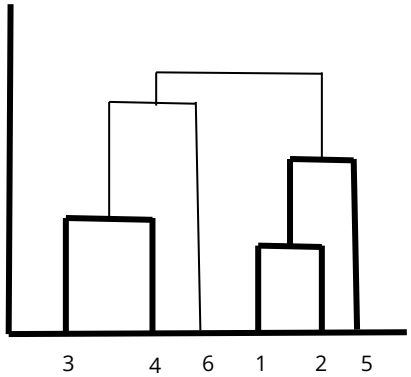

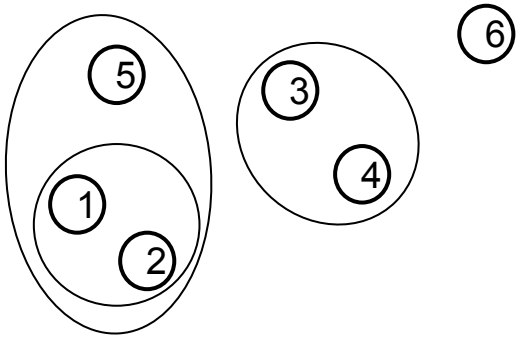

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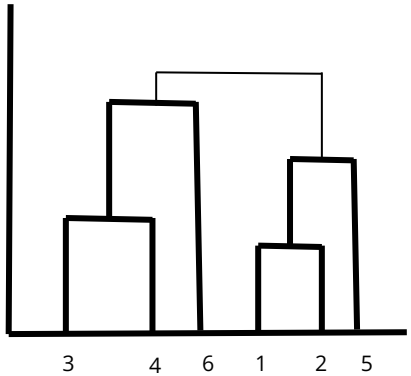

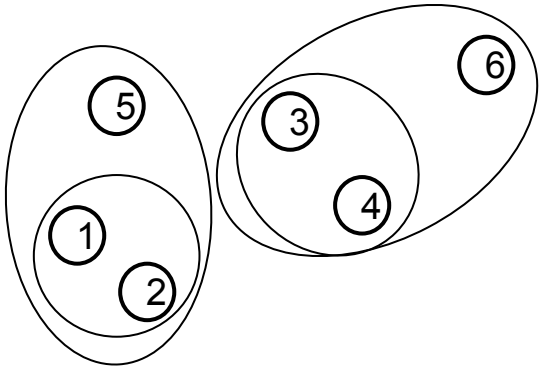

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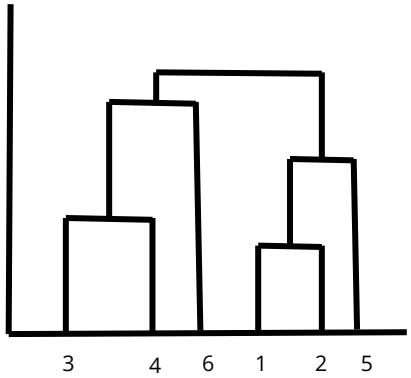
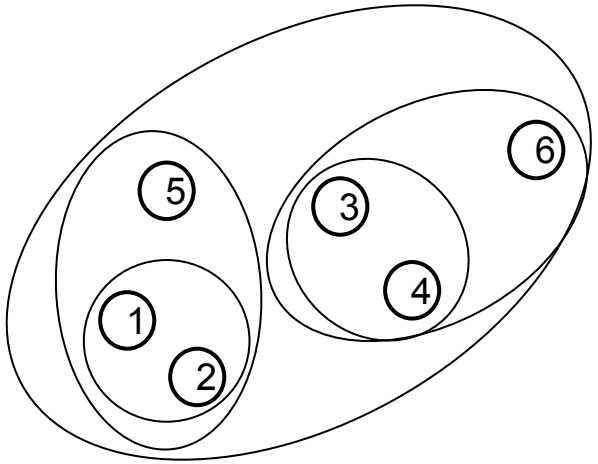
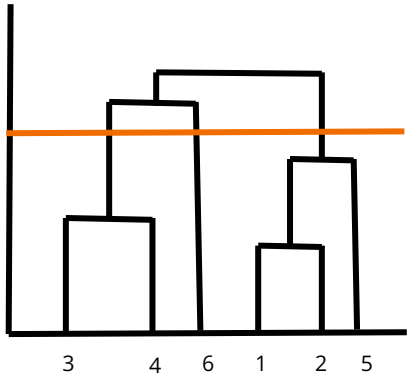
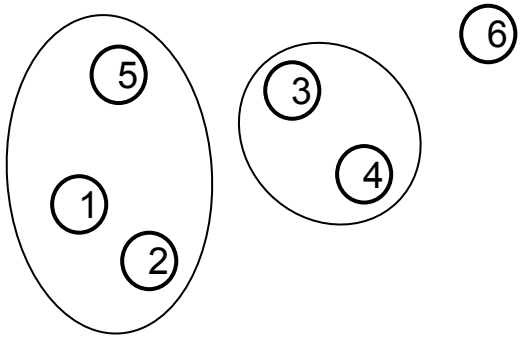




Hierarchical Clustering

We can “cut” the dendrogram at any threshold to produce any number of clusters





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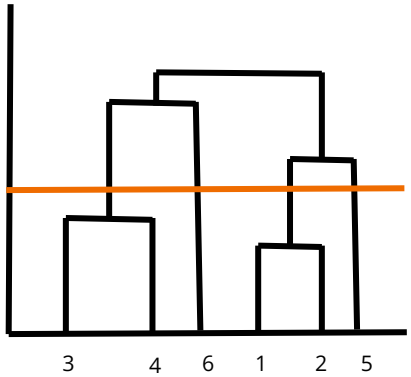

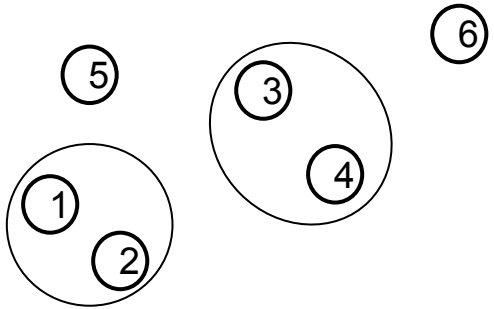

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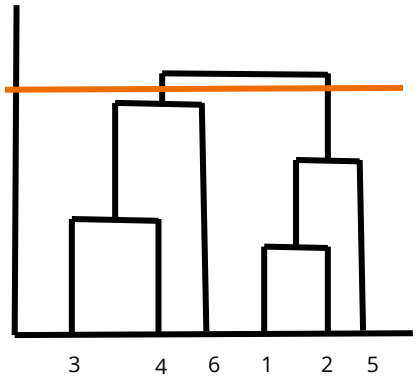
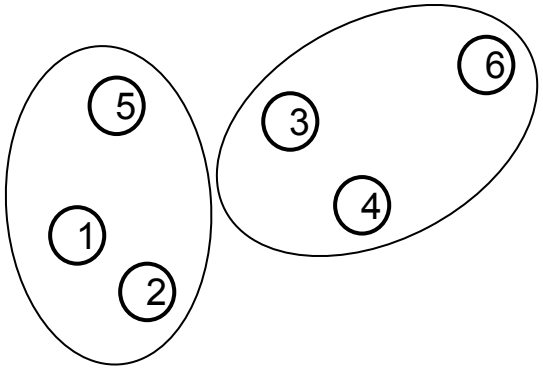




Example

https://www.catalogueoflife.org/

Hierarchical Clustering

Two types of hierarchical clustering:

Agglomerative:

1. Start with every point in its own cluster
2. At each step, merge the two closest clusters
3. Stop when every point is in the same cluster

Divisive:

1. Start with every point in the same cluster
2. At each step, split until every point is in its own cluster

Agglomerative Clustering Algorithm

1. Let each point in the dataset be in its own cluster
2. Compute the distance between all pairs of clusters
3. Merge the two closest clusters
4. Repeat 3 & 4 until all points are in the same cluster

Hierarchical Clustering

Can we implement this? Are we missing anything?

How would you define distance between clusters?

Hierarchical Clustering - Distance Functions

Let's first define:

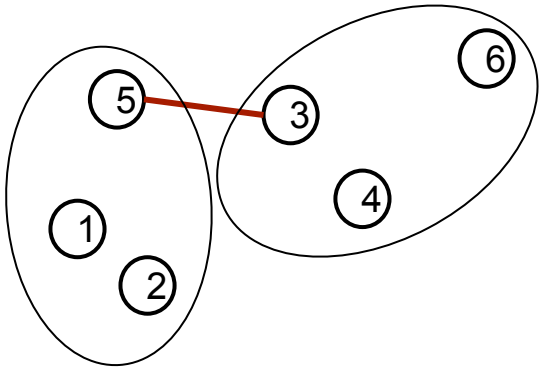
Distance between points: $\mathbf{d(p_1, p_2)}$

Distance between clusters: $\mathbf{D(C_1, C_2)}$

Single-Link Distance

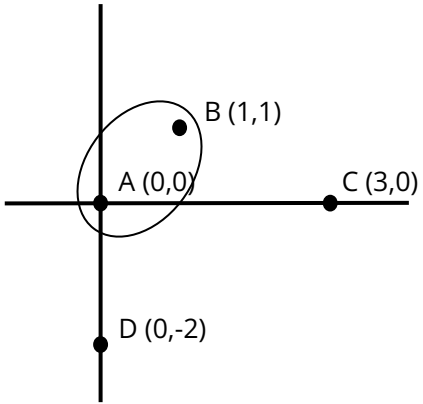
Is the **minimum** of all pairwise distances between a point from one cluster and a point from the other cluster.

$$D_{SL}(C_1, C_2) = \min \{d(p_1, p_2) \mid p_1 \in C_1, p_2 \in C_2\}$$



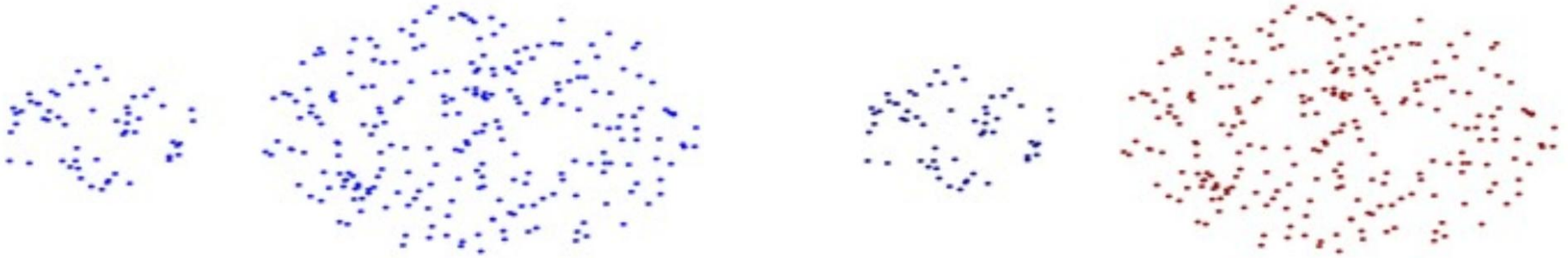
Depends on choice of **d**

Q: Single-Link Distance



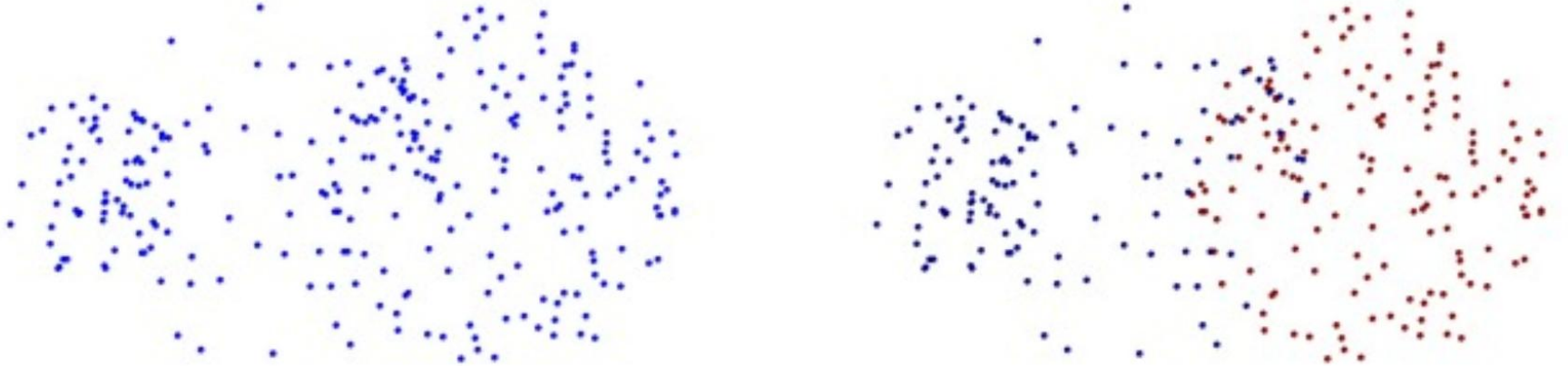
Is C or D closer to {A, B} ?

Single-Link Distance



Can handle clusters of different sizes

Single-Link Distance

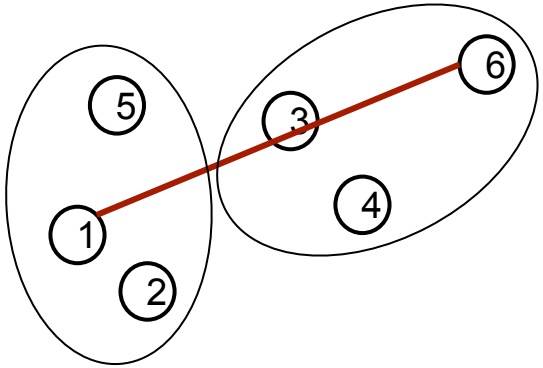


But... Sensitive to noise points
Tends to create elongated clusters

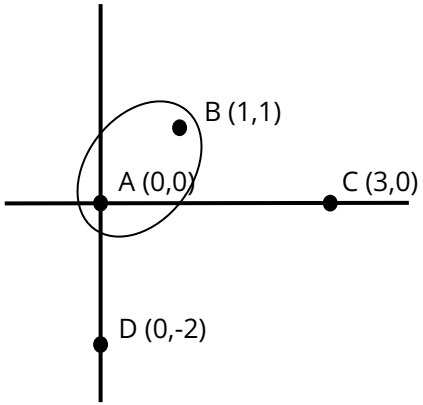
Complete-Link Distance

Is the **maximum** of all pairwise distances between a point from one cluster and a point from the other cluster.

$$D_{CL}(C_1, C_2) = \max \{ d(p_1, p_2) \mid p_1 \in C_1, p_2 \in C_2 \}$$

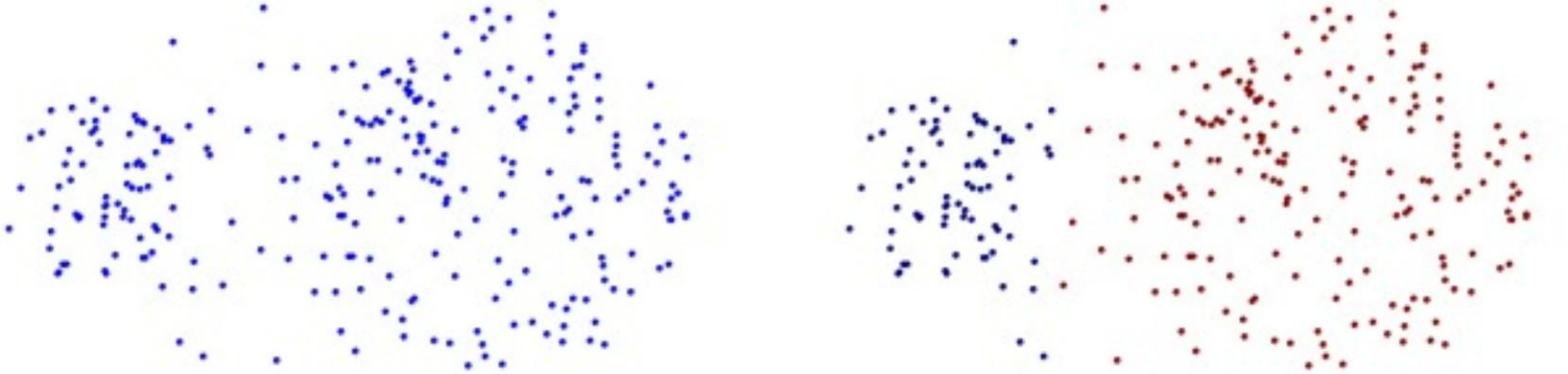


Q: Complete-Link Distance



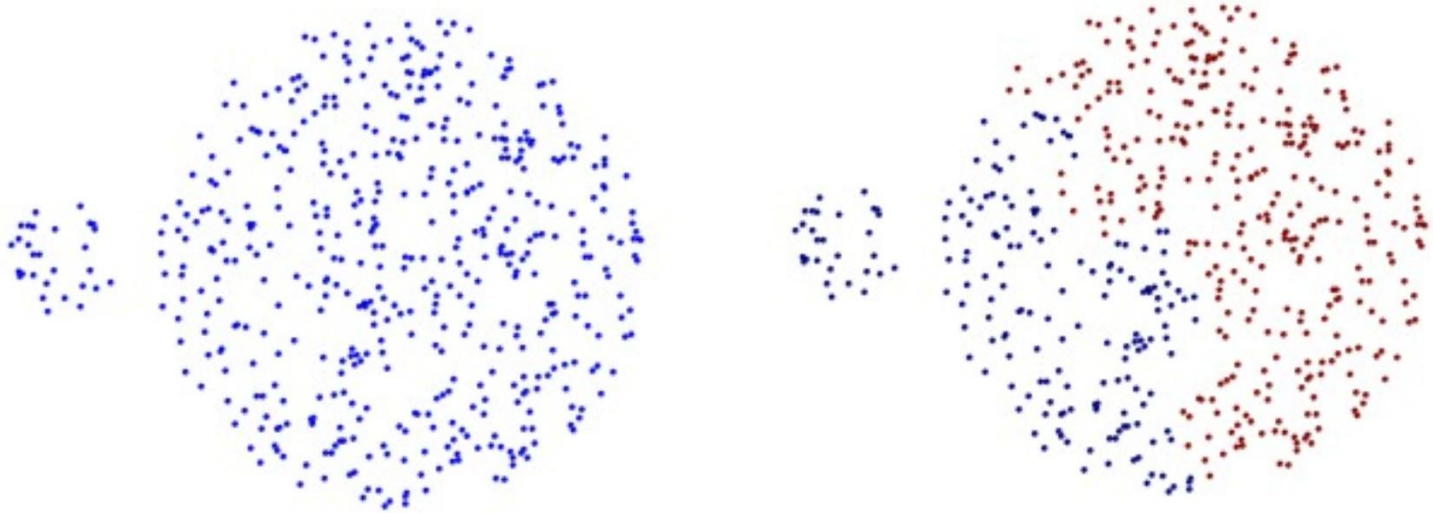
Is C or D closer to {A, B} ?

Complete-Link Distance



Less susceptible to noise
Creates more balanced (equal diameter) clusters

Complete-Link Distance

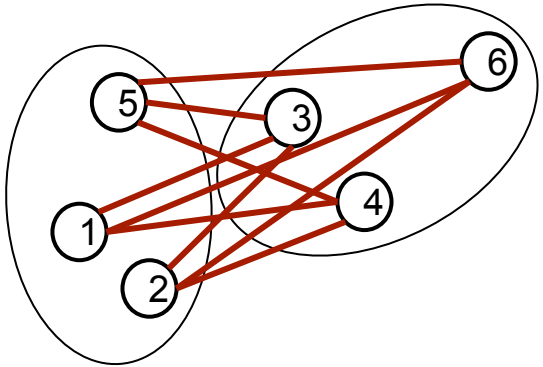


But... Tends to split up large clusters.
All clusters tend to have the same diameter

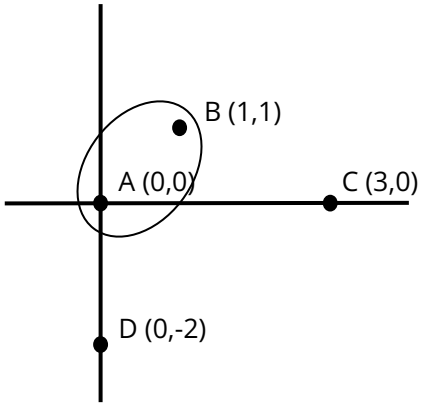
Average-Link Distance

Is the **average** of all pairwise distances between a point from one cluster and a point from the other cluster.

$$D_{AL}(C_1, C_2) = \frac{1}{|C_1| \cdot |C_2|} \sum_{p_1 \in C_1, p_2 \in C_2} d(p_1, p_2)$$



Q: Average-Link Distance



Is C or D closer to {A, B} ?

Average-Link Distance

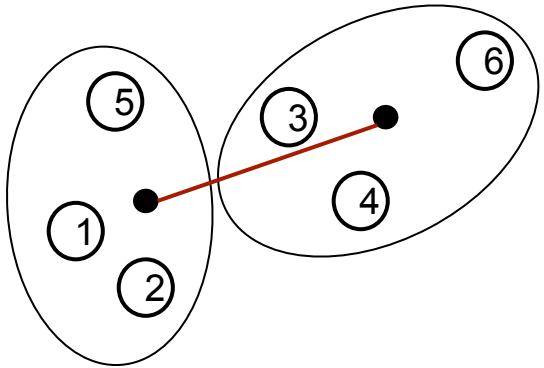
Less susceptible to noise and outliers.

But… Tends to be biased toward globular clusters

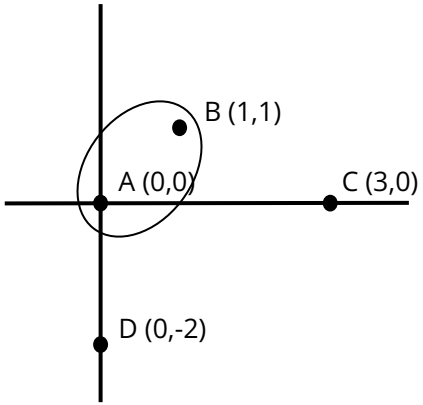
Centroid Distance

The distance between the centroids of clusters.

$$D_C(C_1, C_2) = d(\mu_1, \mu_2)$$



Q: Centroid Distance

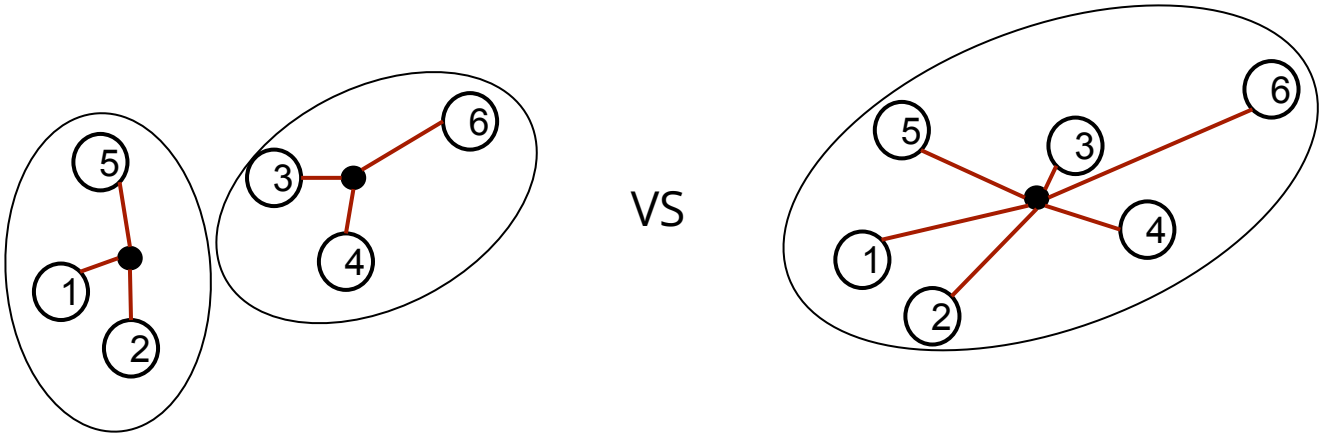


Is C or D closer to {A, B} ?

Ward's Distance

Is the difference between the spread / variance of points in the merged cluster and the unmerged clusters.

$$D_{WD}(C_1, C_2) = \sum_{p \in C_{12}} d(p, \mu_{12}) - \sum_{p_1 \in C_1} d(p_1, \mu_1) - \sum_{p_2 \in C_2} d(p_2, \mu_2)$$



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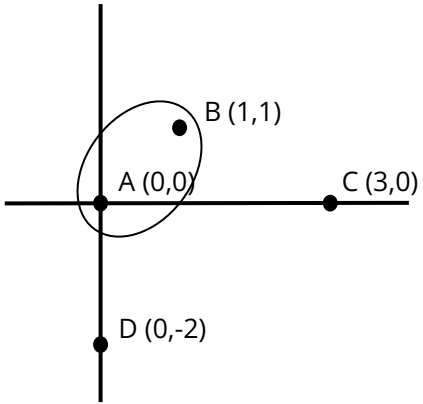

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Example

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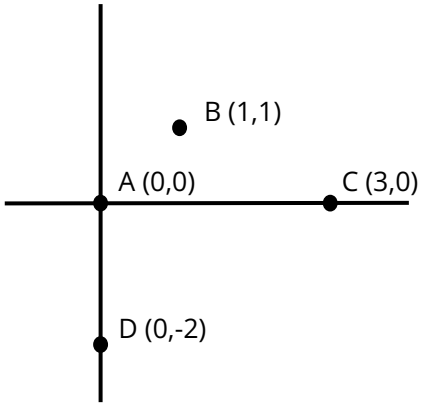
D = Single-Link



Distance Matrix

	A	B	C	D
A				
B				
C				
D				

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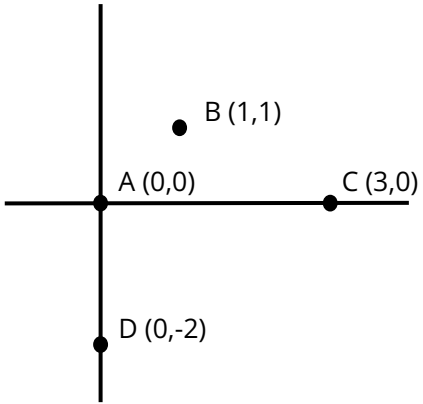

Distance Matrix

	A	B	C	D
A	0			
B		0		
C			0	
D				0

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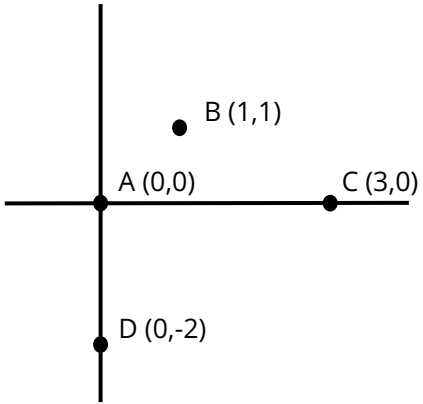

Distance Matrix

	A	B	C	D
A	0	√2	3	2
B	√2	0	√5	√10
C	5	√5	0	√13
D	2	√10	√13	0

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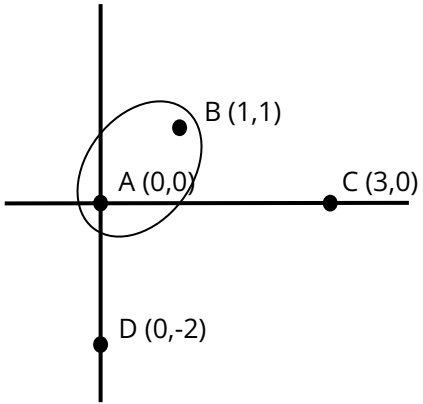

Distance Matrix

	A	B	C	D
A	0	√2	3	2
B	√2	0	√5	√10
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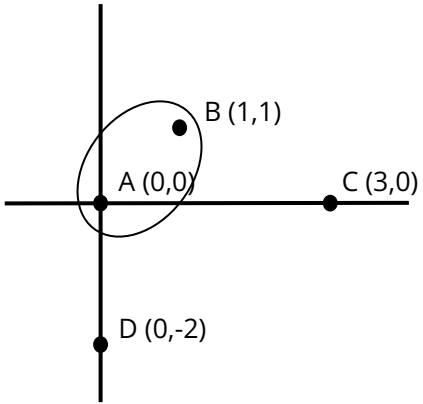
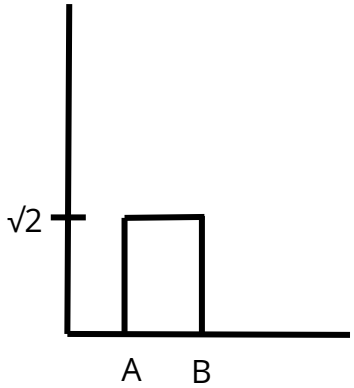


Dendrogram



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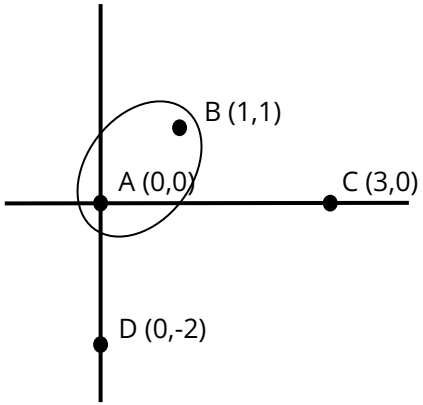

Distance Matrix

	A & B	C	D
A & B	0		
C		0	√13
D		√13	0

Example

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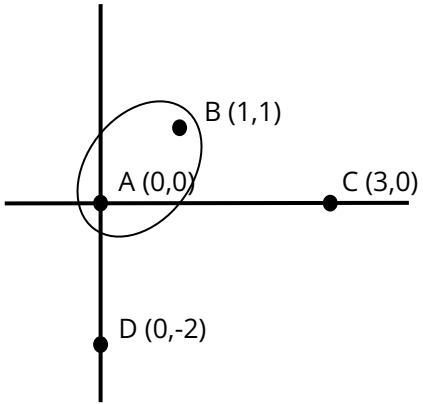

Distance Matrix

	A & B	C	D
A & B	0	√5	2
C	√5	0	√13
D	2	√13	0

Example

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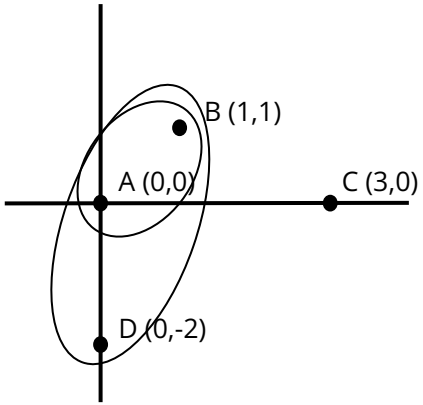
D = Single-Link



Distance Matrix

	A & B	C	D
A & B	0	√5	2
C	√5	0	√13
D	2	√13	0

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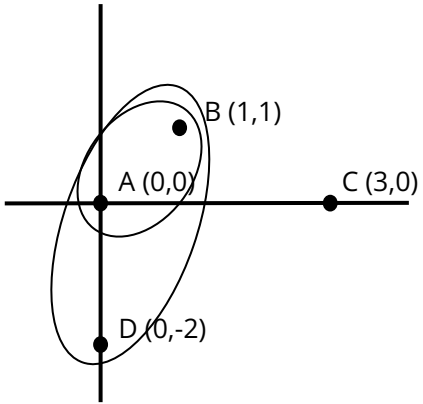

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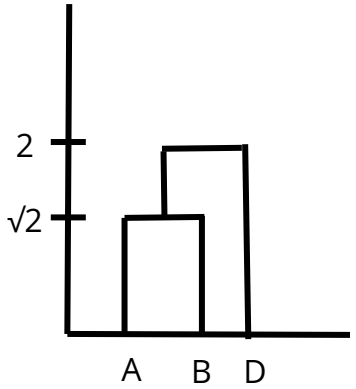

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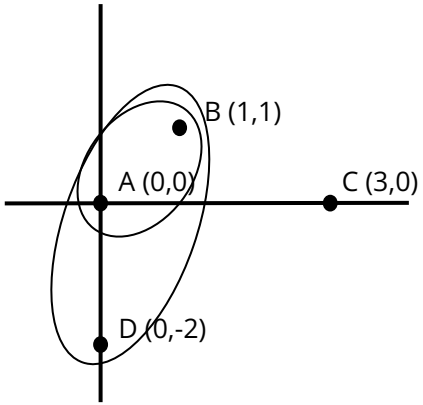
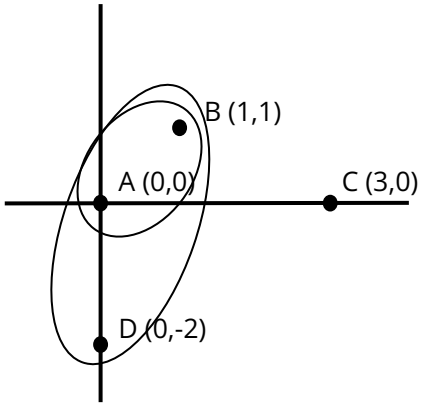


Distance Matrix

	A & B & D	C
A & B & D	0	
C		0

Example

d = Euclidean
D = Single-Link

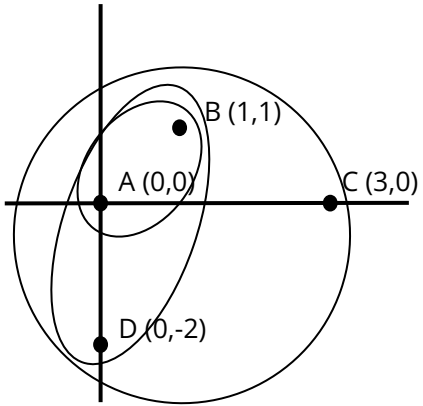


Distance Matrix

	A & B & D	C
A & B & D	0	√5
C	√5	0

Example

d = Euclidean
D = Single-Link

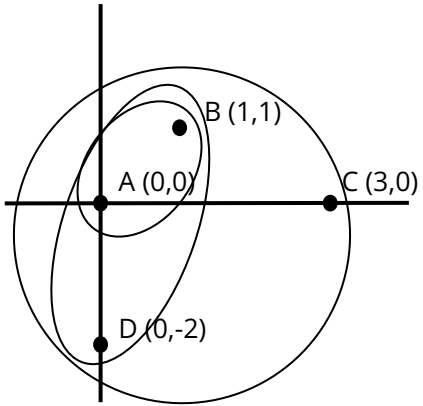


Distance Matrix

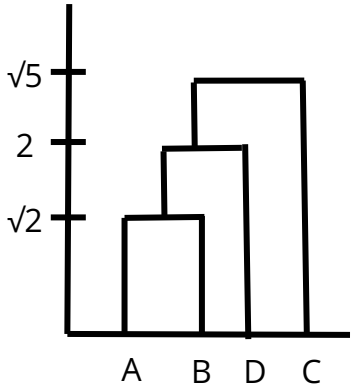
	A & B & D	C
A & B & D	0	√5
C	√5	0

Example

d = Euclidean
D = Single-Link



Dendrogram



Hierarchical Clustering

Finding the threshold with which to cut the dendrogram requires exploration and tuning. But in general hierarchical clustering is used to expose a hierarchy in the data (ex: finding/defining species via DNA similarity).

To capture the difference between clusterings you can use a cost function, or methods that we will discuss later when we look at clustering aggregation.