Hierarchical Clustering

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MACS 40800: Unsupervised Machine Learning

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Lecture Outline

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- Key difference between clustering approaches: **subdividing the data**
  - Hierarchical $\rightsquigarrow$ No
  - Partitioning $\rightsquigarrow$ Yes

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  - Check validation, especially if comparing across clustering algorithms (more next week)

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1. Quick Review
2. Hierarchical Clustering
3. Linkage Methods
4. Dendrograms & Tree Cutting
5. Divisive Hierarchical Clustering
6. Demonstration in R
7. Due Dates

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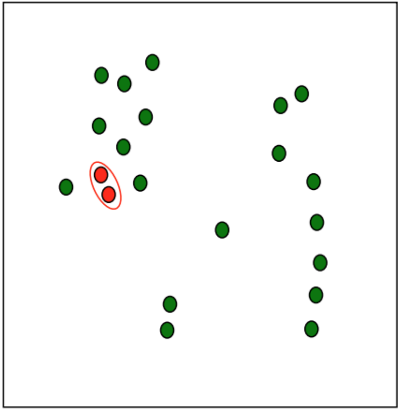
Hierarchical Clustering: The Idea



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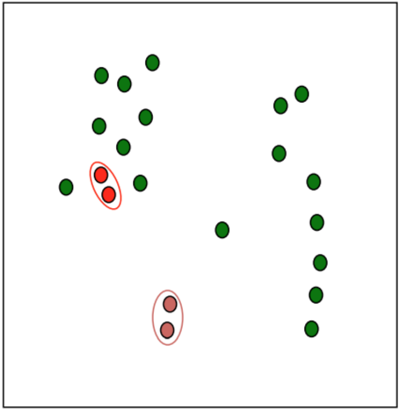

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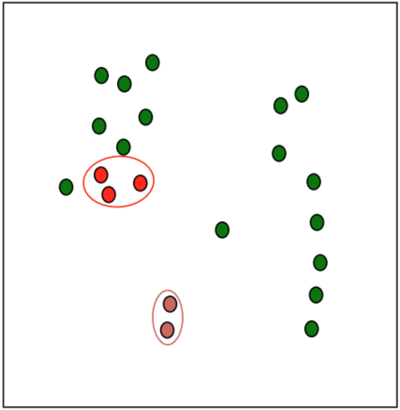

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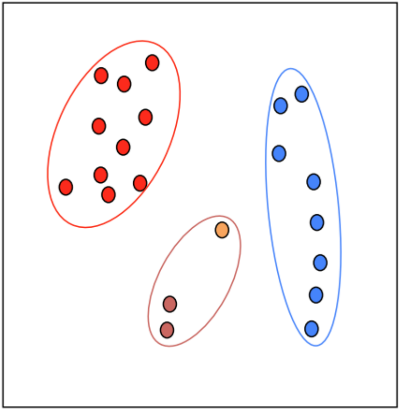

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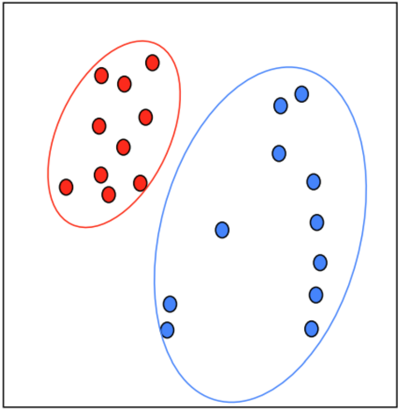

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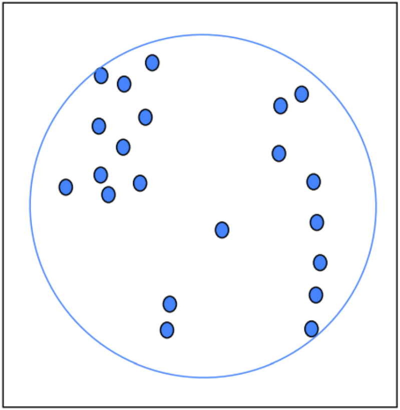

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- Stop when we reach k clusters ($k = 1$ in agglomerative; $k = n$ in divisive)

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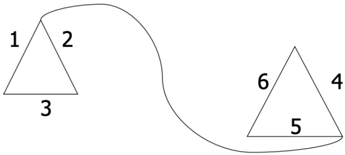

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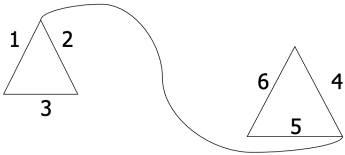

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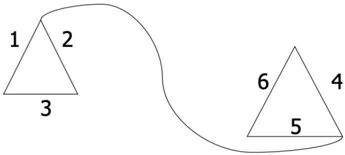

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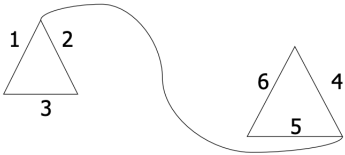

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- So how do we determine what constrains cluster fusion...?

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- There are five common types of linkage: complete, single, Ward's method, average, and centroid

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- **Ward's** linkage method joins the two clusters whose fusion is constrained by the smallest increase in SSE calculated per cluster, C,

$$\sum_{i=1}^{n}(x_i - \bar{x})^2$$

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- **Average** linkage uses the *mean* inter-cluster dissimilarity,

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- Therefore, the input for a hierarchical clustering algorithm is an $N \times N$ distance matrix, from which **inter-cluster distances** are calculated via the selected linkage method

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- So we can get clear clustering when branches along the Y axis are long (suggesting greater distance from other clusters), and less obvious clustering when the branches are shorter

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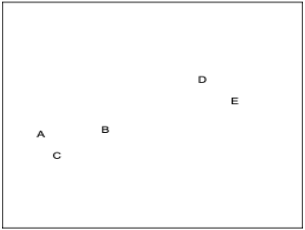

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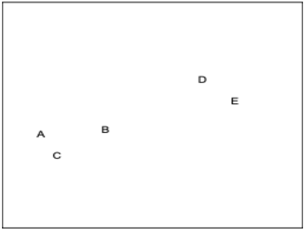

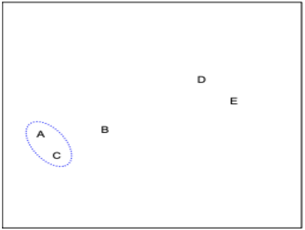

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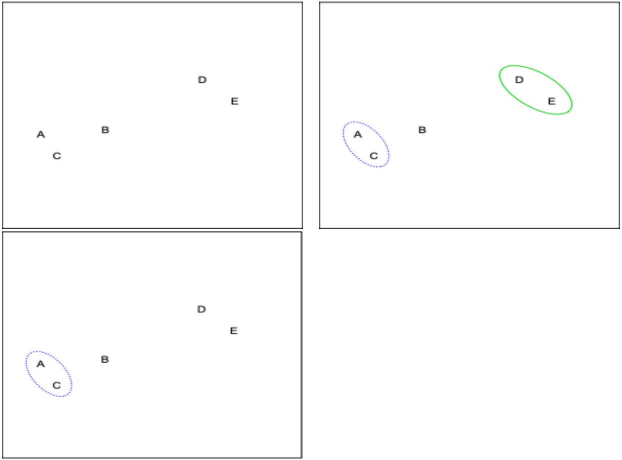

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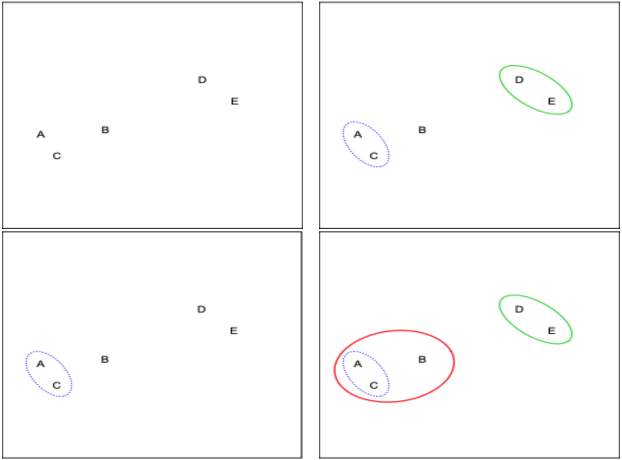

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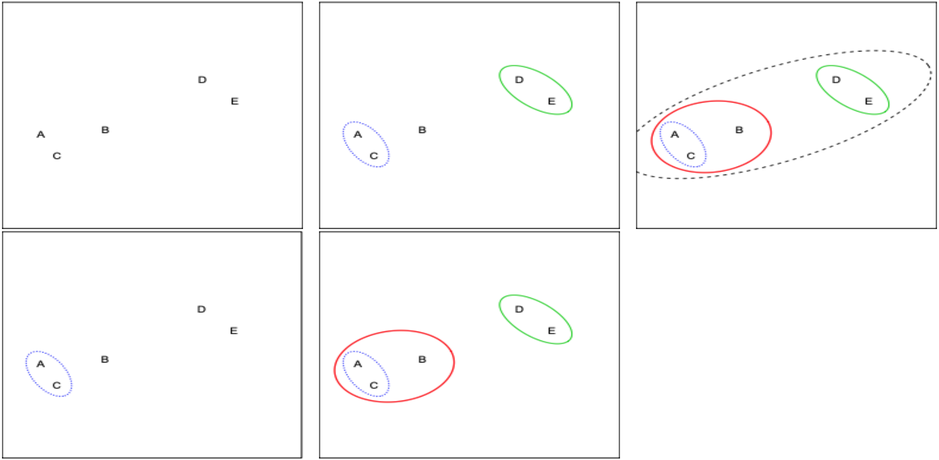

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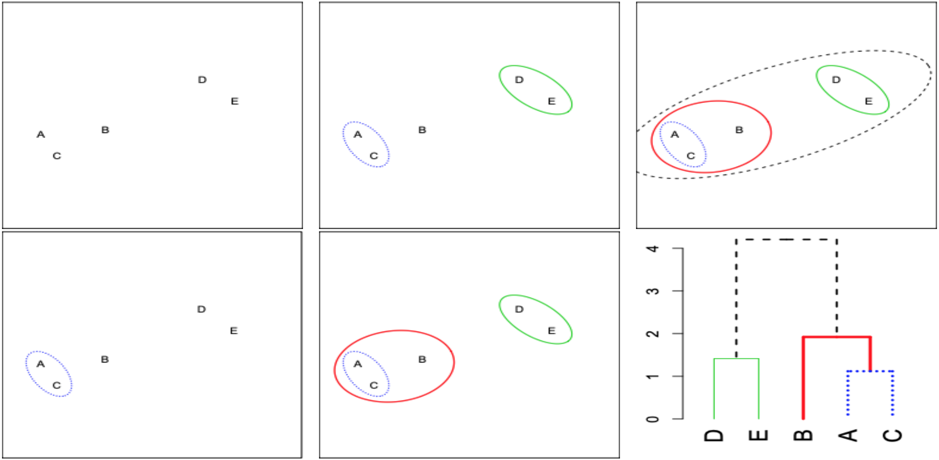

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- So how many clusters *should* accurately characterize the data...?
- That's inherently subjective and largely up to the researcher
- HC is usually most useful in comparison to other approaches allowing for comparison and validation (more next week)

Final Considerations

- Though hierarchical clustering is lauded for being assumption free in that we don't select k *a priori* (as we will in k-means, e.g.), we actually do need to select k, but *post hoc*
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- So how many clusters *should* accurately characterize the data...?
- That's inherently subjective and largely up to the researcher
- HC is usually most useful in comparison to other approaches allowing for comparison and validation (more next week)
- Good to note: HC is pretty computationally inefficient and expensive, especially on large datasets

Lecture Outline

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- We proceed recursively on each cluster until each cluster is a singleton
- This is significantly more expensive even than agglomerative, given the many split calculations required at each split (hence its less popular)

Lecture Outline

Demonstration in R

`HCA_demo.R`

Lecture Outline

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- Take off a bit early and use the time while you're together to polish your proposals