Clustering: Basics & Hierarchical Clustering

Philip D. Waggoner

MACS 40500: Computational Methods for American Politics

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Lecture Outline

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- Thus, the typical goal in clustering is to discover the "natural groupings" present in the data

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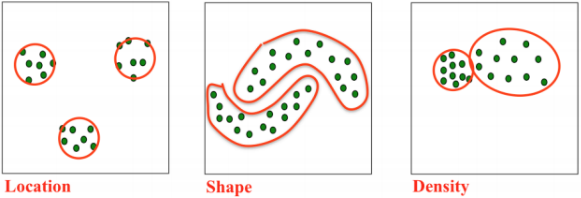

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- *Note*: Next class, also application on presidential vote shares by state in `R`

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  - Visually (VAT/ODI plots)
  - Mathematically (sparse sampling)

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- We can do our best to make sense of a complex feature space, but as our data are unlabeled, we are essentially always “guessing” about what these patterns are revealing
- This is a limitation of UML acorss the board; yet simultaneously the reason it is so important to combine UML with other data reduction and modeling processes

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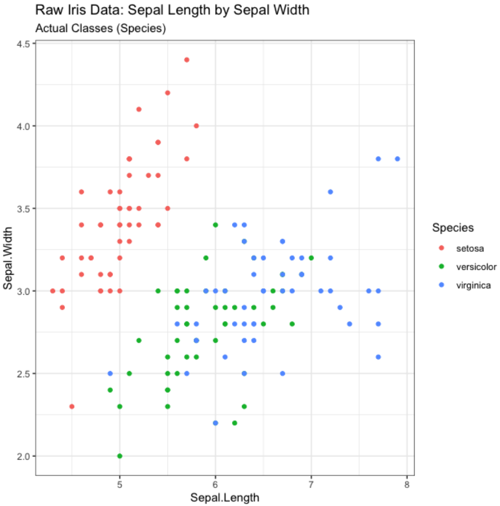
  - 3 Species: setosa, versicolor, and virginica
  - 150 observations (50 of each)

Diagnosing Clusterability: Informally (Sepal Length by Sepal Width)



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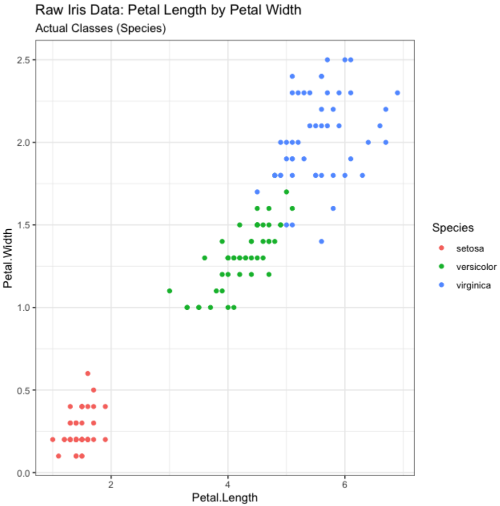

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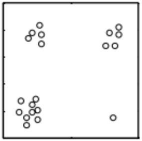
- The visual result becomes darker blocks along the diagonal reflect greater spatial similarity, compared to lighter shaded blocks, which inversely suggest greater dissimilarity

Order is Important



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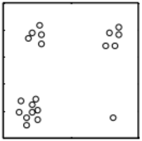

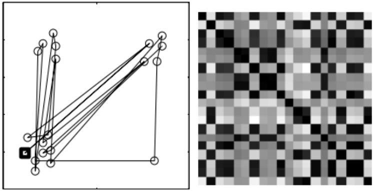

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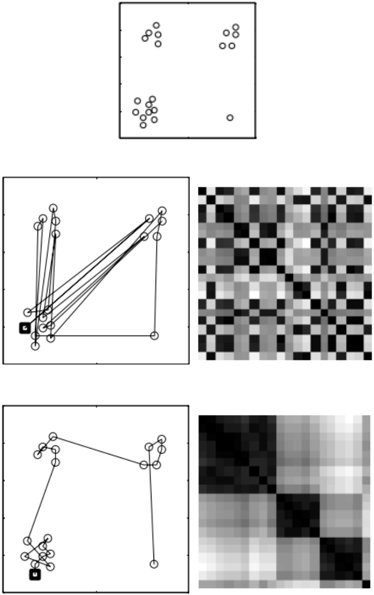
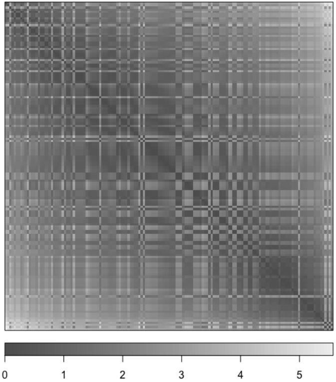


VAT (ODI): Iris Data



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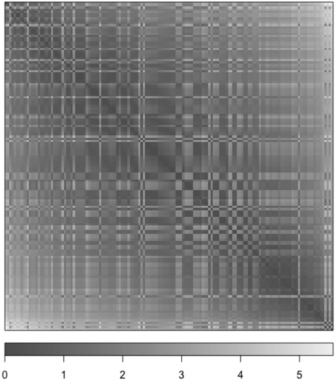

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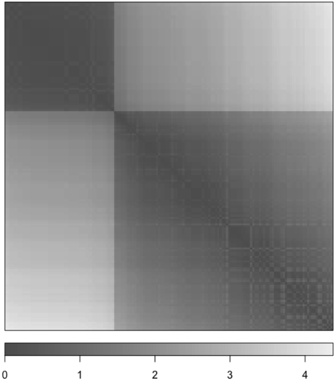

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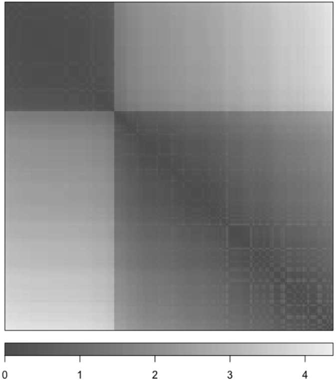

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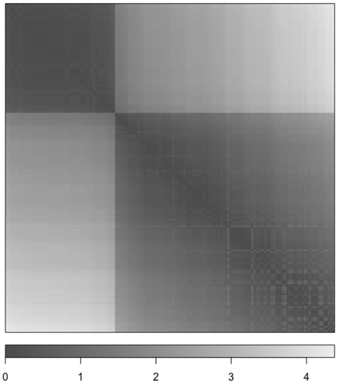

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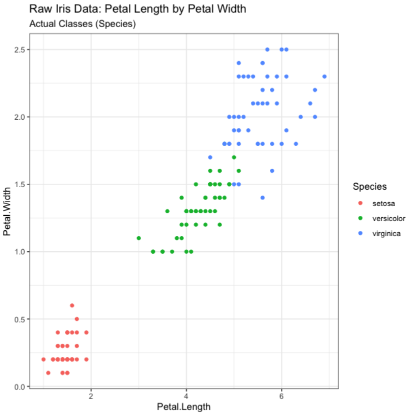

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- The Hopkins (or "H") statistic tests the the null hypothesis of spatial randomness in the data using a sparse sampling test
- It calculates the probability that a given dataset is generated by a uniform (random noise, with no clusters) distribution or not (non-random, with clustering likely)
- This general procedure is called **sparse sampling**

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- In the form of a question: is the actual data random, compared to the synthetic data set, which we *know* is random?

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- In general, $H > 0.5$ leads to rejection of H_0, suggesting the data are non-random, and are "clusterable"

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- By contrast, *features* are usually grouped on the basis of correlation coefficients (but so can observations)

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- Suppose you had two features on which you wanted to cluster units: weight (lbs.) and household income (dollars)
- In such a case, different units of measurement *and* distributions (skewed) will always return biased results
- Thus first, always standardize input features to ensure they are "unitless" (commonly setting $\mu = 0$ and $\sigma = 1$)

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Similarity and Dissimilarity

- We begin with some configuration of actual data, $\delta(p,q)$, and we want to calculate a measurement of distance, $d(p,q)$, that accurately reflects this, such that $d(p,q) \rightarrow \delta(p,q)$

- Generally a distance measure $d(p,q)$ between two points p and q satisfies the following properties, where g is any other intermediate point:

  - $d(p,q) = d(q,p)$
  - $d(p,q) > 0$, if $p \neq q$
  - $d(p,q) = 0$, if $p = q$
  - $d(p,q) \leq d(p,g) + d(g,q)$

Spatial Measures Starting with Minkowski

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  - Respondents on large surveys
  - Geopolitical studies
  - Market preferences
  - Economies
  - Social media users
  - Perceptual studies
  - Geographic trends
  - And, on Friday, partisan voting by state
  - And, on your HW, state legislative professionalism

Lecture Outline

Agglomerative Hierarchical Clustering

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- Key terms: distance measure, linkage methods, dendrogram, tree-cutting

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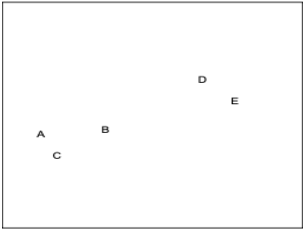

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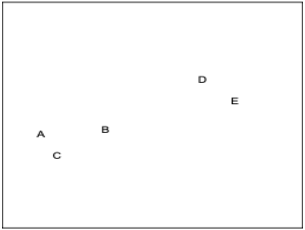

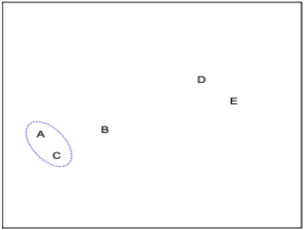

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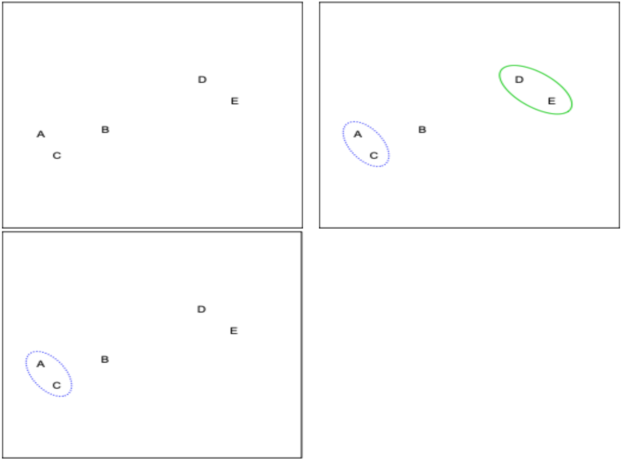

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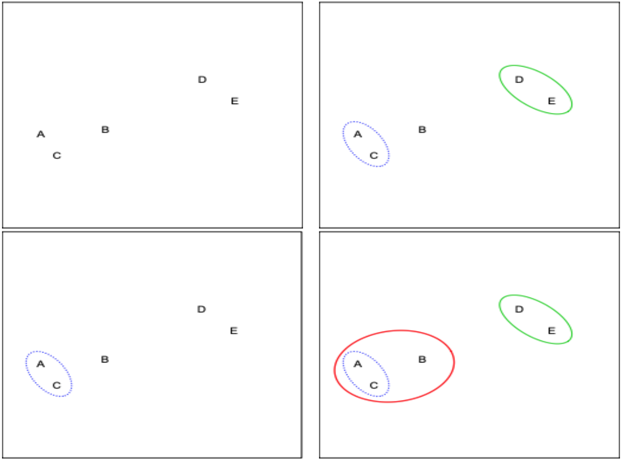

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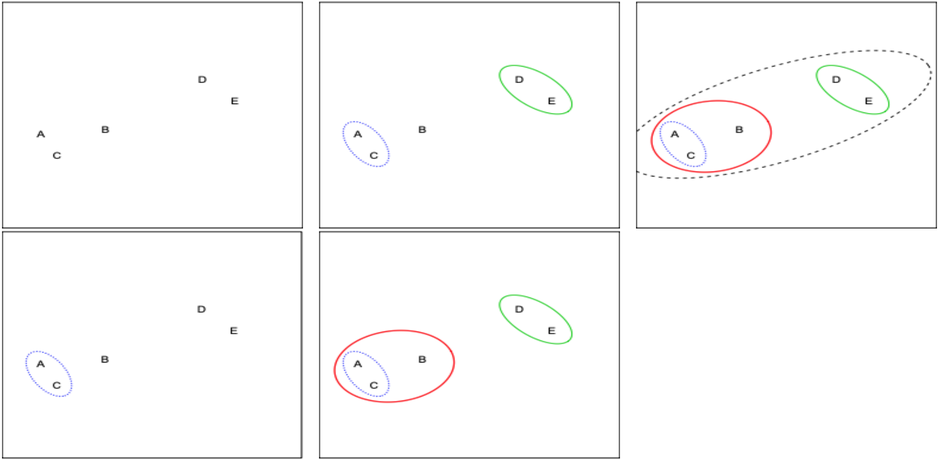

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- Stop when we reach k clusters ($k = 1$ in agglomerative; $k = n$ in divisive)

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- **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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$$d_{average}(C_x, C_y) = \frac{\sum_i \sum_j d_{ij}}{N_{C_x} N_{C_y}}$$

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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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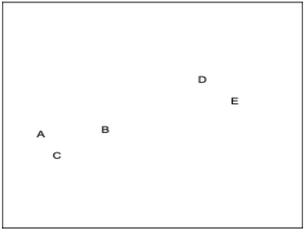

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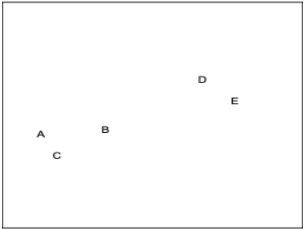

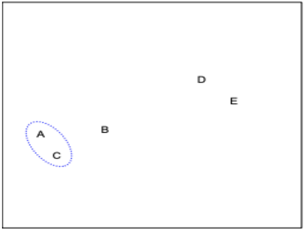

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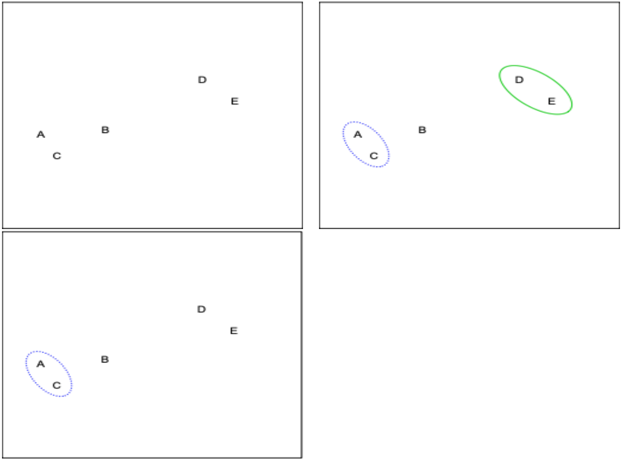

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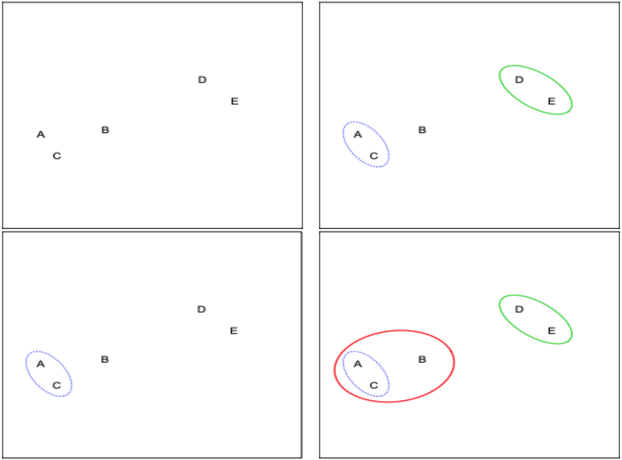

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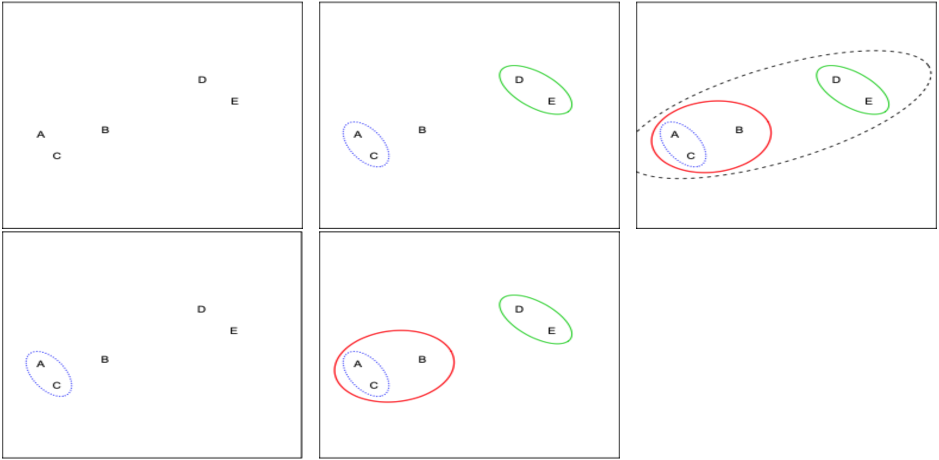

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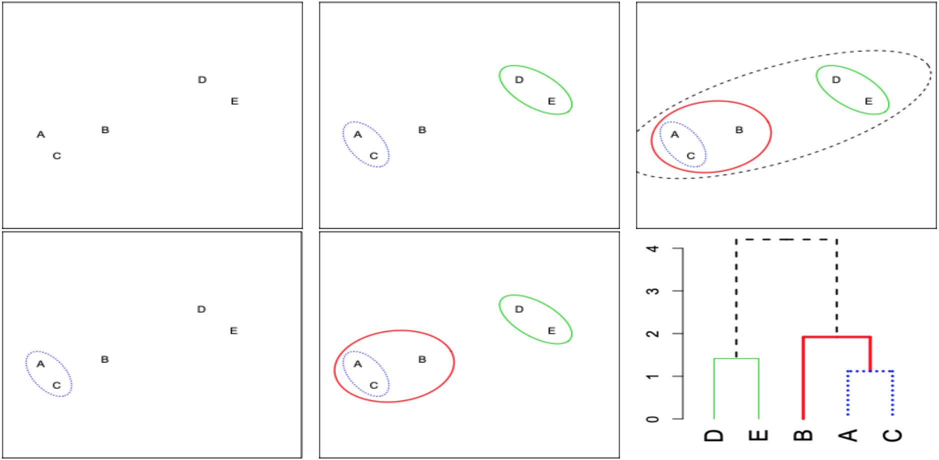

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- HC is usually most useful in comparison to other approaches allowing for comparison and validation (more next class)
- Note: HC is computationally inefficient and expensive, especially on large datasets

Lecture Outline

Divisive Hierarchical Clustering

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- This is significantly more expensive even than agglomerative, given the many split calculations required at each split (hence its less popular)

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Coming Up

- k-means clustering
- Gaussian mixture models
- Demonstration in `R`: 2012 state Democratic vote shares

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- Gaussian mixture models
- Demonstration in `R`: 2012 state Democratic vote shares
- First problem set due **Friday at 5 pm** to our GH repo (quick word on the data and concept)