Introduction to Clustering

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MACS 40800: Unsupervised Machine Learning

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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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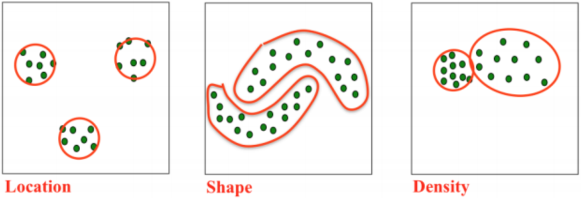

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    - Hard partitioning (focus on k-means clustering, with a few cousins)
    - Soft (model-based) partitioning, can be probabilistic or fractional (focus on the EM algorithm and Gaussian mixture models, with a few cousins)

Lecture Outline

1. Clustering Basics
2. Diagnosing Clusterability
3. Conceptualizing and Calculating Distance
4. Clustering Applications
5. Problem Set 2

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  - Mathematically (sparse sampling)

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- We can do our best to make sense of a complex feature space, but our data are unlabeled, and we have relatively weak (if any) priors on distributions, and so on
- 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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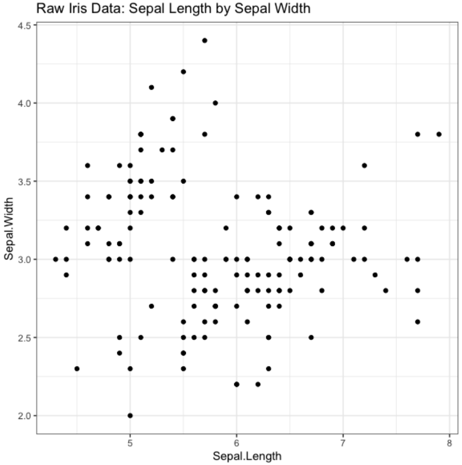
  - 3 Species: setosa, versicolor, and virginica
  - 150 observations (50 of each)

Diagnosing Clusterability: Informally (Sepal Length by Sepal Width)



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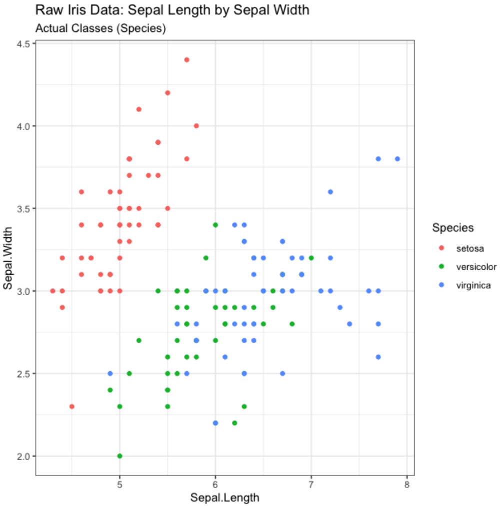

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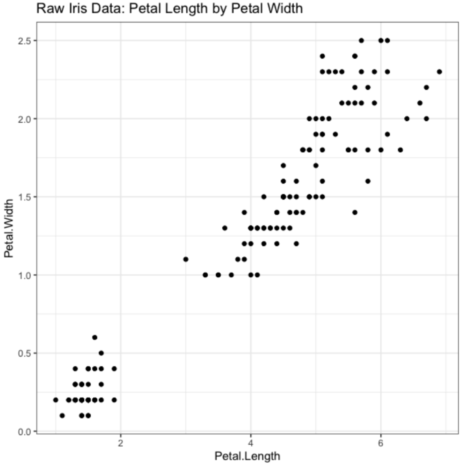

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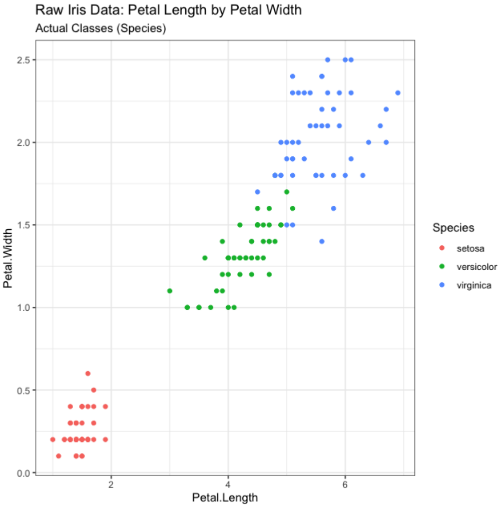
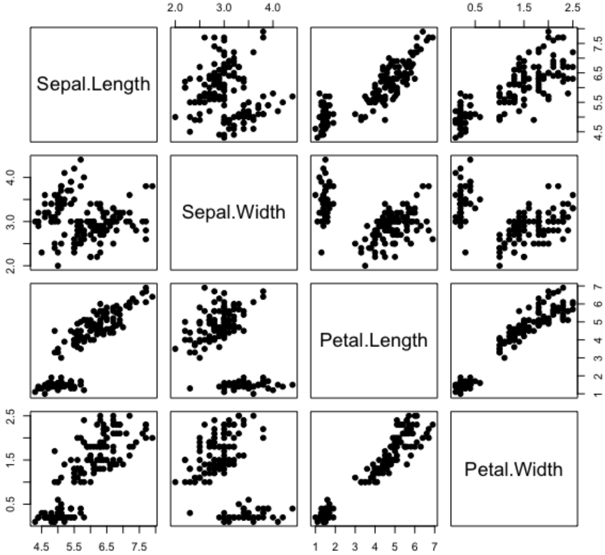


Diagnosing Clusterability: Informally (All Features)



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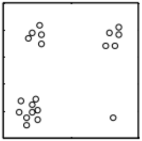
- The visual result becomes darker blocks along the diagonal reflect greater spatial similarity, compared to lighter shaded blocks, which inversely suggest greater dissimilarity

Order is Important



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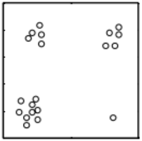

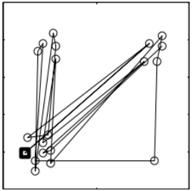

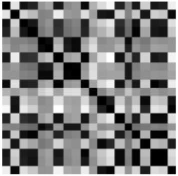

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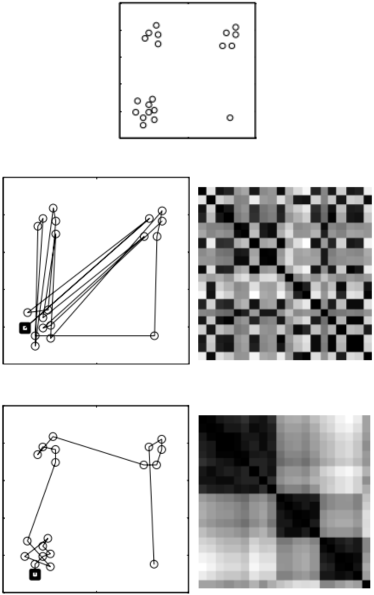

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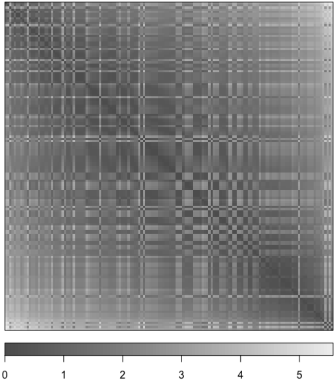

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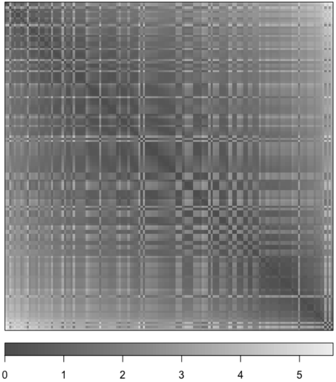

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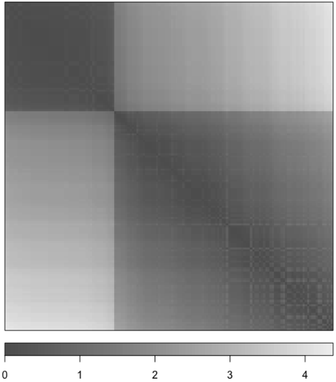

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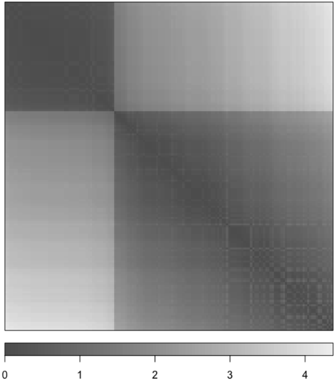

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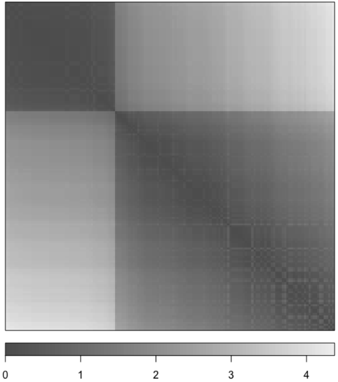

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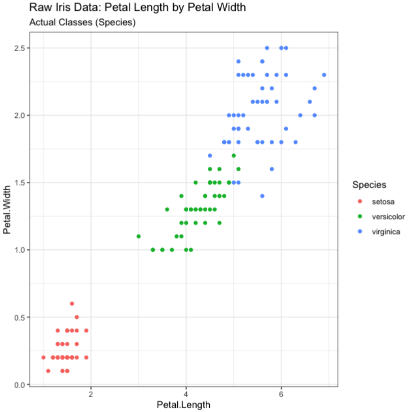

Figure: Raw Data: Petal

In R

Jump to R for a quick demo

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- This general procedure is called **sparse sampling**, of which H is one iteration

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- In other words, we are creating a random, synthetic version of the original data set (the sampling "window"), and we are comparing to see whether these produce similar distributions (i.e., 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 correlations (but also for observations)

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Standardization

- First, *always* standardize when clustering
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- The result is effectly "unit-less" inputs

Similarity and Dissimilarity

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Spatial Measures Starting with Minkowski

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- The problem: **need a distance measure to transform both types of data, without information loss or meaningless values**

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- Gower's measure essentially captures the weighted average of the distances on the different features

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- And numeric features are scaled by dividing the absolute difference by the range of the feature,

$$s_{pqk} = \frac{|p_k - q_k|}{max(k) - min(k)} \tag{6}$$

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    - Geographic trends
    - And a lot more...

Lecture Outline

Problem Set #2: Clustering (part 1)

- **Due Saturday, 10/19, by 12 noon**