

# BIO 682

## Quantitative Biology

### Spring 2010

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<http://www4.nau.edu/shustercourses/BIO682/index.htm>

Lecture 15

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## Classification and Correlation Techniques

Cluster Analysis  
and  
Mantel Test

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## Cluster Analysis

- Seeks to identify homogeneous subgroups of cases in a population.
- Used when the researcher does not know the number of groups in advance but wishes to establish groups and then analyze group membership.
- Contrasts to DFA which analyzes group membership for known groups pre-specified by the researcher.
- Cluster analysis seeks to identify a set of groups which both minimize within-group variation and maximize between-group variation.

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## Cluster Analysis

- The first step in cluster analysis is to select a distance measure to determine how the similarity of each data point is measured
- eg. Euclidean, block distance, Bray-Curtis, etc.

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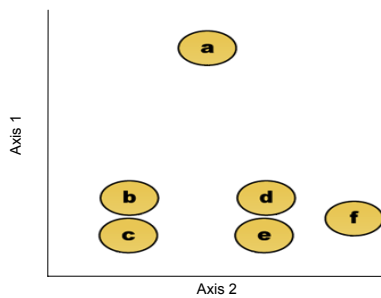
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Samples are ordinated in multidimensional space



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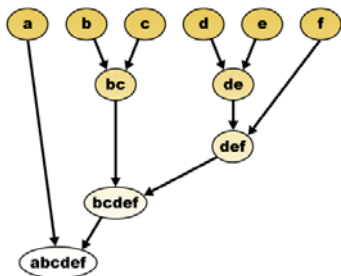
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Clustering can be either agglomerative or divisive



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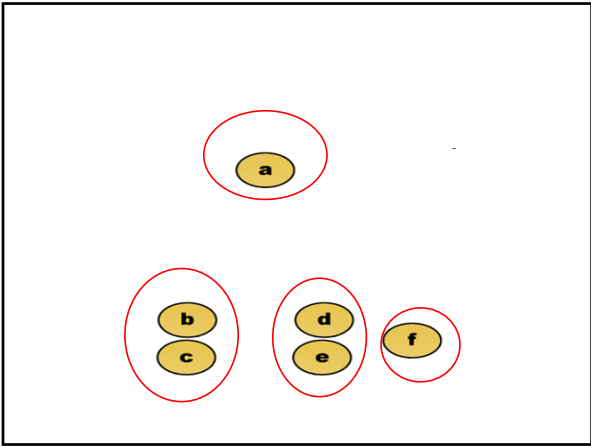
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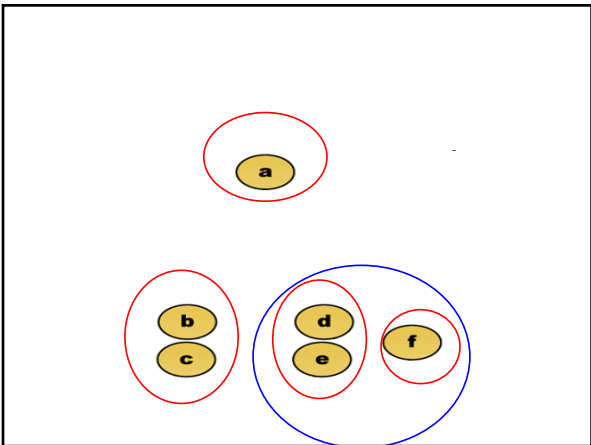
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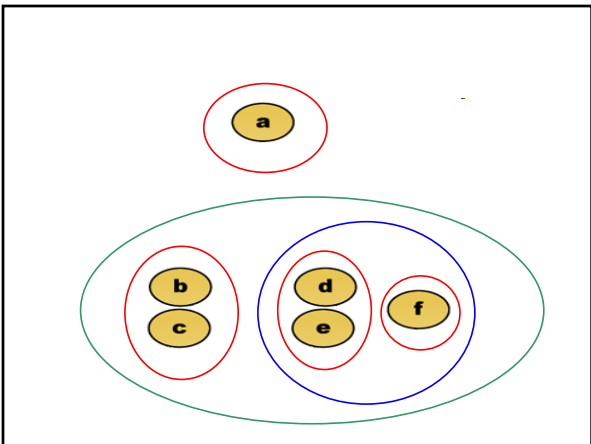
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## Cluster Analysis

- one can decide to stop clustering either when the clusters are too far apart to be merged (distance criterion)
- or when there is a sufficiently small number of clusters (number criterion).

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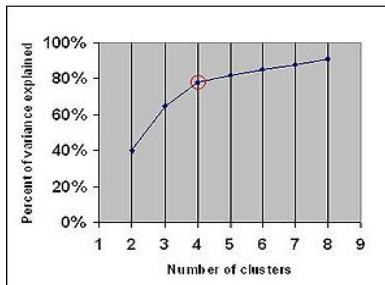
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Choose the minimum number of clusters that explain the most variance



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## Cluster Analysis

- Three general approaches to cluster analysis:
  - Hierarchical clustering.
  - K-means clustering
  - Two-step clustering

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## Hierarchical Clustering

Allows users to select a definition of distance, then select a linking method for forming clusters, then determine how many clusters best suit the data.

Hierarchical clustering generates representation of clusters in dendrograms.

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## Hierarchical Clustering

- Hierarchical clustering is appropriate for smaller samples (typically < 250). When n is large, the solution gets very computationally intensive
- User defines the distance measure and whether clustering is agglomerative or divisive
- Once clusters are grouped together, they stay together

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## K-Means Clustering

The researcher specifies the number of clusters in advance, then the algorithm calculates how to assign cases to the K clusters.

K-means clustering is much less computer-intensive and is therefore sometimes preferred when datasets are large (ex., > 1,000).

K-means clustering generates an ANOVA table showing mean-square error.

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## **K-Means Clustering**

- Researcher specifies the number of groups
- Better for larger groups because all pairwise distance comparisons are not calculated
- Samples may be shifted from one cluster to another during the iterative process of converging on a solution
- the algorithm seeks to minimize within-cluster variance and maximize variability between clusters

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## **Two-step clustering**

- Creates pre-clusters, then it clusters the pre-clusters using hierarchical methods.
- Two step clustering handles very large datasets, is the method chosen when data are categorical (it supports continuous variables also).

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## **Two-step clustering**

- Handles categorical (three or more levels) as well as continuous data
- Identifies pre-clusters in a first step, then treats these as single cases in a second step which uses hierarchical clustering

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**The utility of clusters must be assessed by three criteria**

- **Size.** All clusters should have enough cases to be meaningful.
- One or more very small clusters indicates the researcher has requested too many clusters.
- Analysis resulting in a very large, dominant cluster may indicate too few clusters have been requested

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**The utility of clusters must be assessed by three criteria**

- **Meaningfulness.** Ideally the meaning of each cluster should be readily construed from the variables used to create the clusters

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**The utility of clusters must be assessed by three criteria**

- **Criterion validity.** The number of clusters should be consistent with other variables known from theory or prior research to correlate with the concept which clustering is supposed to reflect

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## Problems

- Failure to meet these criteria may indicate the researcher has requested too many or too few clusters, or possibly that an inappropriate distance measure has been selected.
- It is also possible that the hypothesized conceptual basis for clustering does not exist, resulting in arbitrary clusters.

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## Applications

- Can be used to compare assemblages of taxa from a heterogeneous environment or to determine how heterogeneous an environment is from the perspective of the study organism
- Can be used to create phylogenies based on shared attributes

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## Mantel Test

- The Mantel test is used to test the correlation between two distance matrices
- Originally developed to evaluate spatial and temporal clustering of diseases like leukemia (Mantel 1967)
- It was later introduced to the fields of systematics and biogeography (Sokal 1979)

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## Mantel Test

- Each matrix is calculated from a different set of variables measured on the same sample units

	sp1	sp2	sp3
tree 1	4	1	3
tree 2	3	4	3
tree 3	1	5	3

	height	Stem growth	BTB
tree 1	5	3	3
tree 2	2	5	5
tree 3	2	3	4

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## Mantel Test

- The Mantel test is an alternative to regressing one set of variables against another
- Because the cells of distance matrices are not independent of each other we cannot accept the p-values from standard techniques that assume independence of the observations

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## Mantel Test

- The Mantel test is used to evaluate the congruence between two distance matrices of the same dimensions
- The two matrices must have the same set of sample units in the same order

	sp1	sp2	sp3
tree 1	4	1	3
tree2	3	4	3
tree 3	1	5	3

	height	Stem growth	BTB
tree 1	5	3	3
tree 2	2	5	5
tree3	2	3	4

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## Mantel Test

- Seek linear relationships between two matrices
- The ability to construct the matrices from any distance measure, similarity measure, or design variable leads to high power and flexibility

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## How It Works

- Tests the significance of the correlation between matrices by evaluating results from repeated randomization
  - How often does randomization of one matrix result in a correlation that is as **strong or stronger** than the observed correlation?
- Strong correlation structure between matrices will rarely be preserved or enhanced if one matrix is shuffled

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## Significance

- A test statistic ( $Z$ ) is calculated for each run
$$Z = \sum_{ij} X_{ij} Y_{ij}$$
- Where  $X_{ij}$  and  $Y_{ij}$  represent the matrices of data or each array.

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## Significance

$$Z = \sum_{ij} X_{ij} Y_{ij}$$

- A p-value is calculated from the number of randomizations that yield a test statistic equal to or more extreme than the observed value
- The standardized Mantel statistic (r) is calculated as the Pearson correlation coefficient between the two matrices

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## Mantel Test

- Are trees that are more similar in their arthropod communities also more similar in their growth?

	sp1	sp2	sp3		height	Stem growth	BTD
tree 1	4	1	3	tree 1	5	3	3
tree2	1	4	2	tree 2	2	5	7
tree 3	3	1	3	tree 3	5	3	4

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