FW 599 Special Topics: Multivariate Analysis of Ecological Data in R

Lecture 7: Other Ordination Methods

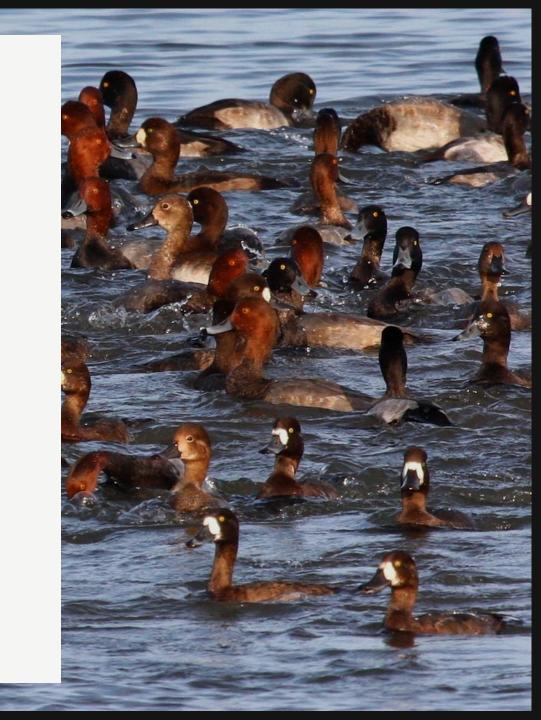
Tuesday, October 22, 2024



Lecture 7: Other Ordination Methods

- Correspondence Analysis (CA)
- Principal Coordinate Analysis (PCoA)
- Nonmetric Multidimensional Scaling (NMDS)





Principal Component Analysis uses eigenanalysis to reduce the dimensionality of large, ecological datasets while retaining as much information as possible.

- Re-projects data in multidimensional space
- Maximizes the variance explained by the first principal axes (eigenvectors)

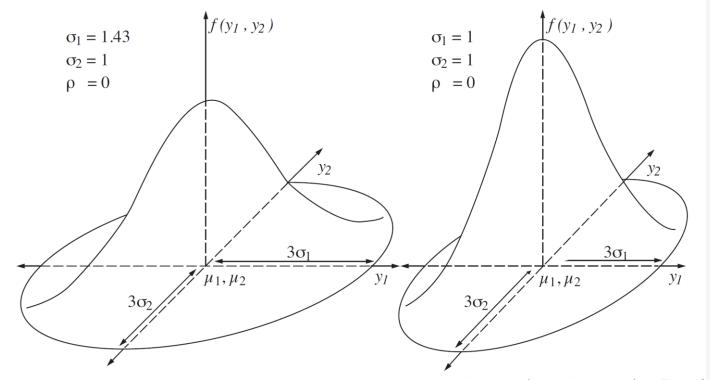


Many methods of multivariate analysis, including PCA, perform better when the response data distributions are **multivariate normal**. *Why?*

- 1. PCA Assumes the relationships between variables are linear
- 2. PCA depends on aligning the principal components with the directions of maximum variability
- 3. Interpretation is influenced by non-linear relationships, skewness, and outliers



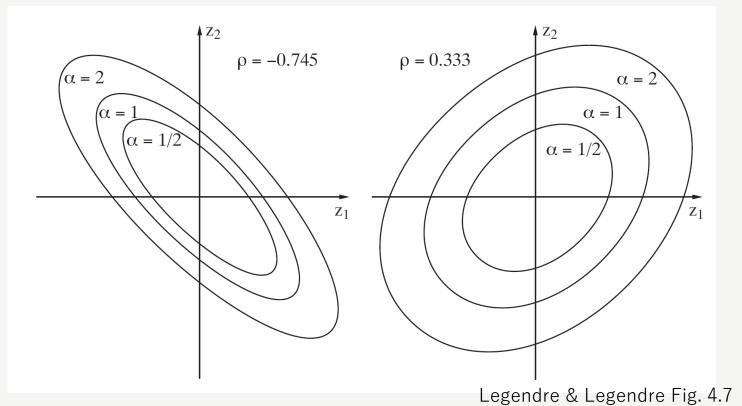
Multivariate normal distribution: Requires mean (μ) , standard deviation (σ) , and <u>correlation</u> (ρ) .



Legendre & Legendre Fig. 4.6



Multivariate normal distribution: Requires mean (μ) , standard deviation (σ) , and <u>correlation</u> (ρ) .



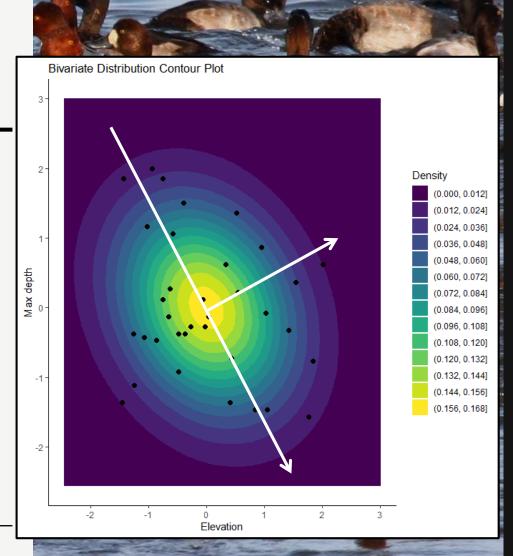


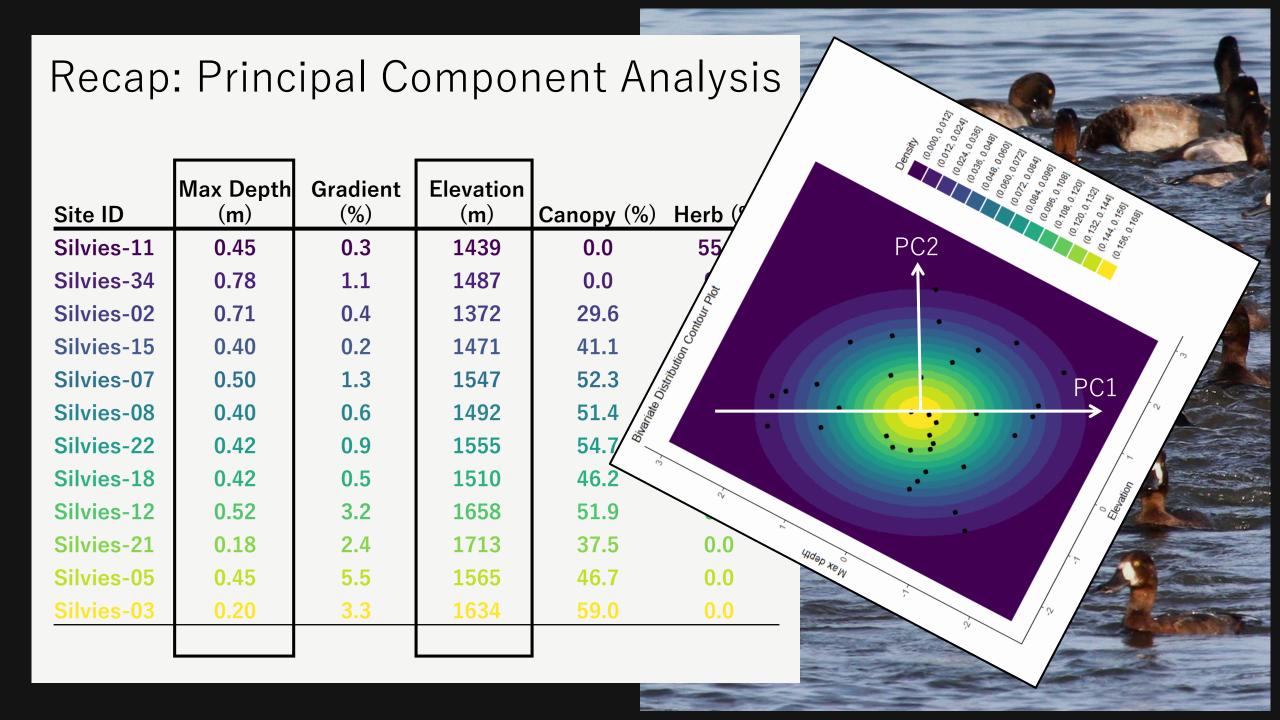
PCA depends on aligning the principal components (axes) with the **directions of maximum variability**.

- The first principal axis is the line that passes through the dimension of greatest variance of the ellipsoid.
- Each subsequent principal axis passes through dimensions of successionally smaller variance.
- All axes are <u>perpendicular</u> to one another in hyperspace.



Site ID	Max Depth (m)	Gradient (%)	Elevation (m)	Canopy (%)	Herb (%)
Silvies-11	0.45	0.3	1439	0.0	55.1
Silvies-34	0.78	1.1	1487	0.0	0.0
Silvies-02	0.71	0.4	1372	29.6	0.0
Silvies-15	0.40	0.2	1471	41.1	0.0
Silvies-07	0.50	1.3	1547	52.3	0.0
Silvies-08	0.40	0.6	1492	51.4	0.0
Silvies-22	0.42	0.9	1555	54.7	0.0
Silvies-18	0.42	0.5	1510	46.2	0.0
Silvies-12	0.52	3.2	1658	51.9	0.0
Silvies-21	0.18	2.4	1713	37.5	0.0
Silvies-05	0.45	5.5	1565	46.7	0.0
Silvies-03	0.20	3.3	1634	59.0	0.0



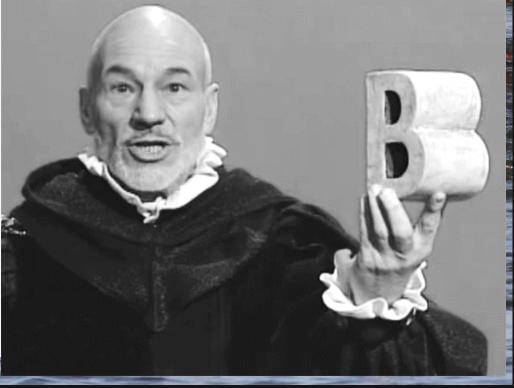


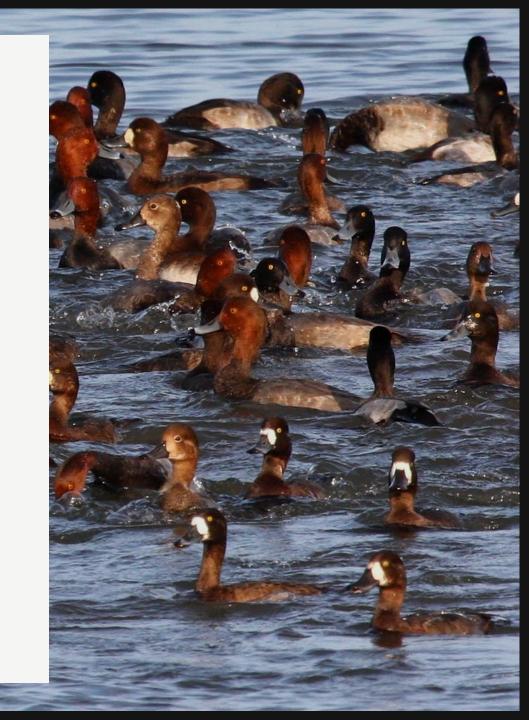
Recap: Limitations

PCA: To use or not to use?

- Optimal use calls for normalization of the data
- If the number of objects is smaller than the number of descriptors (n < p), negative eigenvalues will occur
- PCA is not useful for R-mode analysis
- PCA cannot incorporate multi-state descriptors
- Watch out for the double zero problem!







Species abundance and other kinds of count data are often:

- Non-linear
- Not multinormally distributed
- Highly zero-skewed



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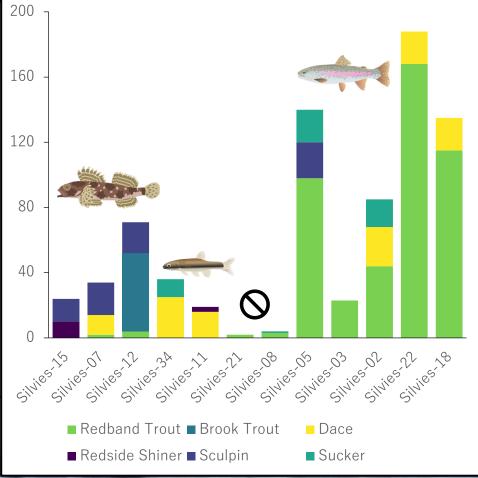
- Non-linear
- Not multinormally distributed
- Highly zero-skewed

Is there a better way?



Site ID	Redband Trout	Brook Trout	Dace	Redside Shiner	Sculpin	Sucker
Silvies-15	0	0	0	10	14	0
Silvies-07	2	0	12	0	20	0
Silvies-12	4	48	0	0	19	0
Silvies-34	0	0	25	0	0	11
Silvies-11	0	0	16	3	0	0
Silvies-21	2	0	0	0	0	0
Silvies-08	3	0	0	0	0	1
Silvies-05	98	0	0	0	22	20
Silvies-03	23	0	0	0	0	0
Silvies-02	44	0	24	0	0	17
Silvies-22	168	0	20	0	0	0
Silvies-18	115	0	20	0	0	0

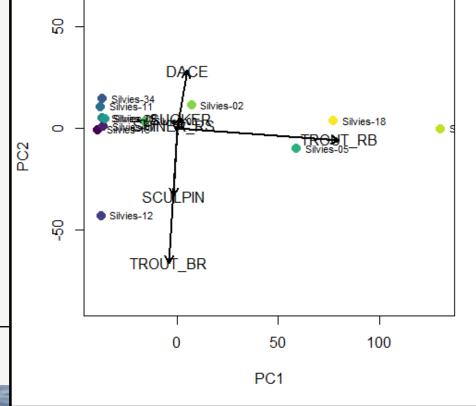




Site ID	Redband Trout	Brook Trout	Dace	Redside Shiner	Sculpin	Sucker
Silvies-15	0	0	0	10	14	0
Silvies-07	2	0	12	0	20	0
Silvies-12	4	48	0	0	19	0
Silvies-34	0	0	25	0	0	11
Silvies-11	0	0	16	3	0	0
Silvies-21	2	0	0	0	0	0
Silvies-08	3	0	0	0	0	1
Silvies-05	98	0	0	0	22	20
Silvies-03	23	0	0	0	0	0
Silvies-02	44	0	24	0	0	17
Silvies-22	168	0	20	0	0	0
Silvies-18	115	0	20	0	0	0



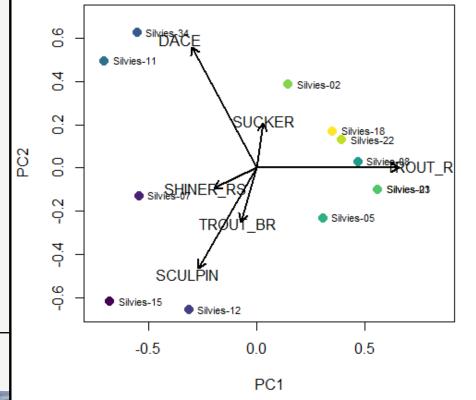
PCA of Raw Fish Abundance Data



Site ID	Redband Trout	Brook Trout	Dace	Redside Shiner	Sculpin	Sucker
Silvies-15	0	0	0	10	14	0
Silvies-07	2	0	12	0	20	0
Silvies-12	4	48	0	0	19	0
Silvies-34	0	0	25	0	0	11
Silvies-11	0	0	16	3	0	0
Silvies-21	2	0	0	0	0	0
Silvies-08	3	0	0	0	0	1
Silvies-05	98	0	0	0	22	20
Silvies-03	23	0	0	0	0	0
Silvies-02	44	0	24	0	0	17
Silvies-22	168	0	20	0	0	0
Silvies-18	115	0	20	0	0	0



PCA of Hellinger Transformed Fish Abundance Data



Correspondence Analysis is an alternative ordination method that preserves the <u>chi-square</u> <u>distances</u> (χ^2) among objects in the principal axes.



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Designed for <u>dimensionally homogeneous</u>, <u>non-negative</u> data (such as counts).

Computed on a two-way <u>contingency table</u> instead of a dispersion matrix.

Excludes double zeros!



Step 1: Transform contingency table into a table of contributions ($\overline{\mathbf{Q}}$) to the Pearson chi-square statistic (χ_p^2).



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Table of frequencies, **Q**:

$$p_{ij} = f_{ij}/f_{++}$$



Table **Q**

Site ID	Redband Trout	Brook Trout	Dace	Redside Shiner	Sculpin	Sucker
Silvies-15	0	0	0	0.013	0.018	0
Silvies-07	0.003	0	0.016	0	0.026	0
Silvies-12	0.005	0.063	0	0	0.025	0
Silvies-34	0	0	0.033	0	0	0.014
Silvies-11	0	0	0.021	0.004	0	0
Silvies-21	0.003	0	0	0	0	0
Silvies-08	0.004	0	0	0	0	0.001
Silvies-05	0.129	0	0	0	0.029	0.026
Silvies-03	0.030	0	0	0	0	0
Silvies-02	0.058	0	0.032	0	0	0.022
Silvies-22	0.221	0	0.026	0	0	0
Silvies-18	0.151	0	0.026	0	0	0



Row weights: p_{i+}

Site ID (Row)	p_{i+}
Silvies-15	0.032
Silvies-07	0.045
Silvies-12	0.093
Silvies-34	0.047
Silvies-11	0.025
Silvies-21	0.003
Silvies-08	0.005
Silvies-05	0.184
Silvies-03	0.030
Silvies-02	0.112
Silvies-22	0.247
Silvies-18	0.177



Column weights: p_{+j}

Species (Column)	$p_{i_{\pm}}$
Redband Trout	0.603
Brook Trout	0.063
Dace	0.154
Redside Shiner	0.017
Sculpin	0.099
Sucker	0.064



Step 1: Transform contingency table into a table of contributions ($\overline{\mathbf{Q}}$) to the Pearson chi-square statistic (χ_P^2).

$$\chi_{ij} = \sqrt{f_{++}} \left[\frac{p_{ij} - p_{i+} p_{+j}}{\sqrt{p_{i+} p_{+j}}} \right]$$



Step 1: Transform contingency table into a table of contributions ($\overline{\mathbf{Q}}$) to the Pearson chi-square statistic ($\chi_{\rm p}^2$).

$$\chi_{ij} = \sqrt{f_{++}} \left[\frac{p_{ij} - p_{i+} p_{+j}}{\sqrt{p_{i+} p_{+j}}} \right]$$

$$\overline{\mathbf{Q}} = \left[\frac{\mathbf{p}_{ij} - \mathbf{p}_{i+} \mathbf{p}_{+j}}{\sqrt{\mathbf{p}_{i+} \mathbf{p}_{+j}}} \right]$$



Step 2: Decompose transformed data table to obtain eigenvalues and eigenvectors.



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Conduct eigenanalysis on the covariance matrix: $\overline{\mathbf{Q}}'\overline{\mathbf{Q}}$



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Conduct eigenanalysis on the covariance matrix: $\overline{\mathbf{Q}}'\overline{\mathbf{Q}}$

$$\lambda_1 = 0.77$$

$$\lambda_2 = 0.48$$

$$\lambda_3 = 0.32$$

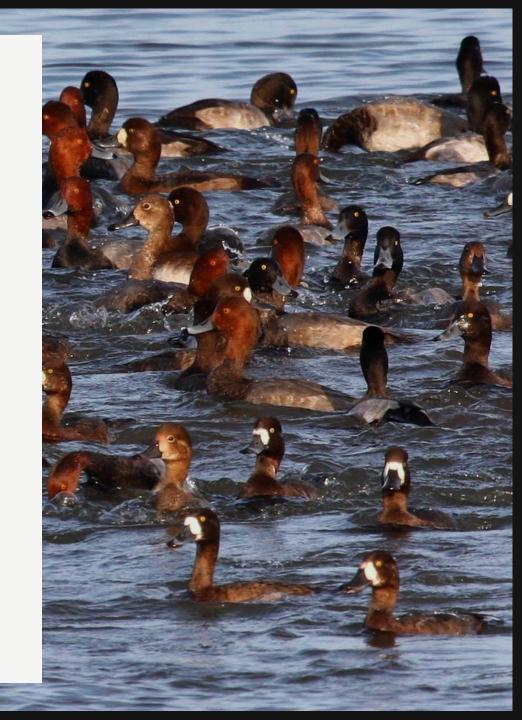
$$\lambda_4 = 0.14$$

$$\lambda_{5} = 0.09$$

$$\lambda_{6} = 0.00$$

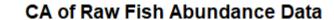


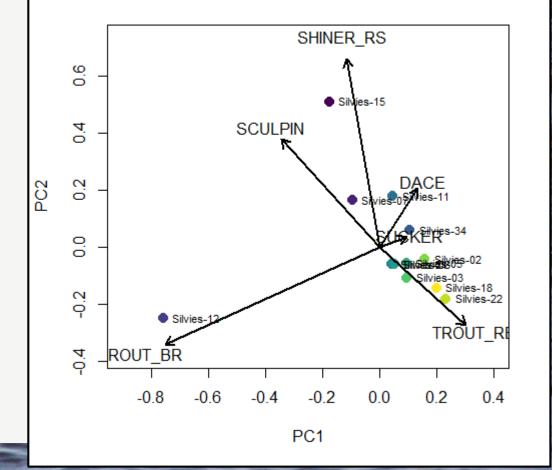
Step 3: Scale as appropriate for plotting and data interpretation.



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Scaling 1: Draw sites at the centroids of the species – most appropriate for representing distances among sites



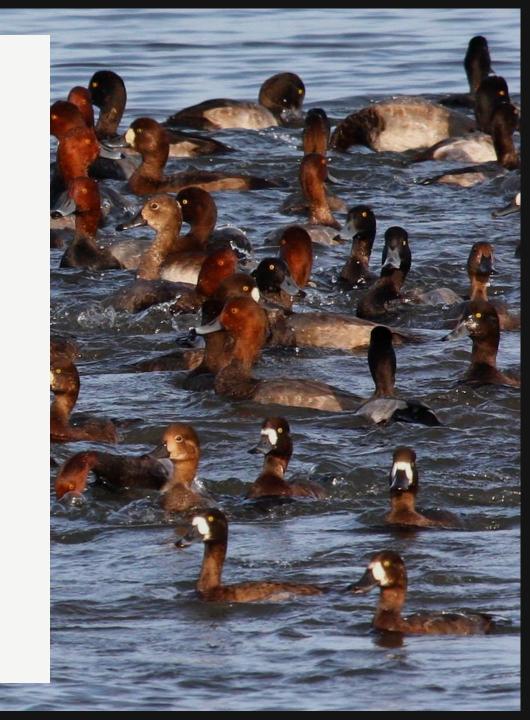
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Scaling 1: Draw sites at the centroids of the species – most appropriate for representing distances among sites

Scaling 2: Draw species at the centroids of the sites – most appropriate for representing distances among species



Correspondence Analysis (CA): Limitations



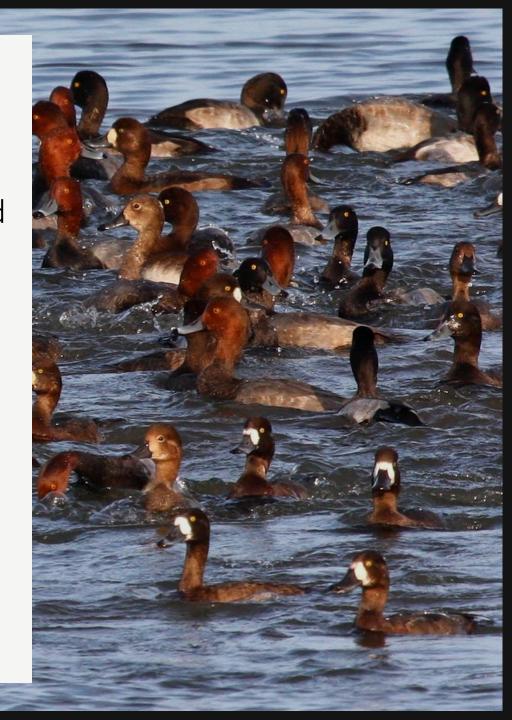
 Data must be dimensionally homogeneous and non-negative



- Data must be dimensionally homogeneous and non-negative
- Assumes linear relationships with environmental gradients



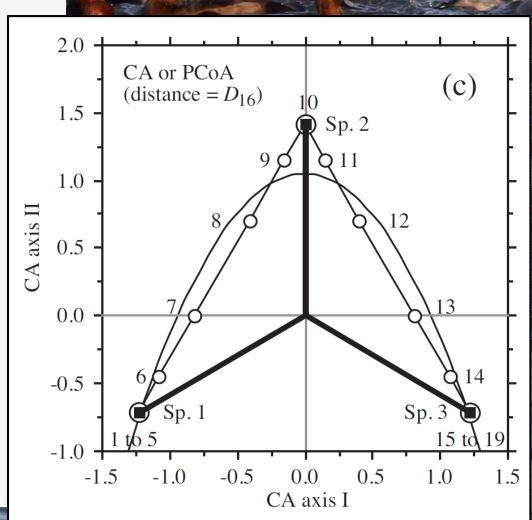
- Data must be dimensionally homogeneous and non-negative
- Assumes linear relationships with environmental gradients
- Assumes linear relationships between objects and descriptors



- Data must be dimensionally homogeneous and non-negative
- Assumes linear relationships with environmental gradients
- Assumes linear relationships between objects and descriptors
- Overly sensitive to rare species

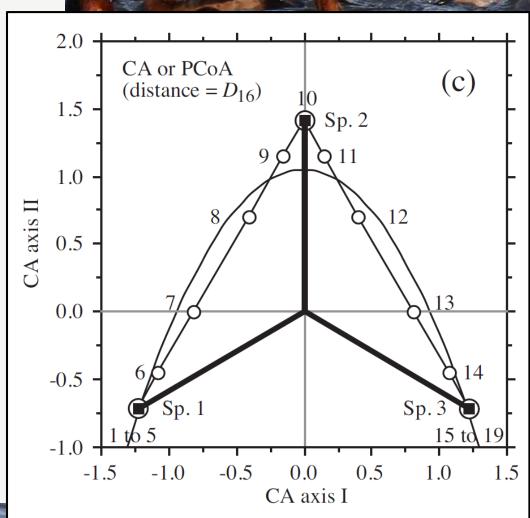


The **arch effect**, also known as the "horseshoe effect" or "Guttman effect," is a common artifact in ordination techniques.

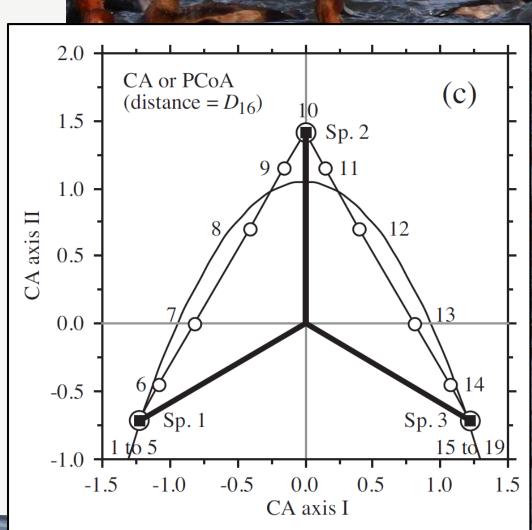


The **arch effect**, also known as the "horseshoe effect" or "Guttman effect," is a common artifact in ordination techniques.

It occurs when the data points form a curved pattern or an arch-shaped (horseshoe) configuration in the ordination space.



The **arch effect**, also known as the "horseshoe effect" or "Guttman effect," is a common artifact in ordination techniques. **But why?**

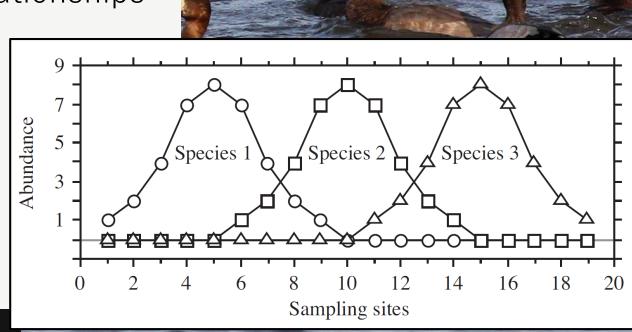


Legendre & Legendre Fig. 9.11

The arch effect, also known as the "horseshoe effect" or "Guttman effect," is a common artifact in ordination techniques. But why?

Non-linear (especially unimodal) relationships

in the underlying data



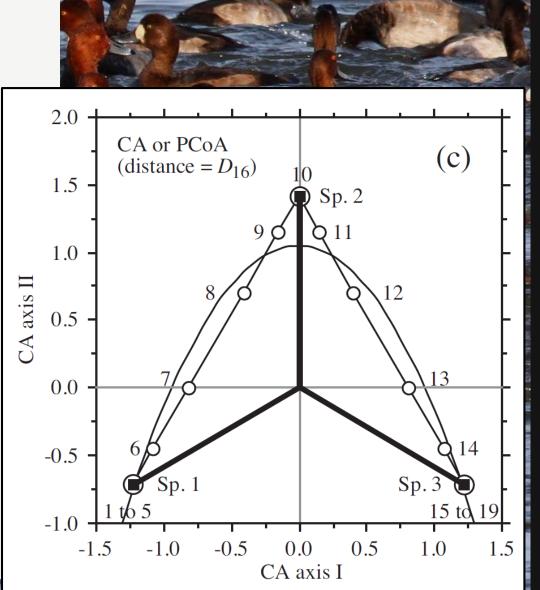
Consequences:

- Misinterpretation: Data points at the ends of the arch may appear closer together in the reduced-dimensionality space, suggesting a stronger similarity than actually exists.
- Loss of Information: Important environmental gradients or other underlying factors are not adequately represented in the first few ordination axes

CA or PCoA (c) (distance = D_{16}) 1.5 1.0 CA axis II 0.5 0.0-0.5 Sp. 3 -0.5 0.00.5 1.0 CA axis I

Solutions:

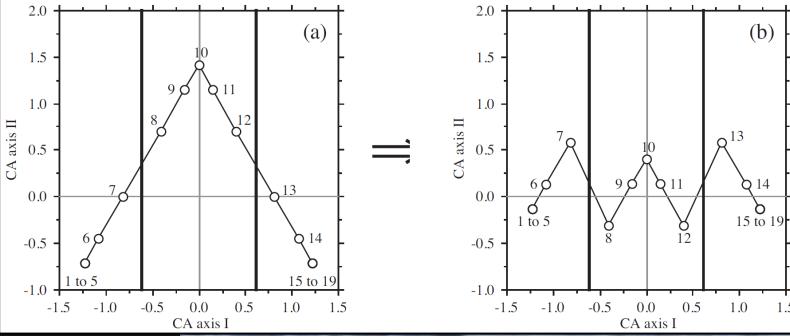
- Detrended Correspondence Analysis (DCA): Explicitly corrects for the curvature by removing the arch, providing a "more accurate" representation of the underlying gradients.
- Non-metric Multidimensional Scaling (NMDS): Is less prone to the arch effect because it focuses on preserving the rank order of distances rather than the exact distances.



Correspondence Analysis (CA): Detrended Correspondence Analysis (DCA)

Detrending by segments: Axis 1 is divided into segments and the mean scores along axis 2 are set to zero.

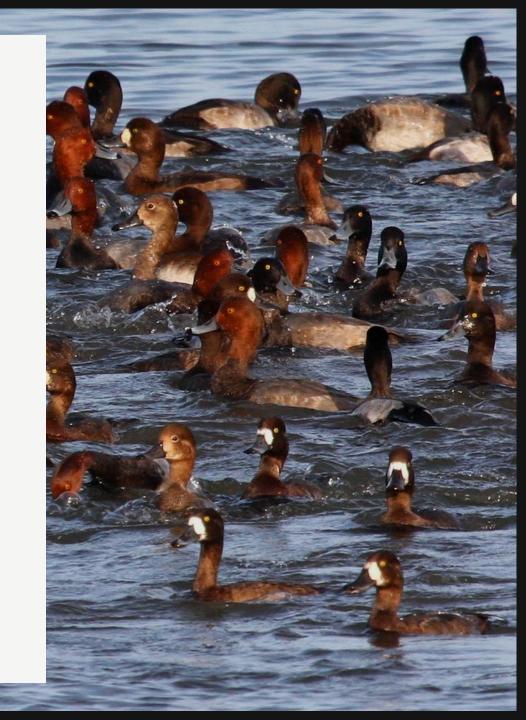




Legendre & Legendre Fig. 9.12

Correspondence Analysis (CA): Detrended Correspondence Analysis (DCA)

Detrending by polynomials: When species are distributed along a "long" environmental gradient, axis 2 is often a quadratic function of axis 1. Thus, a constant is imposed such that axis 2 is uncorrelated with axis 1, etc.

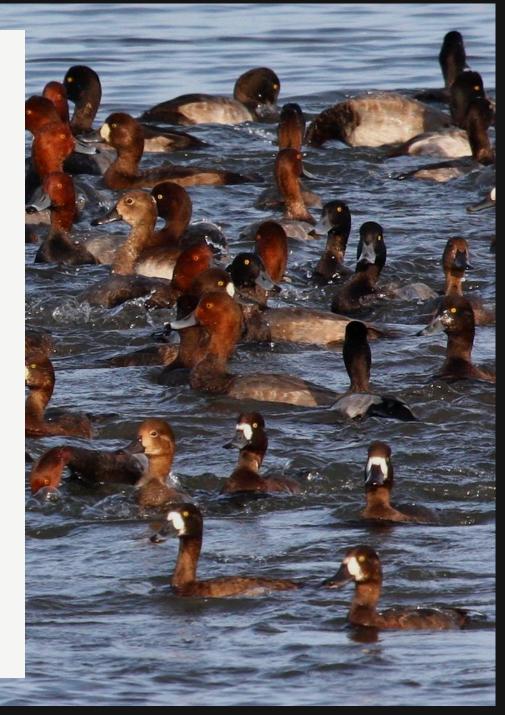


Correspondence Analysis (CA): Detrended Correspondence Analysis (DCA)

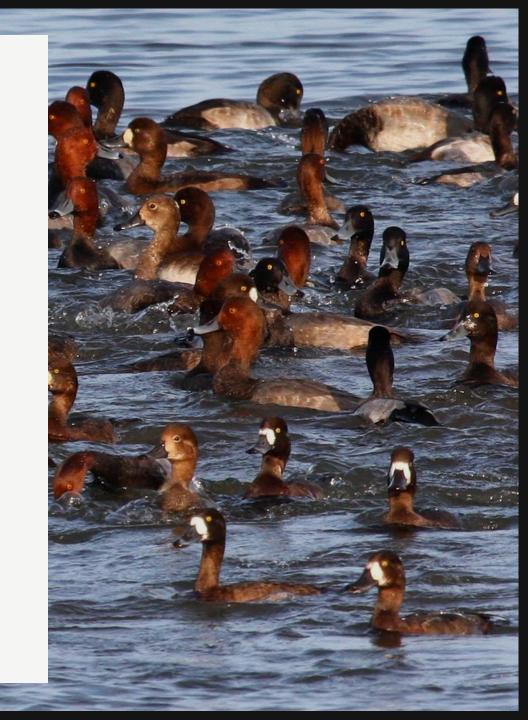
Just don't do it. (Use NMDS instead)







PCA preserves Euclidean distances and CA preserves χ^2 distances. What about other distance relationships?



PCA preserves Euclidean distances and CA preserves χ^2 distances. What about other distance relationships?

- Binary data
- Mixtures of quantitative and qualitative descriptors
- Pretty much any of the other dissimilarity metrics in Legendre & Legendre Chapter 7...



Enter: Principal Coordinate Analysis or Metric Multidimensional Scaling.

Principal coordinates are mediated through a distance function that has been computed among objects.



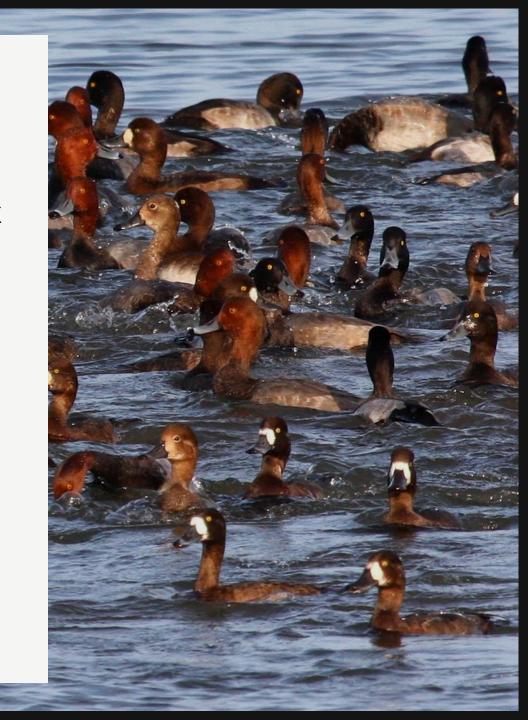
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Improved performance if distances are **metric** (i.e., do not violate the "triangle inequality")



Step 1: Calculate a dissimilarity/distance matrix



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Binary: Jaccard or Sørensen coefficients

Environmental: Euclidean or Manhattan distances (after standardization

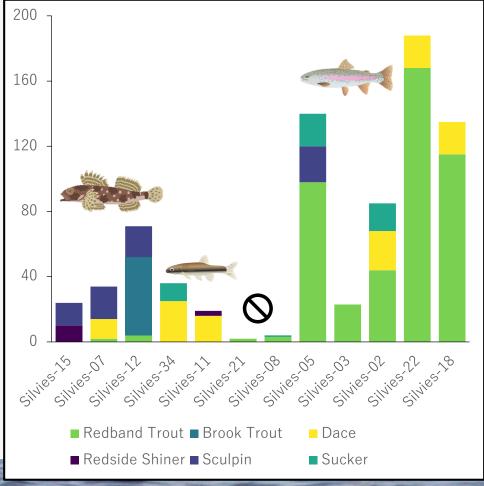
Species abundance: Chi-square distance or Percentage Difference/Bray-Curtis dissimilarity

Mixed data types: Gower's coefficient



	S-15	S-07	S-12	S-34	S-11	S-21	S-08	S-05	S-03	S-02	S-22
Silvies-07	0.52										
Silvies-12	0.73	0.72									
Silvies-34	1.00	0.62	1.00								
Silvies-11	0.88	0.55	1.00	0.54							
Silvies-21	1.00	0.87	0.88	1.00	1.00						
Silvies-08	1.00	0.88	0.89	0.93	1.00	0.33					
Silvies-05	0.75	0.72	0.76	0.80	1.00	0.90	0.81				
Silvies-03	1.00	0.91	0.93	1.00	1.00	0.80	0.73	0.36			
Silvies-02	1.00	0.64	0.95	0.50	0.58	0.86	0.74	0.42	0.41		
Silvies-22	1.00	0.76	0.96	0.81	0.75	0.90	0.86	0.38	0.38	0.41	
Silvies-18	1.00	0.73	0.95	0.79	0.70	0.88	0.83	0.31	0.29	0.34	0.10





Step 2: Transform using equation:

$$A = -1/2*D^2$$

then double-center A by rows and columns



Step 3: Decompose centered dissimilarity matrix to obtain eigenvalues and eigenvectors.



Step 3: Decompose centered dissimilarity matrix to obtain eigenvalues and eigenvectors.

Pretty much the same process as for PCA and CA. **Eigenvalues** correspond to explained variance and **eigenvectors** represent the coordinates of the objects in reduceddimensional space.

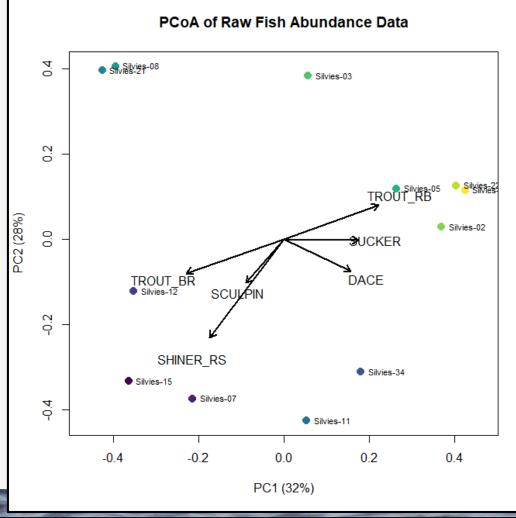


Step 4: Scale each eigenvector by multiplying by the square root of its eigenvalue.



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- Produces of negative eigenvalues when the distance used is semi-metric



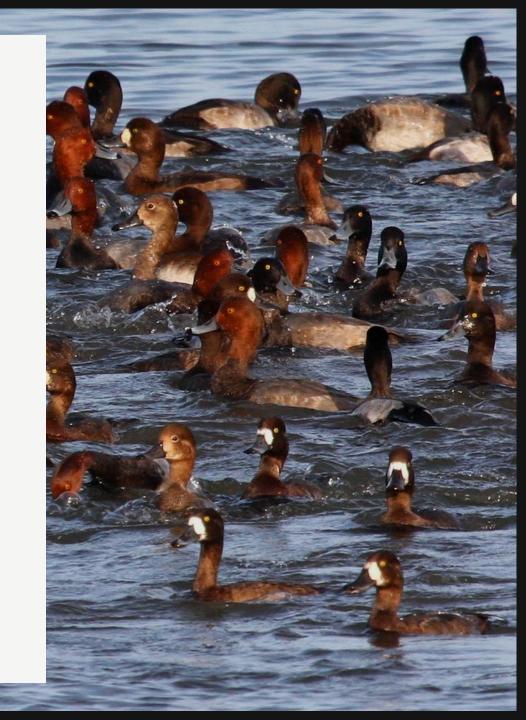
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- Produces of negative eigenvalues when the distance used is semi-metric
- Does not preserve patterns in the original data structure
- Sensitive to outliers
- Reduction in dimensionality may result in arch effect



Nonmetric Multidimensional Scaling (NMDS)



Nonmetric Multidimensional Scaling (NMDS): Introduction

Nonmetric Multidimensional Scaling preserves rank order dissimilarities between objects in a low-dimensional space.



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Useful for examining *relative*, rather than *absolute*, distances among data points.



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Nonmetric Multidimensional Scaling preserves rank order dissimilarities between objects in a low-dimensional space.

Useful for examining *relative*, rather than *absolute*, distances among data points.

NMDS axes *do not* maximize variability in space and are *arbitrary*!



Nonmetric Multidimensional Scaling (NMDS): Steps

Step 1: Calculate distance/dissimilarity matrix



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Step 2: Choose number of dimensions *a priori*



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Step 3: Set initial configuration in *m* dimensions



Step 1: Calculate distance/dissimilarity matrix

Step 2: Choose number of dimensions a priori

Step 3: Set initial configuration in *m* dimensions

Step 4: Iteratively optimize the configuration

Many iterations helps avoid the local minima problem.



Step 1: Calculate distance/dissimilarity matrix

Step 2: Choose number of dimensions *a priori*

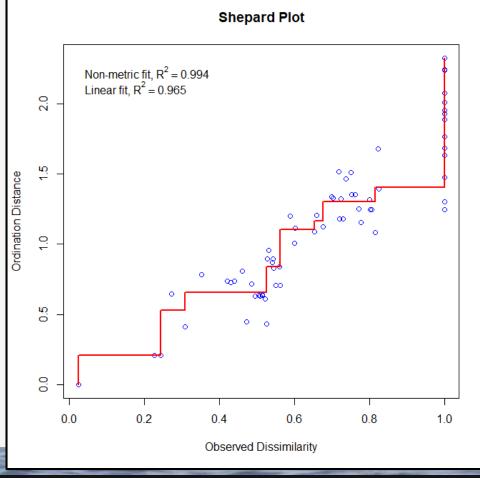
Step 3: Set initial configuration in *m* dimensions

Step 4: Iteratively optimize the configuration

Step 5: Evaluate **Shepard diagram** and **stress**

Stress values below 0.2 are borderline, below 0.1 are good, and 0.05 are excellent.





Step 1: Calculate distance/dissimilarity matrix

Step 2: Choose number of dimensions a priori

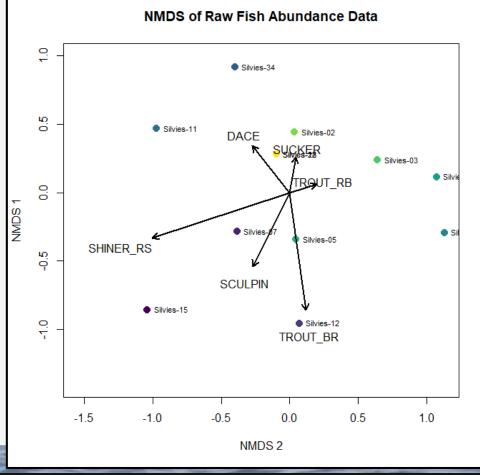
Step 3: Set initial configuration in *m* dimensions

Step 4: Iteratively optimize the configuration

Step 5: Evaluate **Shepard diagram** and **stress**

Step 6: Plot NMDS biplot





Ordination based on rank order rather than exact distances



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- Computationally intensive for large datasets



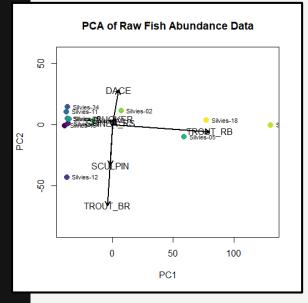
- Ordination based on rank order rather than exact distances
- Computationally intensive for large datasets
- Can be sensitive to starting configuration

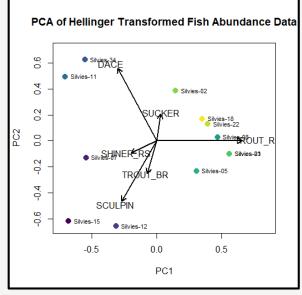


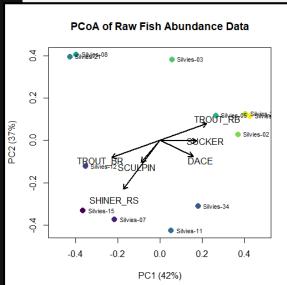
- Ordination based on rank order rather than exact distances
- Computationally intensive for large datasets
- Can be sensitive to starting configuration
- Risk of overfitting

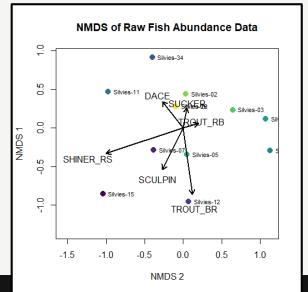


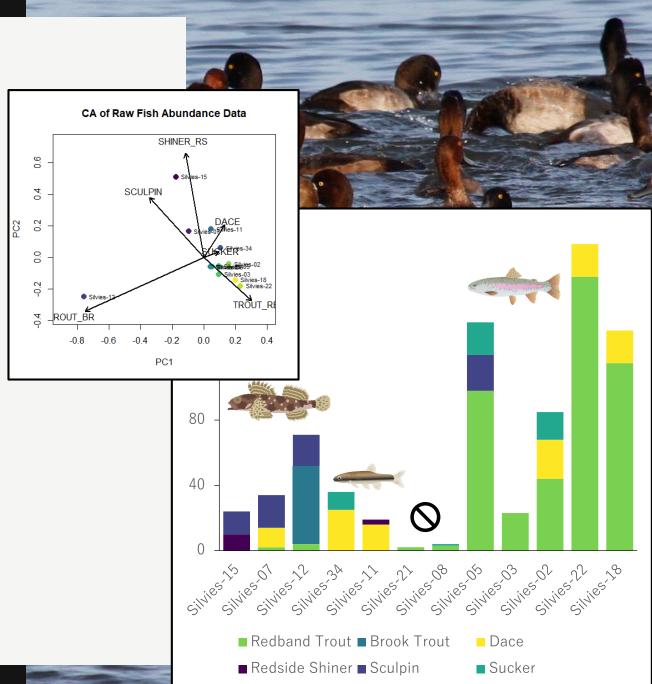
So Which One?











Conclusion: Summary of Key Points

Correspondence Analysis

- Relies on chi-square statistic
- Designed for non-negative, frequency-based data like species abundances
- Over-weighs importance of rare species

Principal Coordinate Analysis

- Can accommodate any distance matrix
- May not capture all variance
- More flexibility = more opportunities to make mistakes

Nonmetric Multidimensional Scaling

- Highly flexible and great for non-metric data
- Axes are arbitrary



Questions?

