

Multivariate Association and Canonical Ordination Methods

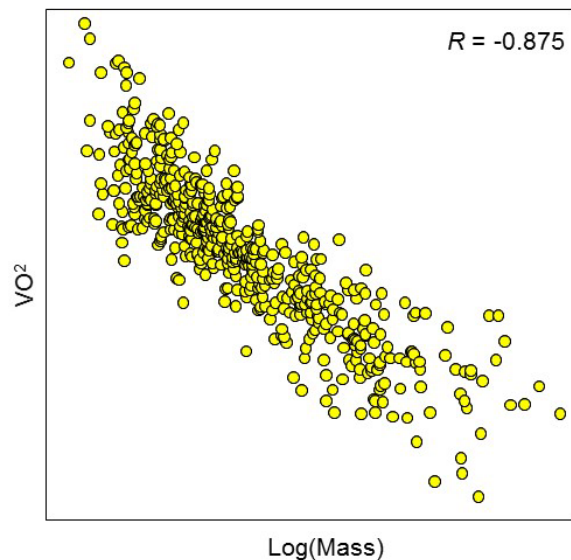
Advanced Biostatistics

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Lecture 10

EEOB 590C

Univariate correlation assesses association between two variables (Y_1 vs Y_2)



Recall: r is a standardized covariance

$$\text{cov}(y_1, y_2) = \frac{1}{n-1} \sum_{i=1}^n (y_{i1} - \bar{y}_{11})(y_{i2} - \bar{y}_{12})$$
$$\text{cor}(y_1, y_2) = r_{12} = \frac{1}{n-1} \sum_{i=1}^n \frac{(y_{i1} - \bar{y}_{11})}{s_1} \frac{(y_{i2} - \bar{y}_{12})}{s_2}$$

But what if \mathbf{Y}_1 & \mathbf{Y}_2 are *sets* of variables (i.e., multivariate matrices)?

How can we determine the extent to which \mathbf{Y}_1 & \mathbf{Y}_2 are correlated or covary?

Four main approaches

- Mantel tests
- Escoffier's RV
- Two-block partial least squares
- Canonical correlation

Mantel test evaluates association using distance matrices (Mantel, 1967)

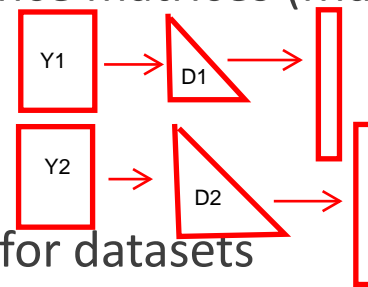
Procedure

Based on the type of input data. Binary? Jacard distance. Abundance? Bray-Curtis.

Data matrix
(Must have same number of rows)

Distance matrix

Unfolded matrices into vectors



1. Calculate appropriate distance matrices for datasets
2. 'Unfold' matrices into vectors of length $n(n-1)/2$ (only off-diagonal elements)
3. Mantel statistic:

$$z_M = \sum_{i=1}^{n-1} \sum_{j=i+1}^n X_{ij} Y_{ij}$$

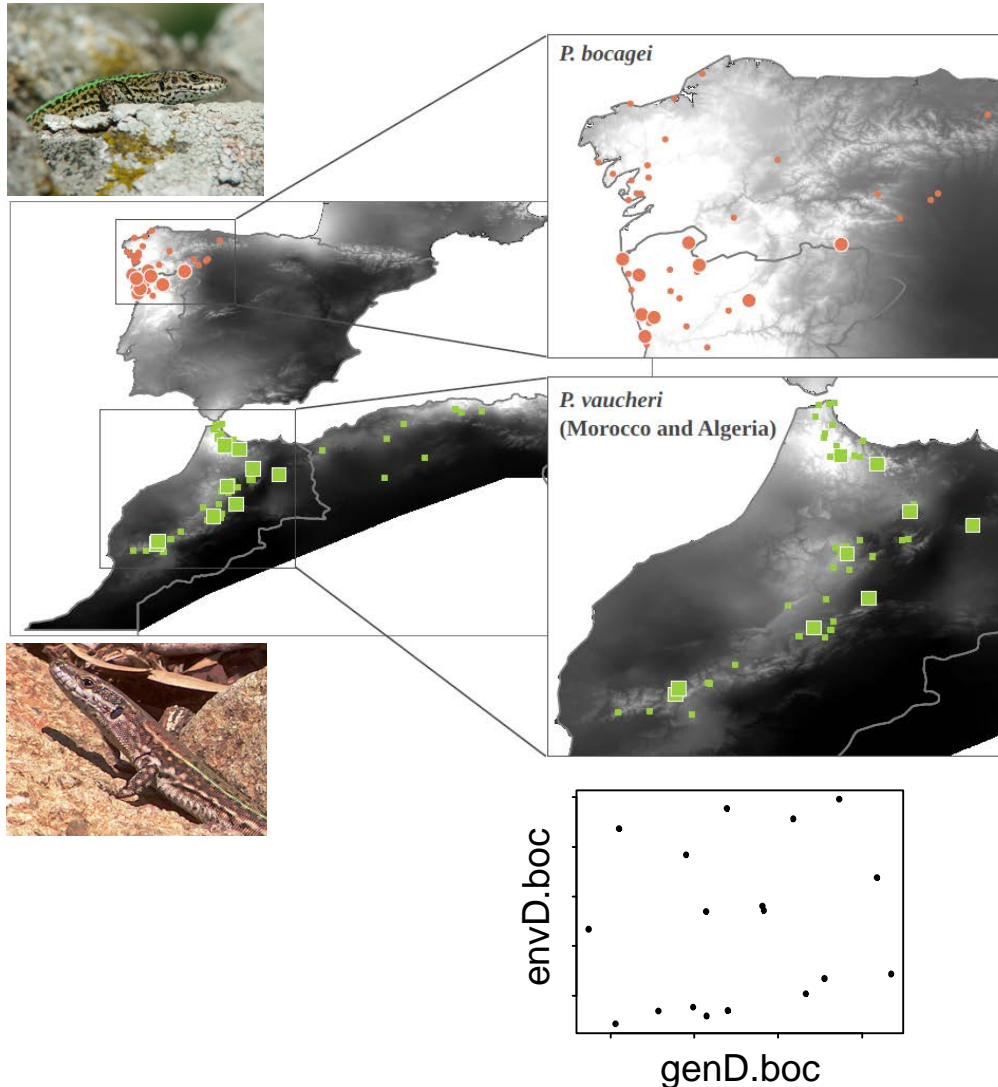
4. Standardized Mantel coefficient of matrix association:

$$r_M = z_M / [n(n-1)/2] - 1$$

5. Assess significance through permutation test*

* Permutation is performed on objects in the distance matrix, NOT on the vector!!!

Is genetic differentiation between populations associated with environmental factors (examined in each of 2 species)?



```
> mantel(genD.boc, envD.boc)
```

Mantel statistic r : 0.068

Significance: 0.380

```
> mantel(genD.vau, envD.vau)
```

Mantel statistic r : 0.446

Significance: 0.010

```
> mantel(genD.vau, geogD.vau)
```

Mantel statistic r : 0.569

Significance: 0.003

Third matrix! What to do?

1: Three-way Mantel Test: for accounting for correlated structure (e.g., spatial)

-Test r_{XY} while accounting for Z ← Testing two data sets while accounting for a third.

-partial Mantel coefficient (analogous to a partial correlation coefficient)

The correlation of x and y while holding z constant. →
$$r_{XY.Z} = \frac{r_{XY} - r_{XZ}r_{YZ}}{\sqrt{1 - r_{XZ}^2} \sqrt{1 - r_{YZ}^2}}$$

Significance found from either:

← Don't bother with this one anymore as computer speed isn't as important. Also can have higher type 1 error.

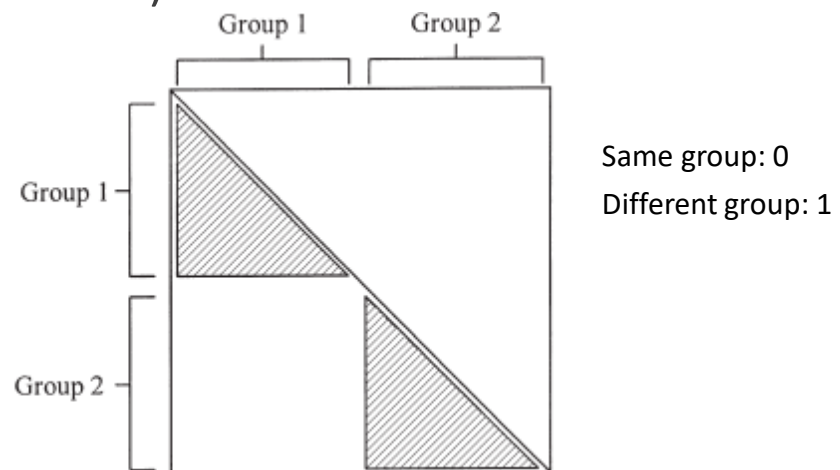
1: Obtain X_{resid} , Y_{resid} from regression on Z , use these and permute

2: Perform full 3-way using $r_{xy.z}$ as above

Residual method faster, but can have higher type I error rates for small N (see Legendre & Legendre 2012)

2: Mantel on design matrices (akin to ANOVA)

-Mantel stat SS_{between}



General and straightforward approach for associating multivariate datasets

Major Weaknesses:

- Can have inflated type I error rates and low power
- Can have significant bias in estimates with autocorrelated data (e.g., spatial)
- Has lower power than GLM or permutational-MANOVA when data can be analyzed as such

Conclusion: though widely used (especially in ecology), Mantel tests not optimal

Recommendation: Use other multivariate covariation methods

See:

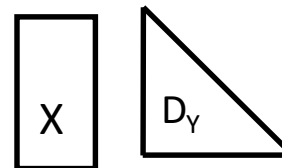
Oden and Sokal 1992. *J. Classif.*

Legendre 2000. *J. Stat. Comp. Simul.*

Harmon and Glor 2010. *Evolution.*

Guillot and Rousset 2013. *Methods Ecol. Evol.*

Sometimes datasets are in various forms:



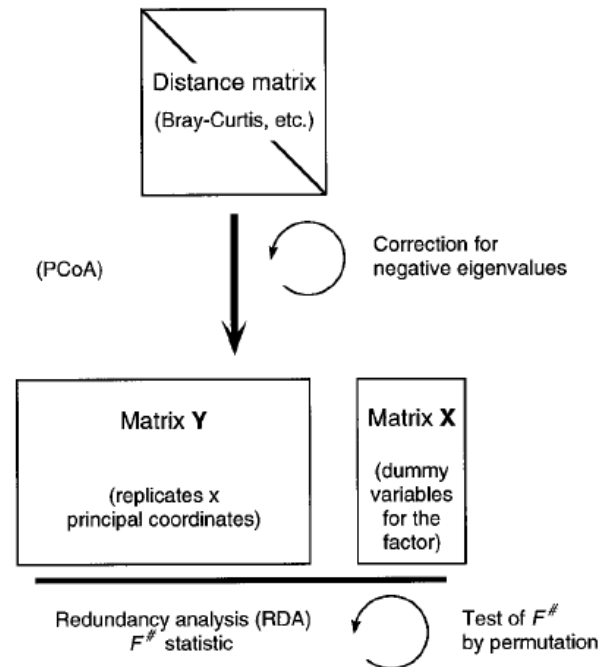
Could use Mantel test, but type I error/power/bias issues

Instead:

- Use PCoA on D_x to obtain multivariate data
- Run GLM or permutational GLM*

$$\hat{\mathbf{Y}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}$$

NOTE: same procedure potentially useful for combining data of different types (binary/continuous)



*NOTE: Legendre & Anderson proposed standard GLM, but we've seen that permutational GLM is more flexible for many situations

Revisiting correlation and covariation:

Univariate: 2 variables

$$\mathbf{Y} = [y_1 \quad y_2]$$

$$\mathbf{SSCP} = \mathbf{Y}^t \mathbf{Y} = \begin{bmatrix} SS_{y_1} & SC_{y_1 y_2} \\ SC_{y_2 y_1} & SS_{y_2} \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} s^2_{y_1} & cov(y_1, y_2) \\ cov(y_1, y_2) & s^2_{y_2} \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} 1 & r_{12} \\ r_{21} & 1 \end{bmatrix}$$

Multivariate: 2 blocks

$$\mathbf{Y} = [\mathbf{Y}_1 \quad \mathbf{Y}_2]$$

$$\mathbf{Y}_1 = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix} \quad \text{Block 1}$$

$$\mathbf{Y}_2 = \begin{bmatrix} d_1 & e_1 & e_1 \\ d_2 & e_2 & e_2 \\ d_3 & e_3 & e_3 \end{bmatrix} \quad \text{Block 2}$$

$$\mathbf{SSCP} = \begin{bmatrix} \mathbf{SS}_{11} & \mathbf{SC}_{12} \\ \mathbf{SC}_{21} & \mathbf{SS}_{22} \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{R}_{21} & \mathbf{R}_{22} \end{bmatrix}$$

$$\mathbf{Y} = [y_1 \quad y_2]$$

For p variables, SSCP, covariance, and correlation matrices have $p \times p$ dimensions

$$\mathbf{Y} = [\mathbf{Y}_1 \quad \mathbf{Y}_2]$$

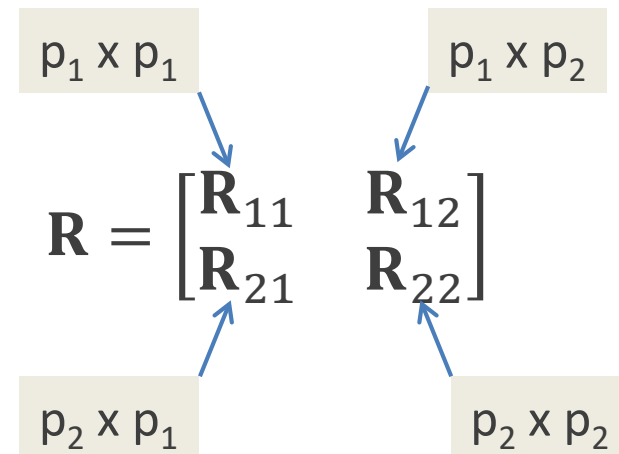
$$\mathbf{Y}_1 \quad n_1 \times p_1$$

$$\mathbf{Y}_2 \quad n_2 \times p_2$$

For two blocks, SSCP, covariance, and correlation matrices have $(p_1 + p_2) \times (p_1 + p_2)$ dimensions

$$\text{SSCP} = \begin{bmatrix} \mathbf{SS}_{11} & \mathbf{SC}_{12} \\ \mathbf{SC}_{21} & \mathbf{SS}_{22} \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix}$$



S^2 for Y_1

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix}$$

Cov across
blocks

$$\mathbf{S}_{21} = \mathbf{S}_{12}^T$$

S^2 for Y_2

Association across variables (correlation):

Univariate (note: can also be from SSCP of centered data)

$$\mathbf{S} = \begin{bmatrix} S^2_{y_1} & Cov_{y_1 y_2} \\ Cov_{y_2 y_1} & S^2_{y_2} \end{bmatrix}$$

$$r_{12} = \frac{Cov_{y_2 y_1}}{\sqrt{S^2_{y_1} S^2_{y_2}}} \quad r_{12}^2 = \frac{Cov_{y_2 y_1}^2}{S^2_{y_1} S^2_{y_2}}$$

Multivariate

$$RV = \frac{tr(\mathbf{S}_{12} \mathbf{S}_{21})}{\sqrt{tr(\mathbf{S}_{11} \mathbf{S}_{11}) tr(\mathbf{S}_{22} \mathbf{S}_{22})}}$$

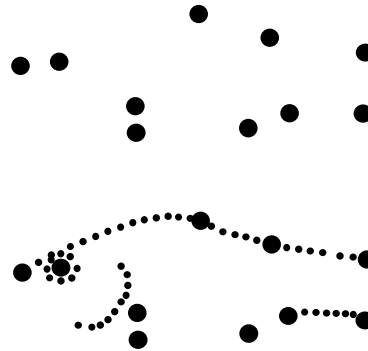
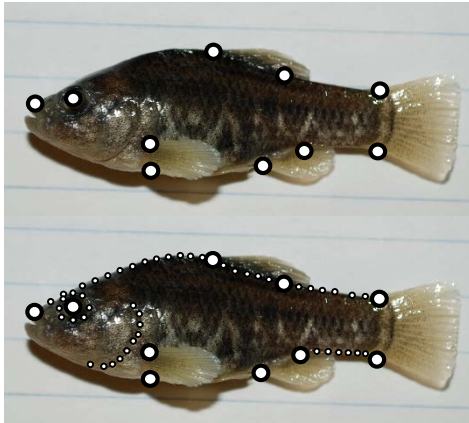
**tr*: the trace of the matrix, the sum of diagonal elements

- Strength of association between subunits: Escoffier's RV
 1. Calculate the covariance among traits, partitioned into subunits
 2. RV is then calculated as:

$$RV = \frac{\text{tr}(\mathbf{S}_{12}\mathbf{S}_{21})}{\sqrt{(\text{tr}(\mathbf{S}_{11}\mathbf{S}_{11})\text{tr}(\mathbf{S}_{22}\mathbf{S}_{22}))}}$$

- Expresses covariation between subunits relative to covariation within ($0 < RV < 1$)
- Statistical assessment via permutation
 - Row-wise permutation of \mathbf{Y}_1 , obtain distribution of RV_{rand}

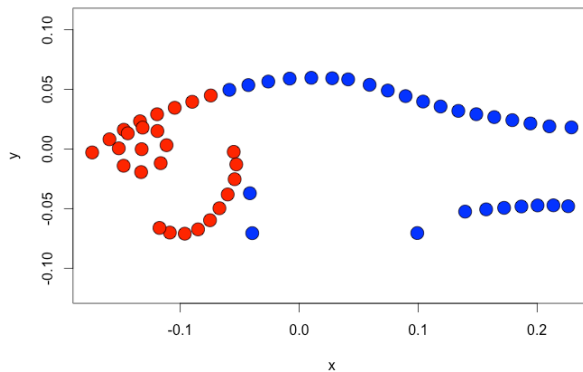
Covariation between body regions in desert pupfish



$$RV = \frac{tr(\mathbf{S}_{12}\mathbf{S}_{21})}{\sqrt{tr(\mathbf{S}_{11}\mathbf{S}_{11})tr(\mathbf{S}_{22}\mathbf{S}_{22})}} = 0.608$$

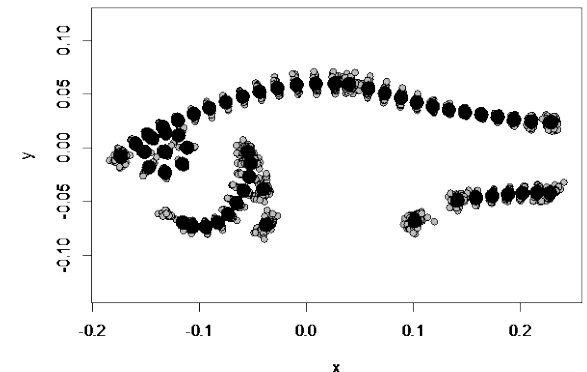
$$\sqrt{RV} = 0.779$$

$$P_{rand} < 0.001$$



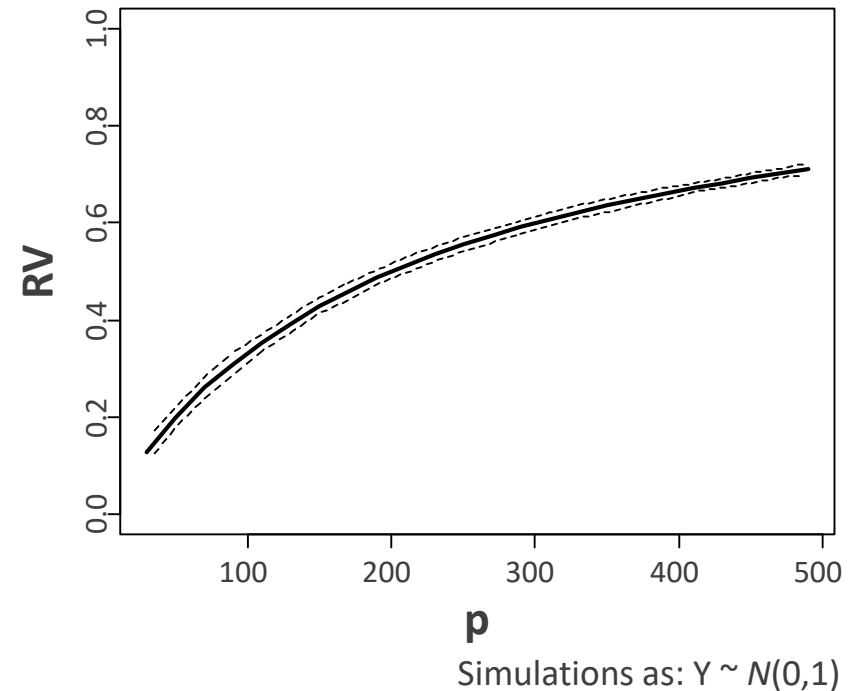
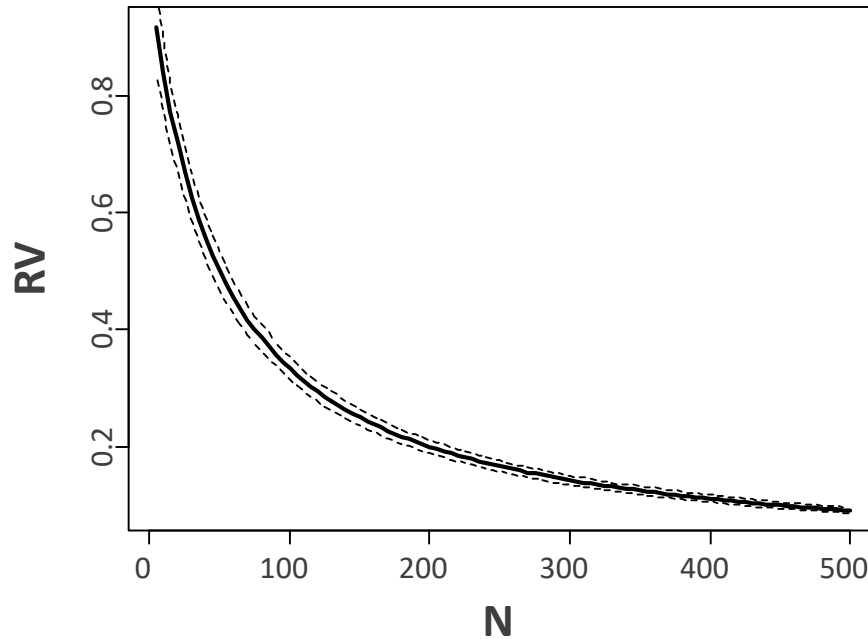
- $N = 54$
- $Y_1 = 54$ (on head)
- $Y_2 = 58$ (on body)

Conclusion: head shape and body shape covary and are correlated with one another



RV coefficient useful for evaluating degree of covariation between two blocks

However, RV is sensitive to N and p_{var}



Conclusion: Cannot compare RV values across datasets to determine which dataset displays 'greater degree' of covariation.

To compare across datasets, need another measure (CR coefficient: Adams 2016)

Evaluates degree of covariation between sets of variables and describes *how* the two blocks are related

Cross-covariance (\mathbf{S}_{12}) expresses relationship between variables in \mathbf{Y}_1 & \mathbf{Y}_2

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix}$$

Decompose this to find rotational solution that describes greatest covariation between the two data sets, \mathbf{Y}_1 & \mathbf{Y}_2

$$\mathbf{S}_{12} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$$

$$S_{12} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$$

Left singular vectors,
eigenvectors of \mathbf{Y}_1 aligned to
the direction of maximum
covariation between \mathbf{Y}_1 and \mathbf{Y}_2

Right singular vectors,
eigenvectors of \mathbf{Y}_2 aligned to
the direction of maximum
covariation between \mathbf{Y}_1 and \mathbf{Y}_2

Eigenvalues (singular values),
they allow evaluation of the %
covariance explained

$$\frac{\lambda_1^2}{\sum \lambda_i^2} \times 100\%$$

$$\mathbf{S}_{12} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$$


Projection of centered variable matrices on corresponding singular vectors provide ordination scores

$$\mathbf{P}_1 = \mathbf{Y}_{1c}\mathbf{U} = [\mathbf{p}_{11} \quad \mathbf{p}_{12} \quad \cdots \quad \mathbf{p}_{1\min(p_1, p_2)}]$$

$$\mathbf{P}_2 = \mathbf{Y}_{2c}\mathbf{U} = [\mathbf{p}_{21} \quad \mathbf{p}_{22} \quad \cdots \quad \mathbf{p}_{2\min(p_1, p_2)}]$$

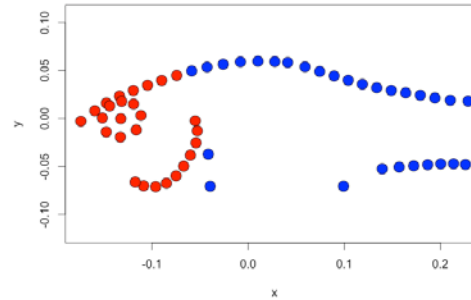
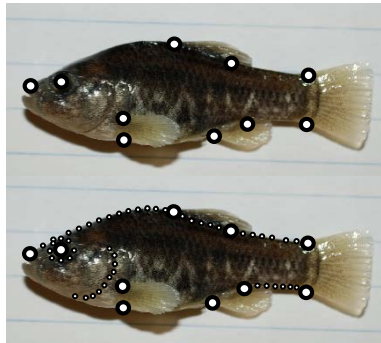
Only the first vectors are meaningful for describing and interpreting maximum covariation

The Pearson correlation between these vectors is a measure of matrix association


$$r_{PLS} = \text{cor}(\mathbf{p}_{11}, \mathbf{p}_{21})$$

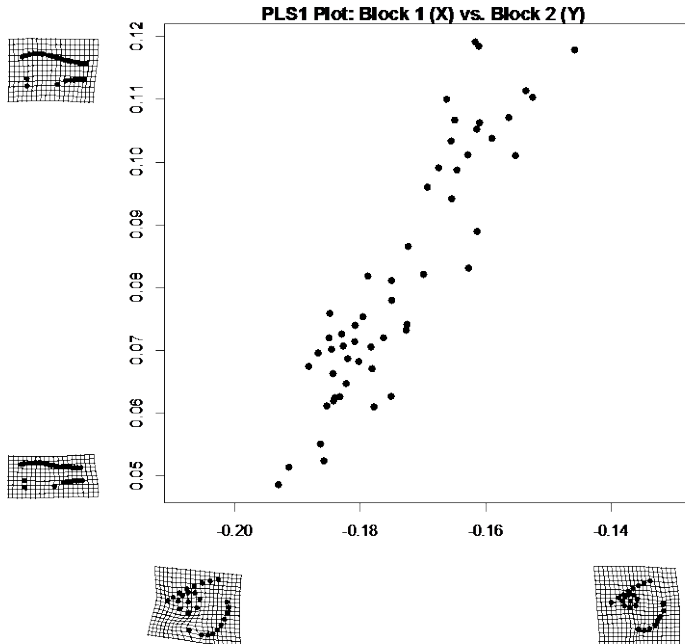
Association can be tested by row-permutation of \mathbf{Y}_2

Covariation between body regions in desert pupfish



$$RV = \frac{tr(\mathbf{S}_{12}\mathbf{S}_{21})}{\sqrt{tr(\mathbf{S}_{11}\mathbf{S}_{11})tr(\mathbf{S}_{22}\mathbf{S}_{22})}} = 0.608$$

$$\sqrt{RV} = 0.779$$



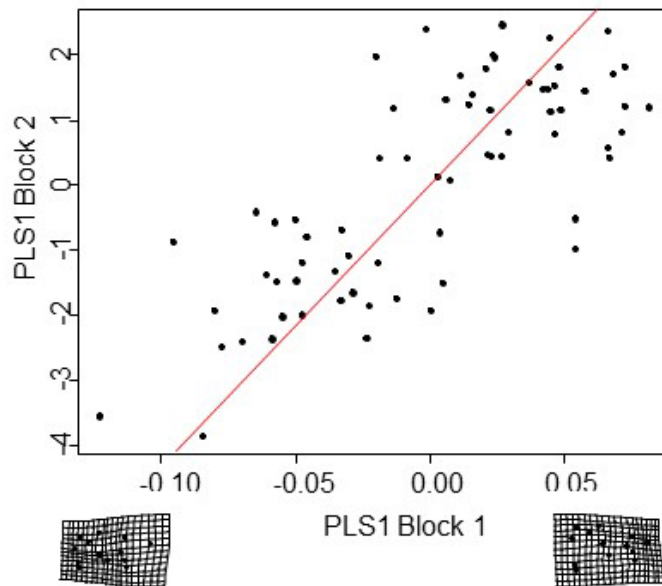
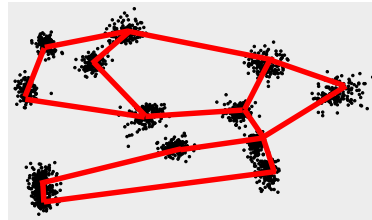
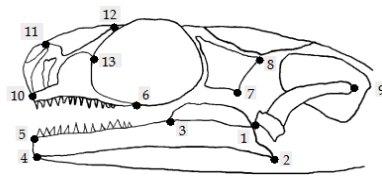
$$r_{PLS} = cor(\mathbf{p}_{11}, \mathbf{p}_{21}) = 0.917$$

$$P_{rand} < 0.001$$

Conclusion: head shape and body shape covary and are correlated with one another

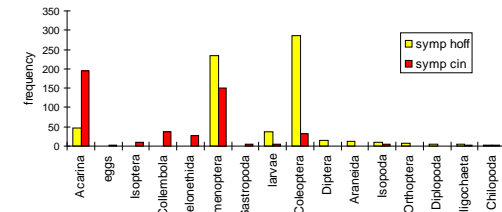
Note: Examining PLS loadings (as in PCA) allows discovery of important variables

Covariation between morphology and food use in salamanders



$$r_{PLS} = 0.759$$

$$P_{rand} < 0.001$$



Conclusion: morphology and food use covary

Loadings on food axis (PLS2): mainly a contrast of small vs. large prey items

oligo	gastro	isopo	diplo	chilop	acar	aranei	chelo	coleo	collem	dipter	hymen	isopt	orthop	larvae	eggs
0.09	-0.018	0.0424	0.0551	0.0933	-0.507	0.2537	-0.112	0.4949	-0.394	0.1658	0.3649	-0.119	0.1263	0.2158	-0.071

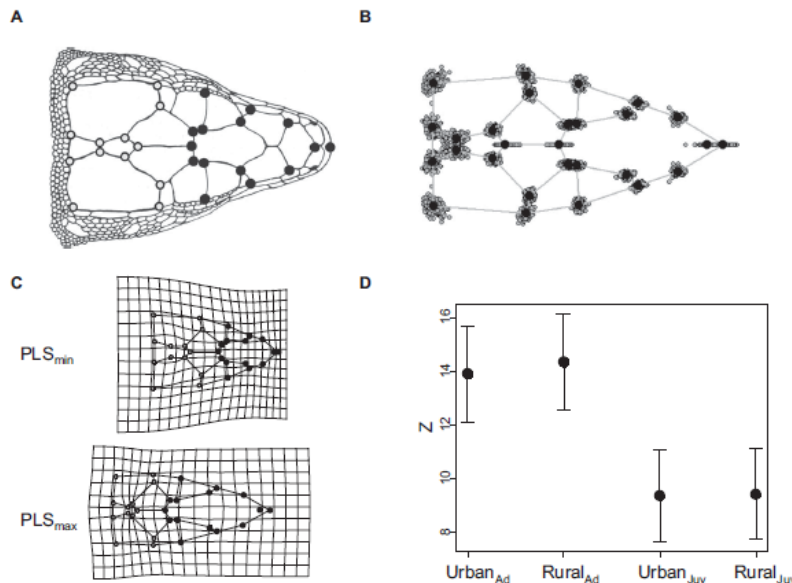
Like the RV, r_{pls} can be sensitive to p_{var}

To compare across datasets, obtain Z-score from permutation distribution

$$Z = \frac{r_{obs} - \mu_r}{\sigma_r}$$

Compare 2 values as: $\hat{z}_{12} = \frac{|(r_1 - \hat{\mu}_1) - (r_2 - \hat{\mu}_2)|}{\sqrt{\hat{\sigma}_{r_1}^2 + \hat{\sigma}_{r_2}^2}}$. (under standard normal distribution)

Example: PLS (anterior/posterior head shape) in juveniles vs. adults



Significantly greater covariation in adults

Identify maximal correlation between blocks \mathbf{Y}_1 & \mathbf{Y}_2

- Like 2B-PLS, r_{12} found from linear combinations (LC) in \mathbf{Y}_1 & \mathbf{Y}_2
- More constrained than PLS
 - Orthogonality within blocks (same as PCA and PLS)
 - Orthogonality across blocks (i.e. $\mathbf{Y}_{11} \perp \mathbf{Y}_{21}$)

If one block has $p=1$ variable, CCorA = multiple regression

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{R}_{21} & \mathbf{R}_{22} \end{bmatrix}$$

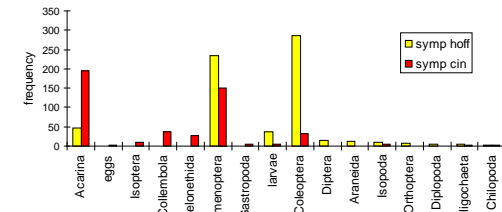
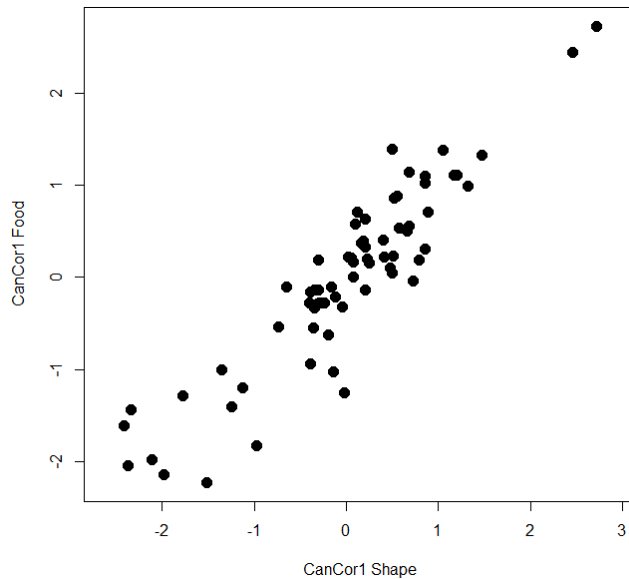
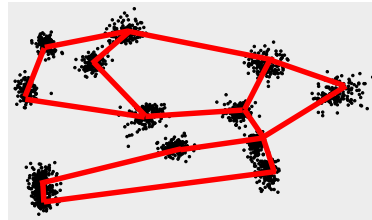
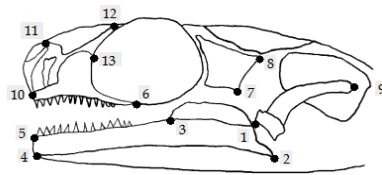
$$\mathbf{A} = \mathbf{R}_{11}^{-1/2} \mathbf{R}_{12} \mathbf{R}_{22}^{-1} \mathbf{R}_{21} \mathbf{R}_{11}^{-1/2} \xrightarrow{\text{eigenanalysis}} \mathbf{U}: \text{canonical vectors for } \mathbf{Y}_1$$

$$\mathbf{B} = \mathbf{R}_{22}^{-1/2} \mathbf{R}_{12} \mathbf{R}_{11}^{-1} \mathbf{R}_{21} \mathbf{R}_{22}^{-1/2} \xrightarrow{\text{eigenanalysis}} \mathbf{V}: \text{canonical vectors for } \mathbf{Y}_2$$

$$\mathbf{C} = \mathbf{R}_{22}^{-1} \mathbf{R}_{21} \mathbf{R}_{11}^{-1} \mathbf{R}_{12} \xrightarrow{\text{eigenanalysis}} \lambda: \text{canonical correlations}$$

Significance from Pillai's trace of \mathbf{C} (& often permutation)

Covariation between morphology and food use in salamanders



Higher correlation than before because of higher mathematical constraints.

$$r_{CCorA} = 0.916$$

$$P_{rand} < 0.001$$

Conclusion: morphology and food use covary

Note: r_{CCorA} is higher than r_{PLS} because of additional mathematical constraints

Various approaches to multivariate association

1: Mantel Tests: associate distance matrices

- High type I error, low power, and bias



Abandon this.

2: RV: strength of association


- RV_{Null} varies with N & p

3: PLS: maximum covariation between sets of variables

- Can use Z-score transform to compare across datasets

4: CCorA: maximum correlation between sets of variables

- Elegant, but many (unrealistic) mathematical constraints



Don't like this.

PLS is most general and with fewest mathematical constraints

Considers association of two matrices (**X** & **Y**)

Provides visualization (ordination) from $\mathbf{Y} \sim \mathbf{X}$ (differing from PCA/PCoA)

Several canonical ordination methods

- Canonical Variates Analysis (CVA) / Discriminant Analysis (DA)

- Redundancy Analysis (RDA)

- Canonical Correspondence Analysis (CCA)

*Mathematically, the canonical form (from Greek $\kappa\alpha\upsilon\omega\nu$, 'kanôn') is the simplest and most comprehensive representation of relationship, without losing generality

Recall univariate multiple regression: $Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \dots + \varepsilon_i$

-Here, predicted values ($\hat{\mathbf{Y}}$) are a 1-dimensional 'ordination' of original \mathbf{Y} along the regression line

-Regression maximizes R^2 between \mathbf{Y} and $\hat{\mathbf{Y}}$

-Represents the optimal LS relationship between \mathbf{X} and \mathbf{Y}

Canonical analyses share this property for multivariate \mathbf{Y} , and generate ordinations of \mathbf{Y} constrained by the maximal LS relationship to \mathbf{X}

Consider these different ways of dealing with joint-variation in \mathbf{X} & \mathbf{Y}

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_{XX} & \mathbf{S}_{XY} \\ \mathbf{S}_{YX} & \mathbf{S}_{YY} \end{bmatrix}$$

RDA and CCA do so in a predictive sense (i.e., regression)

Canonical Correlation and 2B-PLS also deal with this, but in a 'correlational' sense

Ordination that maximally discriminates among *known* groups (g)

Variation expressed as ratio of between-group variation (**A**) relative to within-group variation (**V**)

$$\mathbf{V}^{-1}\mathbf{A}$$

Decomposition of $\mathbf{V}^{-1}\mathbf{A}$ results in canonical vector space

- Suggests which groups differ on which variables
- Within-group variation in CVA plot is circular

METHOD COMMONLY MISUSED BY BIOLOGISTS

CVA accomplished via an eigenanalysis:

$$\mathbf{V}^{-1}\mathbf{A} = \mathbf{C}\mathbf{\Lambda}\mathbf{C}^t$$

- Normalized canonical axes found as:

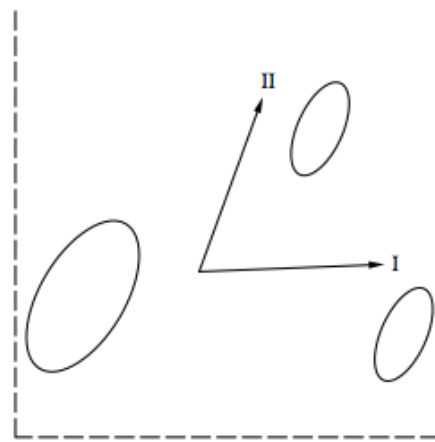
$$\mathbf{C}^* = \mathbf{C}(\mathbf{C}^t\mathbf{V}\mathbf{C})^{-1/2}$$

- Canonical variate scores found via projection

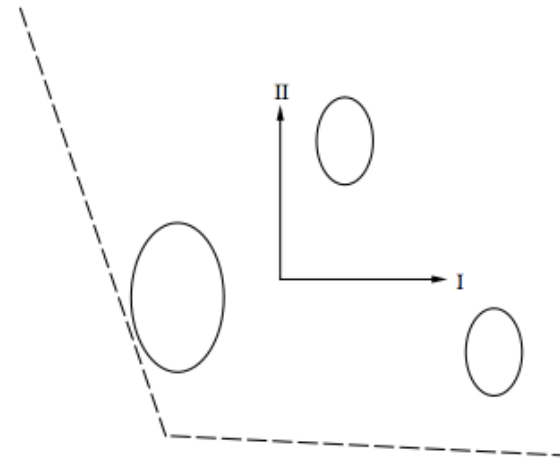
$$\mathbf{Y}_{score} = \left(\mathbf{Y} - \overline{\overline{\mathbf{Y}}}\right)\mathbf{C}^*$$

Visualization accompanied by MANOVA on groups

CVA rotates and shears data space to a spaces of normalized canonical axes
(group variation will be circular)

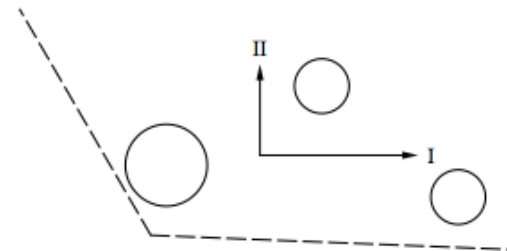


(a)



(b)

Data space (a) →
eigenvectors (b) →
canonical axes (c)



(c)

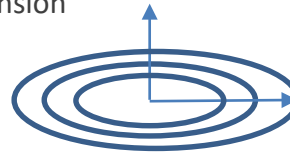
Classify objects (known or unknown) to groups (**VERY useful**)

-Obtain D_{Mahal}^2 objects to group means

$$D_{Mahal}^2 = (\mathbf{Y}_i - \bar{\mathbf{Y}}_2)^t \mathbf{V}^{-1} (\mathbf{Y}_i - \bar{\mathbf{Y}}_2)$$

-Assign objects to group to which it is closest

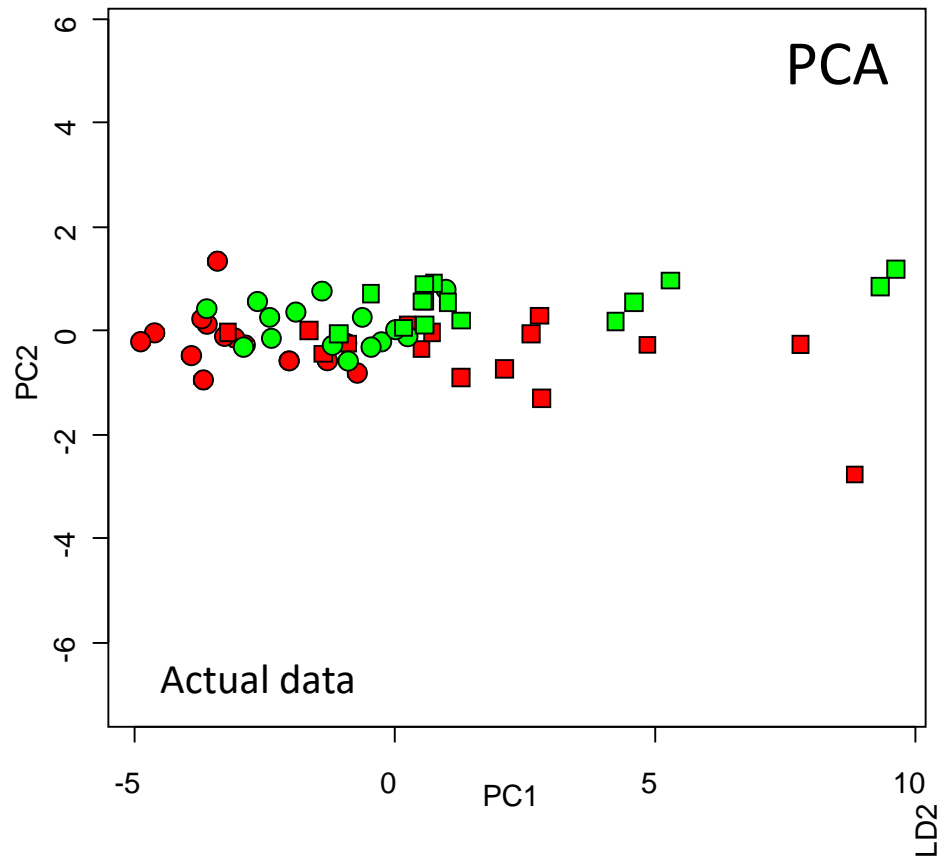
-This weights distance by variation in each dimension



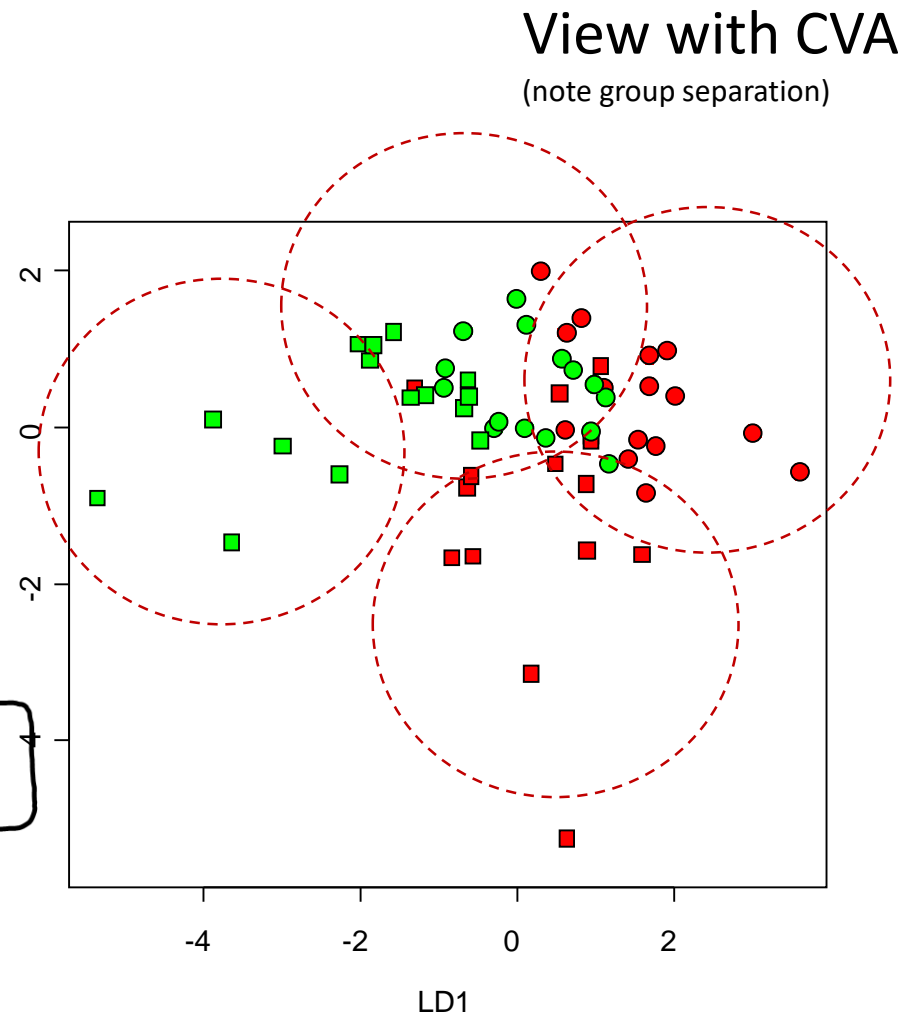
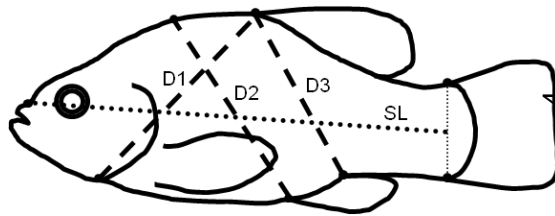
It is 'easier' to shift in the direction of variation, so there is a smaller D_{Mahal} along the main axis of scatter, even if D_{euclid} is similar

-Determine % misclassification

Note: ideally classification rates estimated from second dataset (cross-validation)



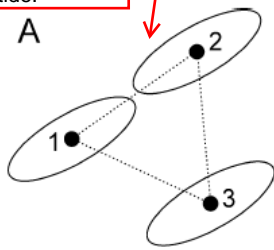
Salty ♀ ●
Salty ♂ ■
Fresh Water ♀ ●
Fresh Water ♂ ■



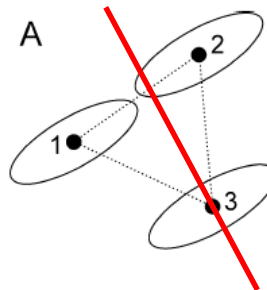
- Ordination provides plot of \mathbf{Y} that maximally separates *a priori* groups
- This is **NOT** a representation of actual space (that is found via PCA/PCoA)
- Plot distorts actual relationships and accentuates group differences (groups appear more distinct than they are)

-Distances and directions distorted in CVA space

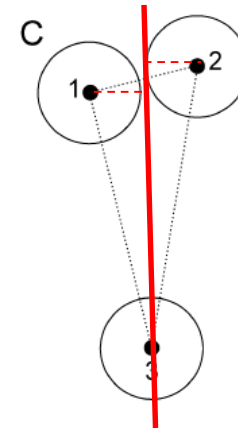
Groups 1 and 2 are both with the same tide; Group 3 is against the tide.



Original data:3
equidistant groups



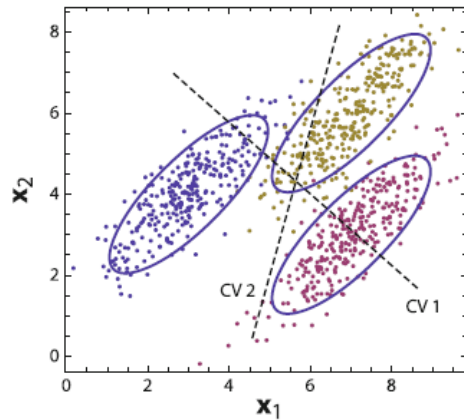
CV1 through data
space



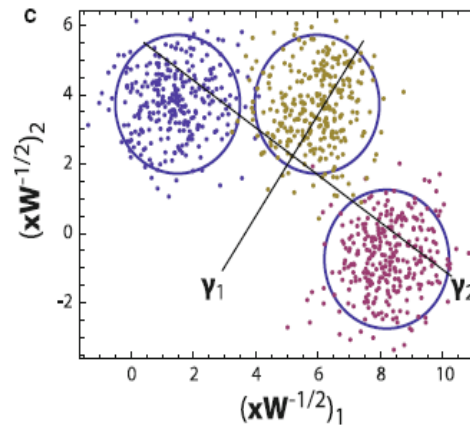
CVA space: groups
NOT equidistant

- CVA should **NOT** be used as a description/representation of variation in multivariate space

CV axes NOT orthogonal in original data space

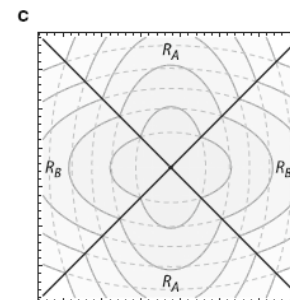
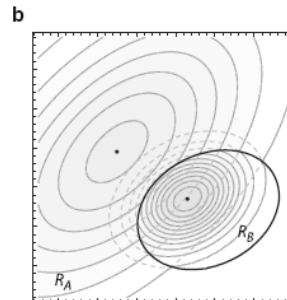
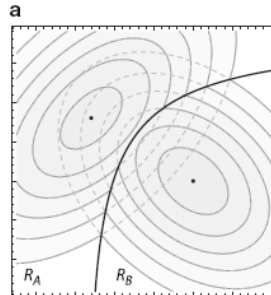
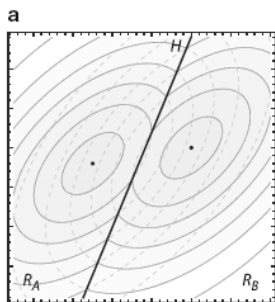


Original
data space

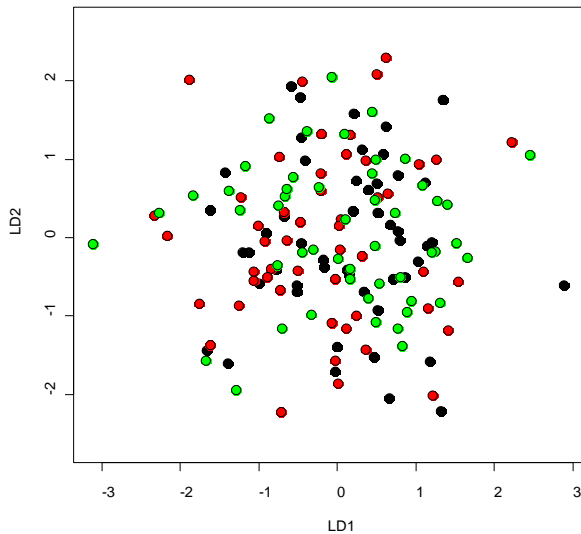


CVA data
space

Linear discrimination ONLY forms linear plane IFF within-group covariances identical (shown as 'equal probability classification lines below)

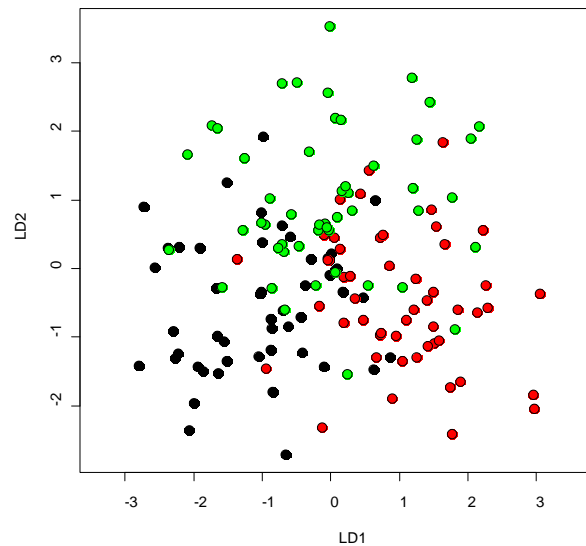


Increasing number of variables enhances *PERCEIVED* group differences, even when groups are identical!

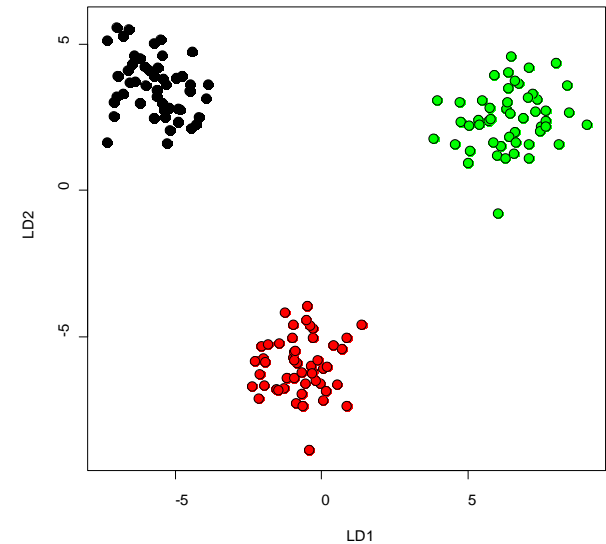


$p = 4$

of variables



$p = 50$



$p = 150$

Simulation: $N=50$, groups = 3

CVA ordination not useful

- Distorts distances and directions in data space
- Misrepresents within-group covariation and group distances
- Perceived group differences increase with additional variables (even for identical groups)

CVA classification *can* be useful

For plot of data space: use PCA/PCoA

Direct extension of multiple regression for multivariate \mathbf{Y}
-*Redundancy* synonymous with 'explained variance'

RDA is a constrained ordination of \mathbf{Y} such that ordination vectors are linear combinations of \mathbf{Y} and linear combinations of \mathbf{X}

RDA is an eigenanalysis of VCV from $(\hat{\mathbf{Y}})$ multivariate multiple regression

Thus, RDA preserves Euclidean distances of objects in space of predicted values $\hat{\mathbf{Y}}$ (appropriate for continuous \mathbf{Y} variables)

- Center **X** and **Y** variables and standardize*
- Perform multivariate multiple regression and obtain predicted values

$$\hat{\mathbf{Y}} = \mathbf{X}(\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{Y}$$

- Calculate VCV of predicted values

$$\mathbf{S}_{\hat{\mathbf{Y}}^t \hat{\mathbf{Y}}} = \frac{1}{n-1} \hat{\mathbf{Y}}^t \hat{\mathbf{Y}} = \mathbf{S}_{\mathbf{YX}} \mathbf{S}^{-1}_{\mathbf{XX}} \mathbf{S}^t_{\mathbf{YX}}$$

- Ordination from PCA of

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_{\mathbf{XX}} & \mathbf{S}_{\mathbf{XY}} \\ \mathbf{S}_{\mathbf{YX}} & \mathbf{S}_{\mathbf{YY}} \end{bmatrix}$$

$$\mathbf{S}_{\hat{\mathbf{Y}}^t \hat{\mathbf{Y}}} = \mathbf{C} \mathbf{\Lambda} \mathbf{C}^t$$

- NOTE: If **X** or **Y** begins as a distance matrix, first perform PCoA to generate a set of 'variables' for RDA (see Legendre and Anderson, 1999. Ecol. Monogr.)

*steps are not absolutely necessary, but simplify computations, and place variables in context for direct comparison

RDA provides ordination of \mathbf{Y} as maximally described by \mathbf{X}

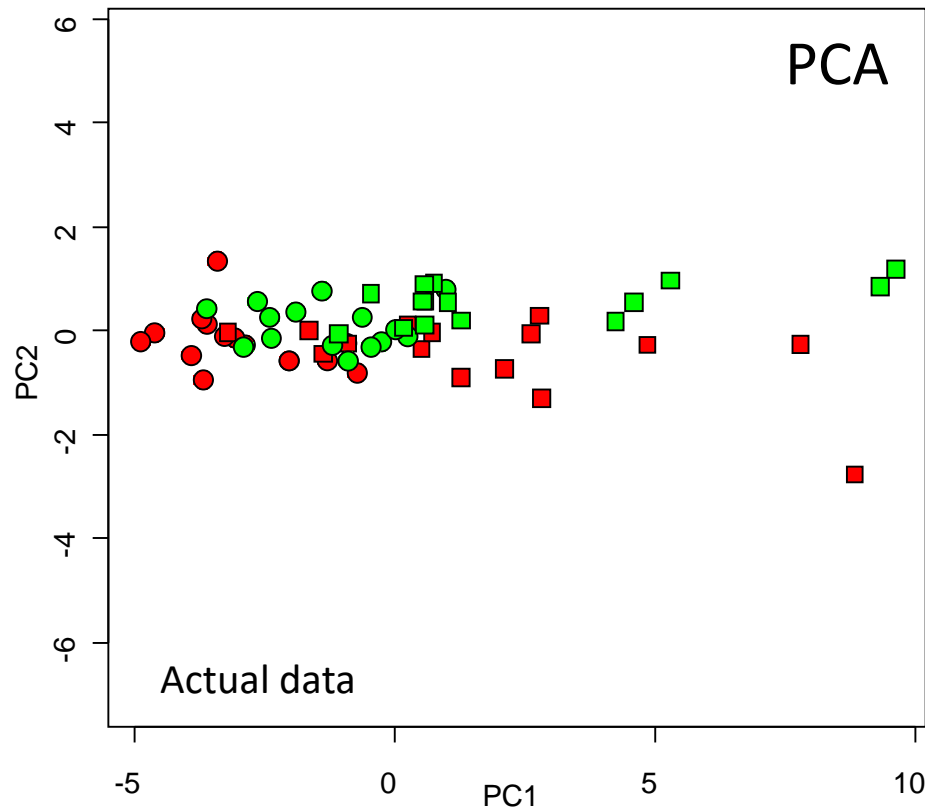
RDA: ordination of 'fitted' values based on GLM ($\hat{\mathbf{Y}}$)

-Eigenvector loadings describe relative contributions of each variable to ordination on that canonical axis (interpret like PC loadings)

-Ordination can be shown as biplot of \mathbf{X} (as vectors) in PCA of $\hat{\mathbf{Y}}$

-Reflects relative importance of variables on ordination

Ordination is 'standardized' for regression of \mathbf{Y} on \mathbf{X}

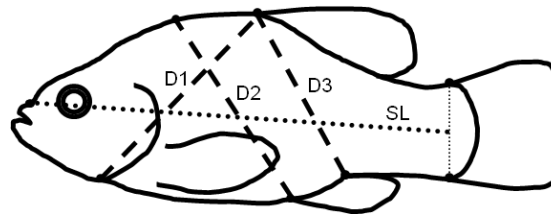


Salty ♀ ●

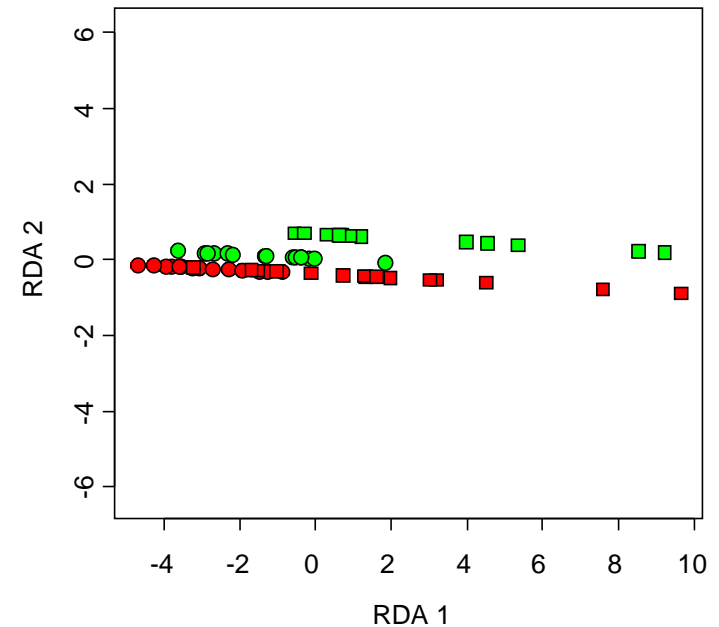
Salty ♂ ■

Fresh Water ♀ ●

Fresh Water ♂ ■



NOTE: in this case, RDA has done exactly what one should NOT do: Fit common slope when groups are diverging (see MANOVA).



RDA

RDA: X: groups and SVL

Y: 3 body depth measurements

- $Y \sim X$ step is useful, though usually through GLM
- Ordination step can lead to biological misinterpretation!
- If wrong model of $Y \sim X$, ordination not representative of pattern
 - RDA should **NOT** be used to describe patterns and variation in data
 - RDA only shows predicted patterns (based on a model, X)
- Exceptionally easy to misuse (knowingly or unknowingly)
 - Provides false sense of pattern relative to error (noise)
 - An incorrect model (X) results in incorrect ordination

- Extends correspondence analysis of \mathbf{Y} to a predictive framework
- CCA is a constrained ordination of \mathbf{Y} given linear combinations of \mathbf{Y} & \mathbf{X}
- Conceptually identical to RDA, but for a different \mathbf{Y} -data input

- Same caveats apply

- Canonical ordination (DA, CVA, RDA, etc.) popular in some disciplines
- They do **NOT** represent a true view of the **Y** data space
 - Views are filtered through some model **$Y \sim X$**
- Actual patterns should always be viewed first (PCA/PCoA)
- Use **EXTREME CAUTION** when interpreting canonical ordinations