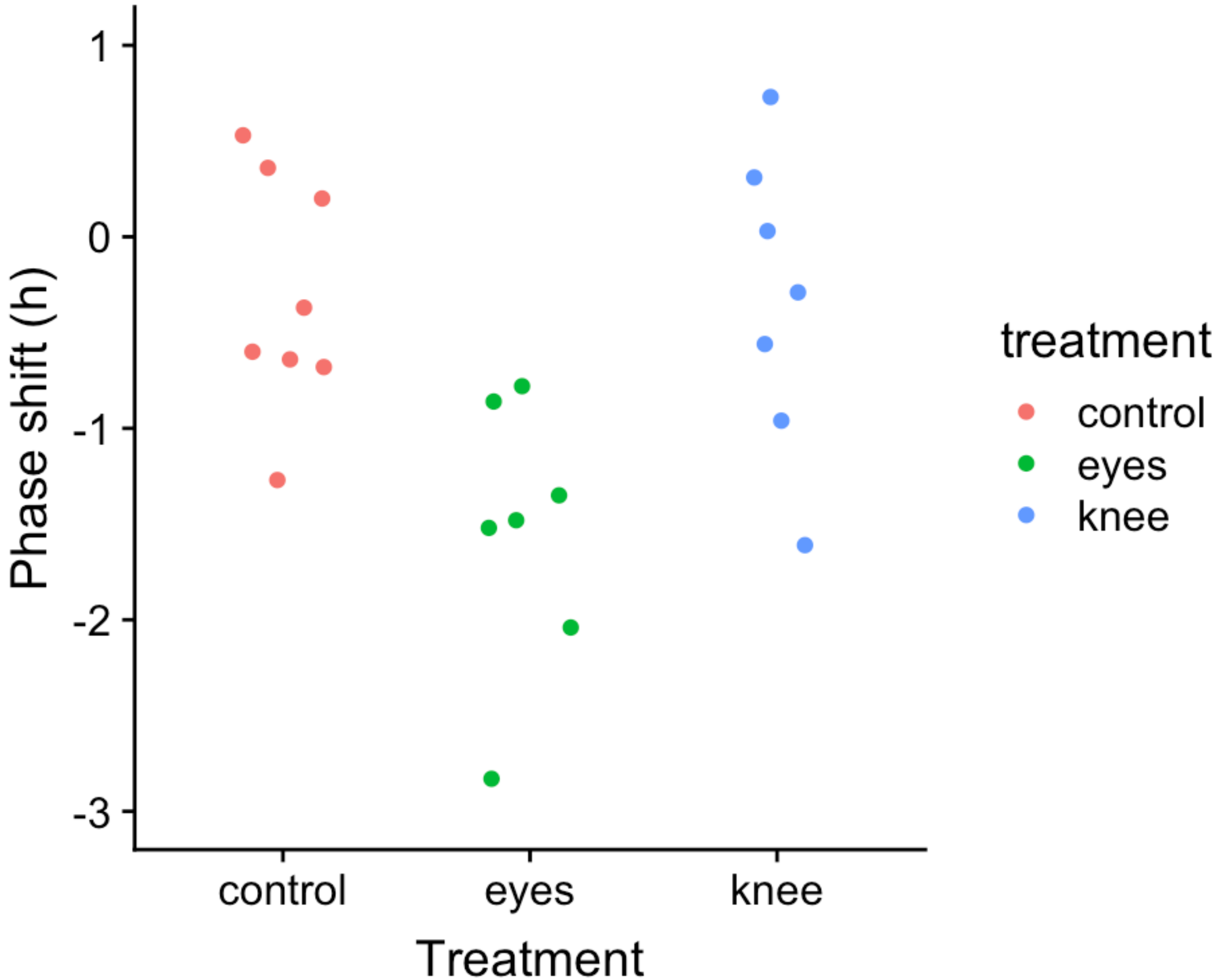
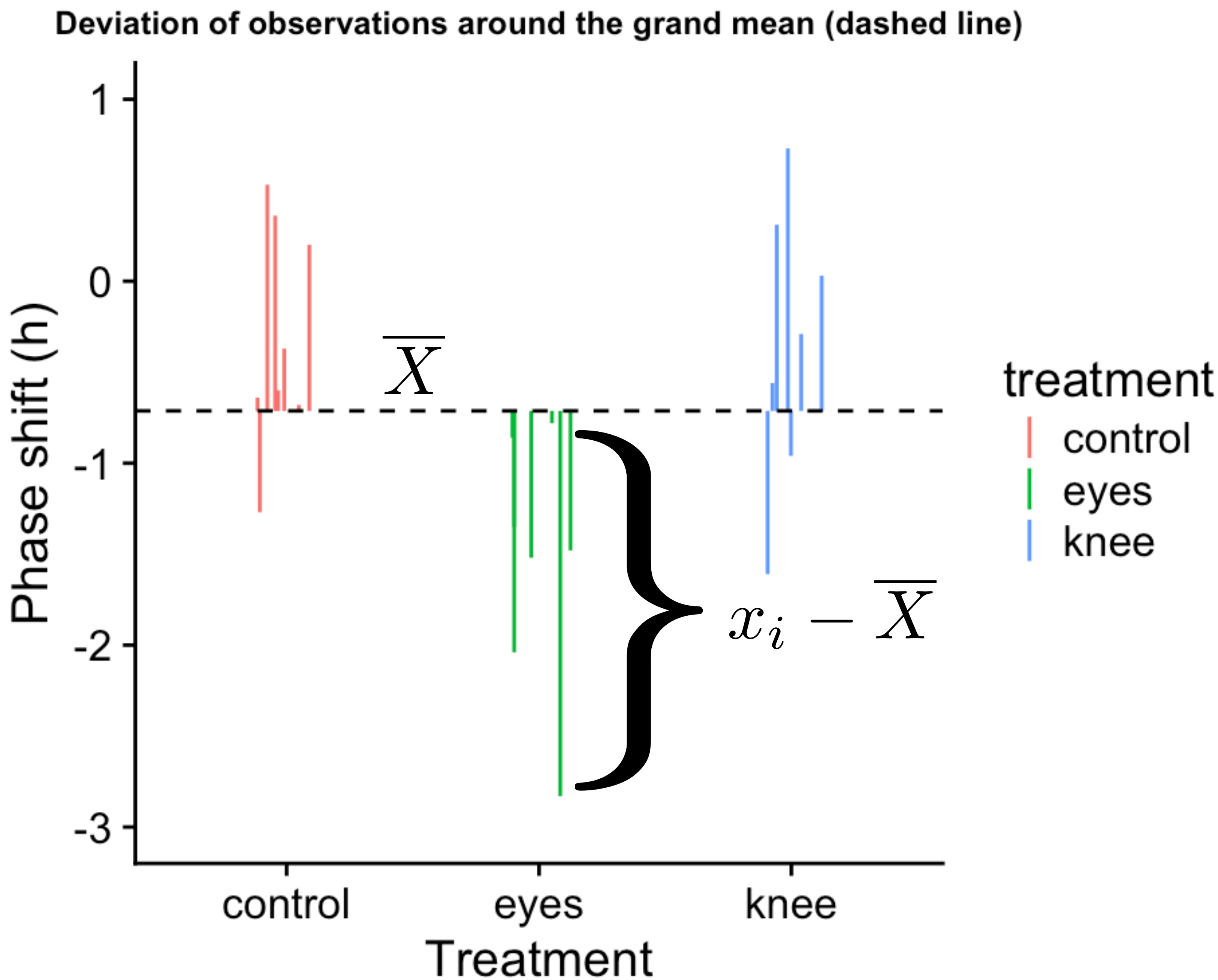
Canonical Variates (Linear Discriminant) Analysis

Review: ANOVA

ANOVA helps us answer the following question:
Does the mean of at least one of the groups differ from the others?

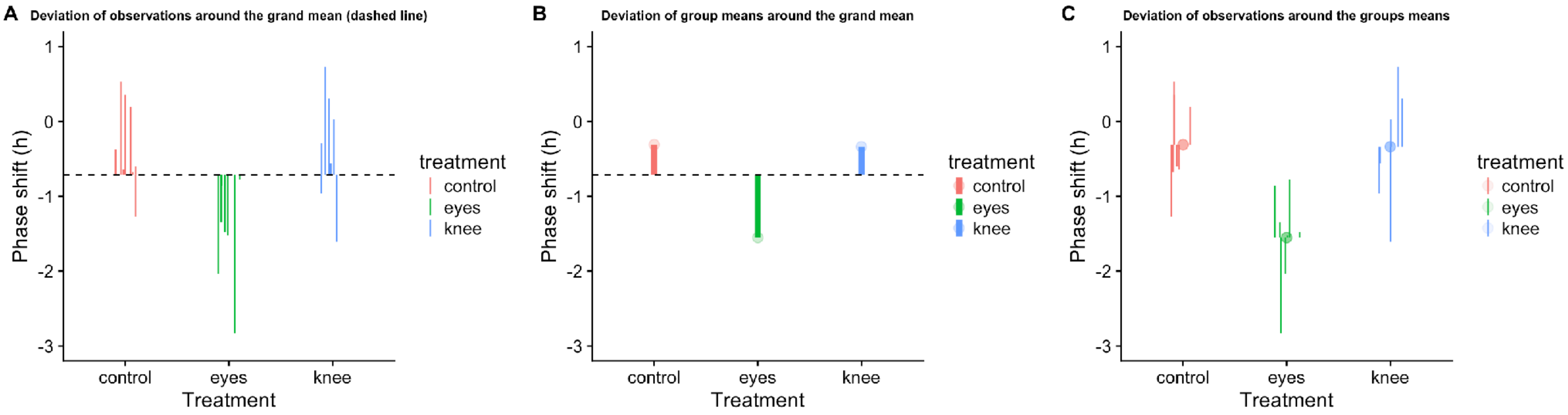


Review: ANOVA - sum of squared deviations



$$SS_{total} = \sum_i (x_i - \overline{X})^2$$

ANOVA: Partitioning of sums-of-squared deviations into "between groups" (group) and "within groups" (error) components



$$SS_{\text{total}} = SS_{\text{group}} + SS_{\text{error}}$$

ANOVA: Test statistic, F

$$F = \frac{\text{between group variation}}{\text{within group variation}} = \frac{\text{MS}_{\text{group}}}{\text{MS}_{\text{error}}}$$

where

$$MS_{\text{group}} = \frac{SS_{\text{group}}}{df_{\text{group}}} = \frac{SS_{\text{group}}}{k-1}$$

$$MS_{\text{error}} = \frac{SS_{\text{error}}}{df_{\text{error}}} = \frac{SS_{\text{error}}}{N-k}$$

If F >> 1, is evidence that groups means differ

Overview of Discriminant Analysis

Discrimination

Given an $n \times p$ data matrix, $\boldsymbol{X}$, and a grouping of the n specimens into g groups, find the linear combination of the variables, $\boldsymbol{X}\boldsymbol{a}$, that best discriminates between the groups.

$$\vec{\boldsymbol{y}}_{\text{discrim}} = a_1\vec{\boldsymbol{x}}_1 + a_2\vec{\boldsymbol{x}}_2 + \cdot + a_p\vec{\boldsymbol{x}}_p$$

Classification

Given g groups, define a function that assigns an object with unknown assignment to the 'best' group.

Fisher's Discriminant Function

- Applies to the two-group case.
- Solution: find $\boldsymbol{a}$ that maximizes the ratio of the squared group mean difference to within-group variance:

$$F = \frac{(\bar{\boldsymbol{x}}_1\boldsymbol{a} - \bar{\boldsymbol{x}}_2\boldsymbol{a})^2}{\boldsymbol{a}'W\boldsymbol{a}}$$

where

- $\bar{\boldsymbol{x}}_1 = \frac{1}{n_1}\sum_{i=1}^{n_1}\boldsymbol{x}_{1i}$ (row-vector of means of group 1)
- $\bar{\boldsymbol{x}}_2 = \frac{1}{n_2}\sum_{i=1}^{n_2}\boldsymbol{x}_{2i}$ (row-vector of means of group 2)
- $W = \frac{1}{n_1+n_2-2}\sum_{i=1}^{2}\sum_{j=1}^{n_i}(\boldsymbol{x}_{ij} - \bar{\boldsymbol{x}}_i)(\boldsymbol{x}_{ij} - \bar{\boldsymbol{x}}_i)'$ (w/in-group pooled covariance matrix)
- n_i indicates the number of observations in the ith group and the $\boldsymbol{x}_{i1}, \ldots, \boldsymbol{x}_{in_i}$ represent the specific observations (as vectors).

Geometry of the Two-Group Discriminant Function

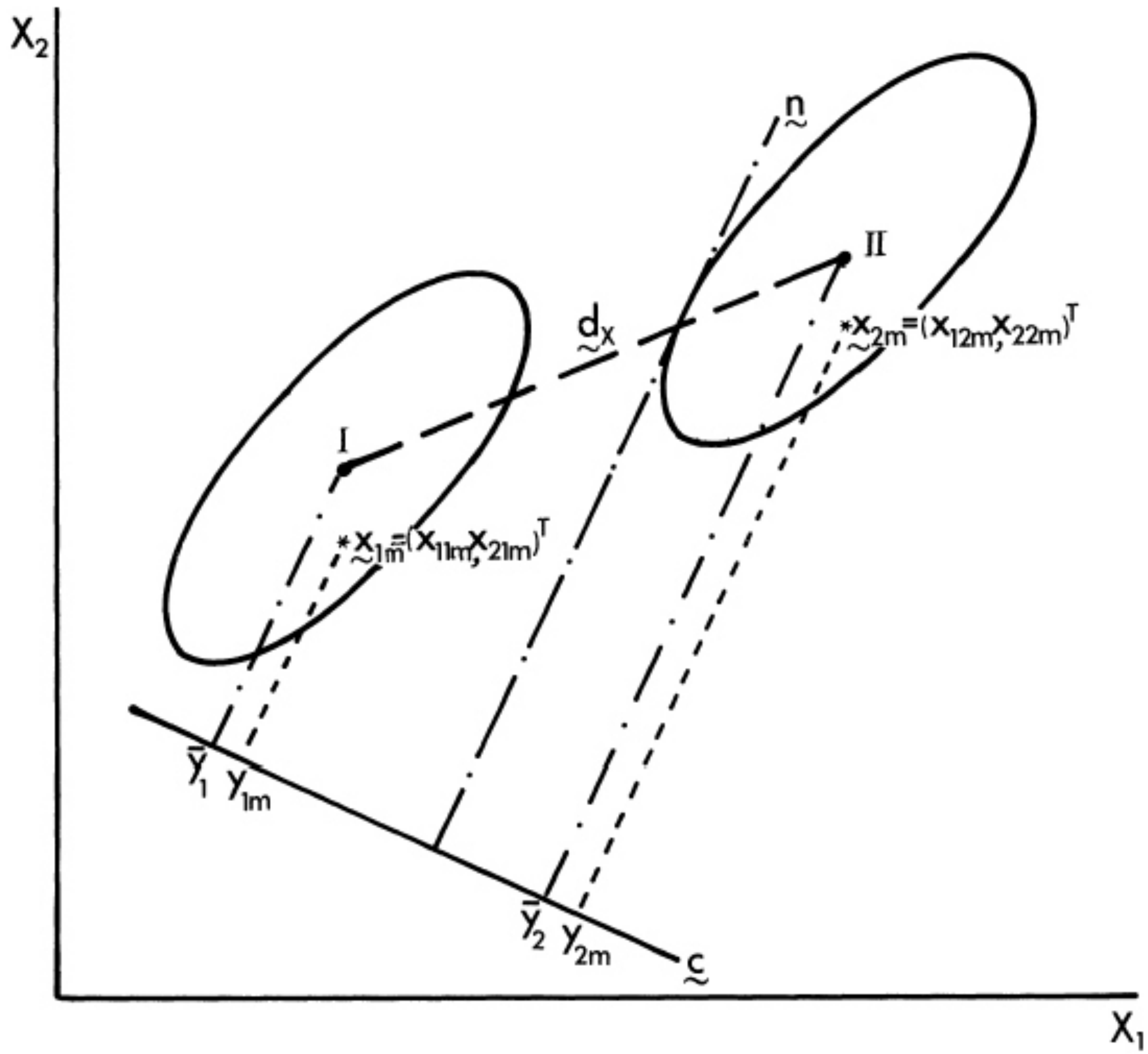


FIG. 4.—Representation of the discriminant function for two groups and two variables, showing the group means and associated 95% concentration ellipses. The vector **c** is the discriminant vector. The points $\bar{y}_1$ and $\bar{y}_2$ represent the discriminant means for the two groups.

The discriminant vector can be constructed by drawing the tangent **n** to the concentration ellipse at the point of intersection with the line **d** joining the group means; the discriminant vector is orthogonal to the tangent **n**.

Fisher's LDF

$$F = \frac{(\boldsymbol{a}'\bar{\boldsymbol{x}}_1 - \boldsymbol{a}'\bar{\boldsymbol{x}}_2)^2}{\boldsymbol{a}'\boldsymbol{W}\boldsymbol{a}}$$

Maximizing F gives:

$$\boldsymbol{a} = c\boldsymbol{W}^{-1}(\bar{\boldsymbol{x}}_1 - \bar{\boldsymbol{x}}_2)'$$

where c is an arbitrary constant (usually taken to be 1).

Fisher's LDF as Classification

Fisher's solution can also be setup as a classification solution using regression.

- setup a dummy variable, $\boldsymbol{y}$ that takes the values:
  - $y_1 = n_2/(n_1 + n_2)$ for observations in group 1
  - $y_2 = -n_1/(n_1 + n_2)$ for observations in group 2
- Solve the standard multivariate regression, $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{b} + \boldsymbol{e}$
- Allocate unknown individual to group 1 if it's predicted y is closer to y_1 than to y_2, otherwise assign to group 2.

What if there are more than two groups?

The multi-group equivalent of Fisher's LDF is called 'Canonical Variate Analysis' (CVA).

- straight forward extension of Fisher's solution
- Find $\boldsymbol{a}$ that maximizes the ratio of between-group to within-group variance:

$$F = \frac{\boldsymbol{a}'\boldsymbol{B}\boldsymbol{a}}{\boldsymbol{a}'\boldsymbol{W}\boldsymbol{a}}$$

- $\boldsymbol{W}$ is within-group matrix (as defined previously)
- $\boldsymbol{B}$ is the between-group covariance matrix
  - $\boldsymbol{B}_w = \frac{1}{g-1}\sum_{i=1}^{g} n_i(\bar{\boldsymbol{x}}_i - \bar{\boldsymbol{x}})(\bar{\boldsymbol{x}}_i - \bar{\boldsymbol{x}})'$ where $\bar{\boldsymbol{x}}$ is the "grand-mean", $\bar{\boldsymbol{x}}_i$ is the mean in group i, and n_i is the sample size in group i (weighted version)
  - $\boldsymbol{B}_u = \frac{1}{g-1}\sum_{i=1}^{g}(\bar{\boldsymbol{x}}_i - \bar{\boldsymbol{x}})(\bar{\boldsymbol{x}}_i - \bar{\boldsymbol{x}})'$ (unweighted version)

Geometry of CVA

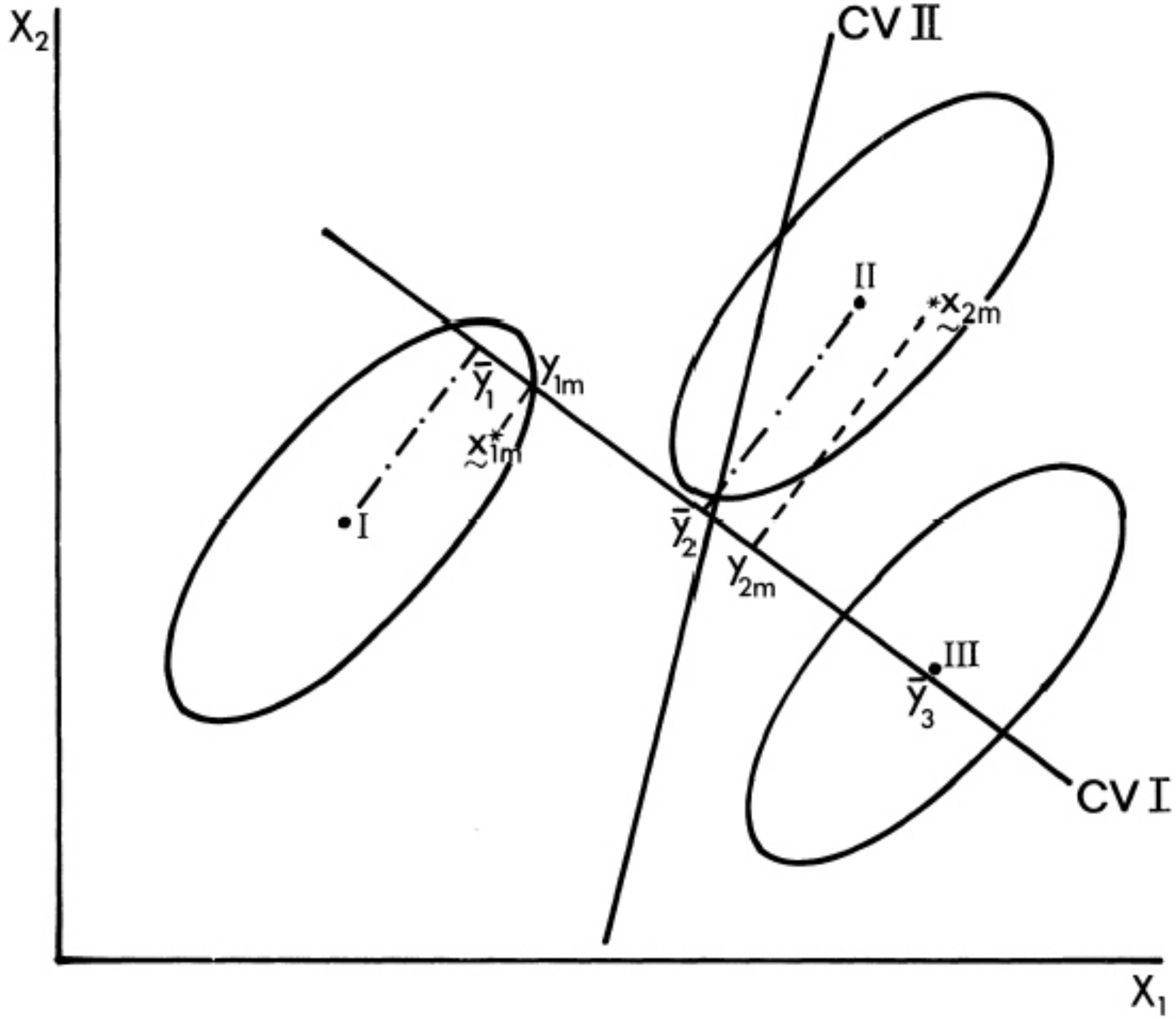


FIG. 2.—Representation of the canonical vectors for three groups and two variables. The group means (I, II and III) and 95% concentration ellipses are shown. The vectors CVI and CVII are the two canonical vectors. In the text, CVI = **e**. The points y_{1m} and y_{2m} represent the canonical variate scores corresponding to the first canonical vector for the observations $\mathbf{x}_{1m}$ and $\mathbf{x}_{2m}$.

CVA Solution

Maximizing F leads to the following:

$$(\boldsymbol{B} - l\boldsymbol{W})\boldsymbol{a} = 0$$

- l is an eigenvalue of $\boldsymbol{W}^{-1}\boldsymbol{B}$
- $\boldsymbol{a}$ is an eigenvector of $\boldsymbol{W}^{-1}\boldsymbol{B}$

There will be $s = \min(p, g - 1)$ non-zero eigenvalues.

Organize the eigenvectors, $\boldsymbol{a}_i$, as columns of a $p \times s$ matrix $\boldsymbol{A}$.

- The ***canonical variates*** are given by $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{A}$
- The mean of the i-th group in the canonical variates space is given by $\bar{\boldsymbol{y}}_i = \bar{\boldsymbol{x}}_i\boldsymbol{A}$, where $\bar{\boldsymbol{x}}_i$ is the mean row-vector for group i.

CVA as a two-stage rotation I

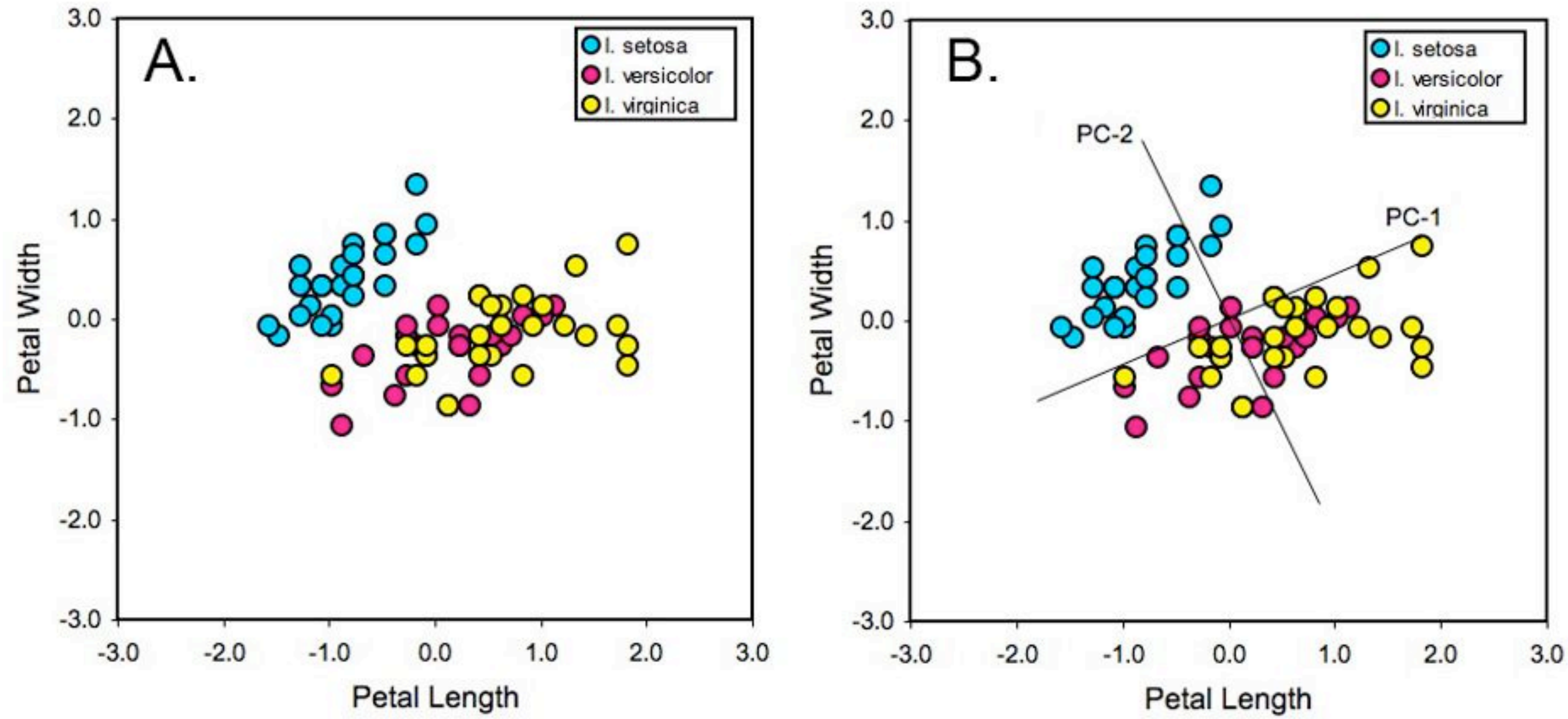


Figure 2. Stage 1 CVA implicit rotation. A. Scatterplot of first two *Iris* variables for example dataset. B. Orientation of the two pooled-sample principal components of the within-groups SSQCP matrix (*W*).

From MacLeod 2010, PalaeoMath newsletter

CVA as a two-stage rotation II

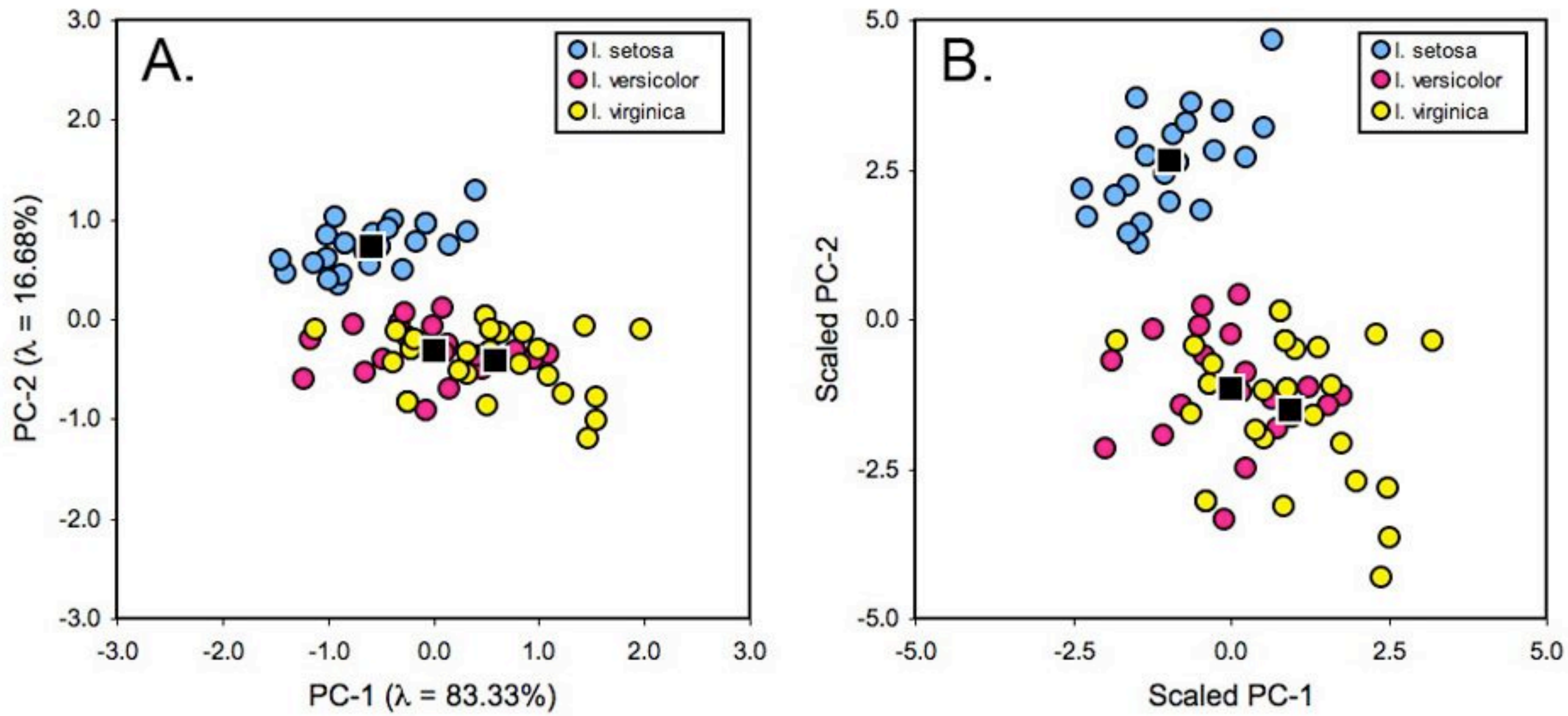


Figure 3. Intermediate scaling operation of a CVA. A. Scatterplot of *Iris* PC scores for the Stage 1 rotation (see Fig. 2). B. Result of scaling the two within-groups principal components by the square roots of their associated eigenvalues. Note difference in separation of the group centroids (black squares) after scaling.

From MacLeod 2010, PalaeoMath newsletter

CVA as a two-stage rotation III

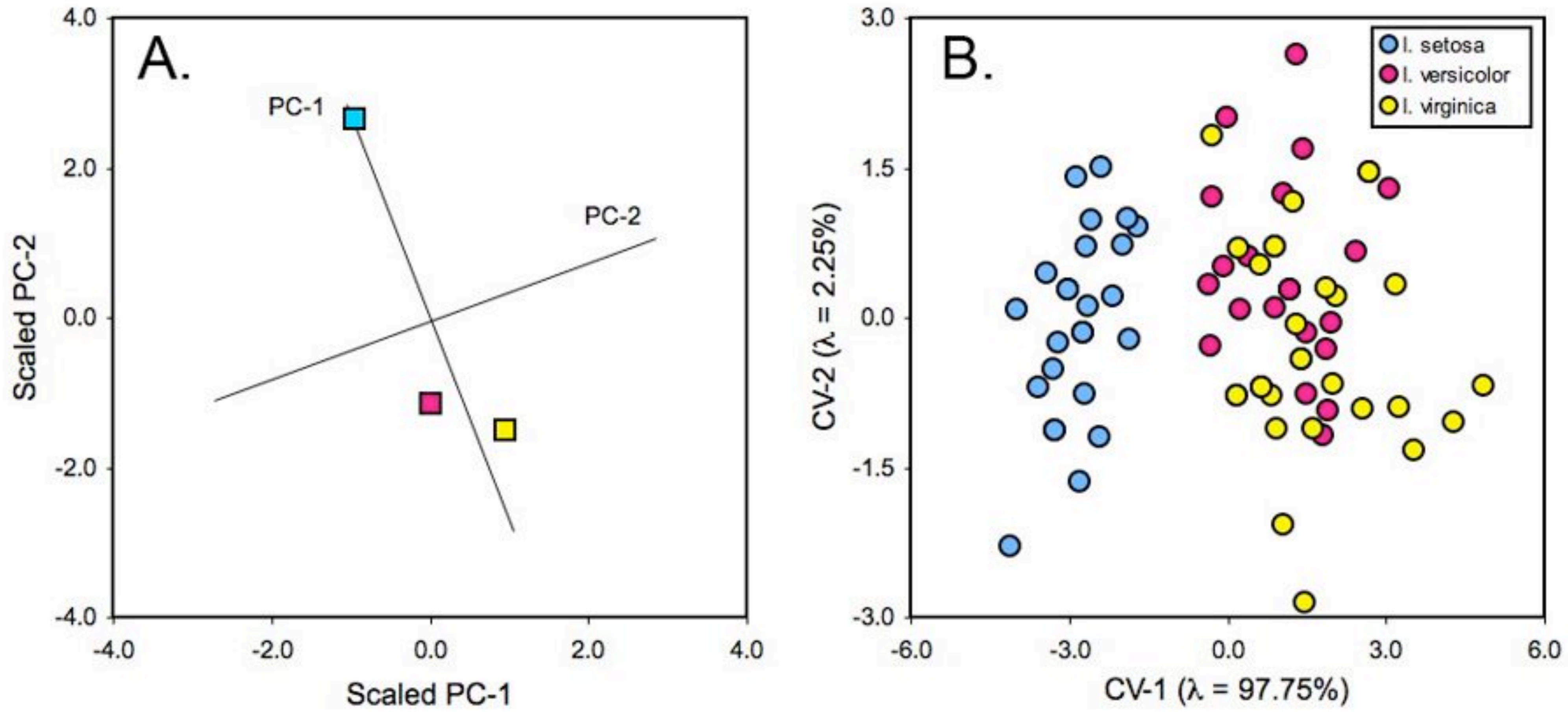


Figure 4. Stage 2 CVA implicit rotation. A. *Iris* group centroids plotted in the within-groups orthogonal-orthonormal space (see Fig. 3B) with between groups PC (= CVA) axes. B. Reduced *Iris* dataset plotted in the space defined by the CVA axes.

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CVA as a two-stage rotation IV

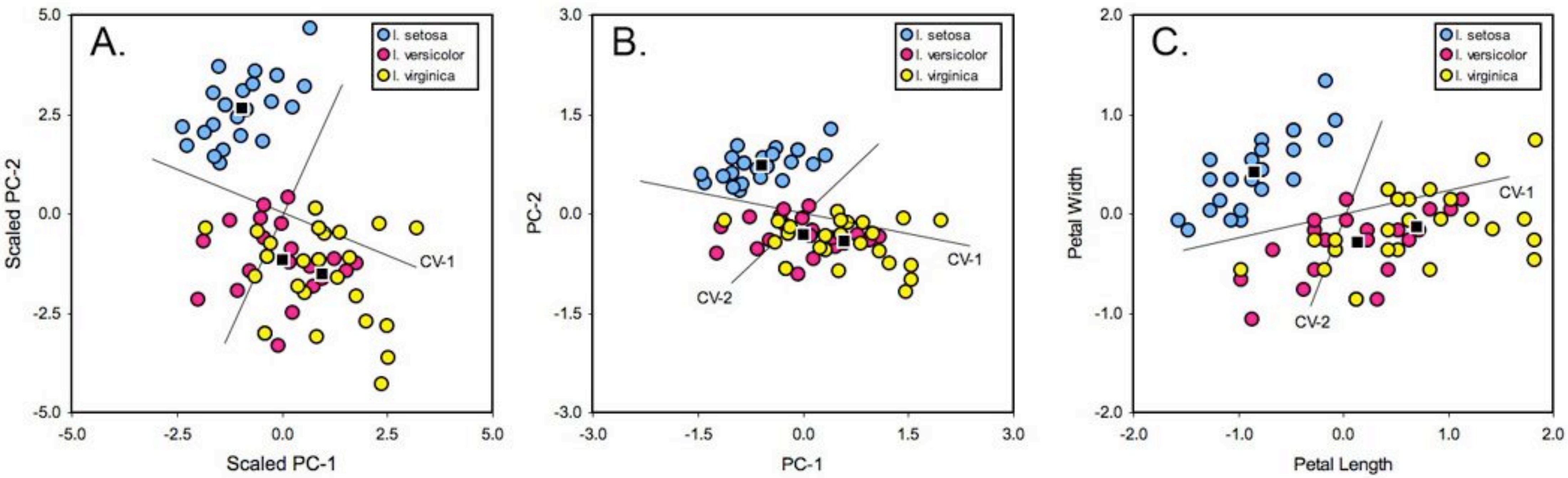

Figure 5. Back-calculation of final CVA axis orientation through the intermediate stages of the canonical rotations and scalings. A. Orientation of final CVA axes in the space of the scaled within-groups principal components (compare to Fig. 3A). B. Orientation of final CVA axes in the space of the raw within-groups principal components (compare to Fig. 3B). C. Orientation of final CVA axes in the space of the original variables (compare to Fig. 2).

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Similarities and Differences between CVA and PCA

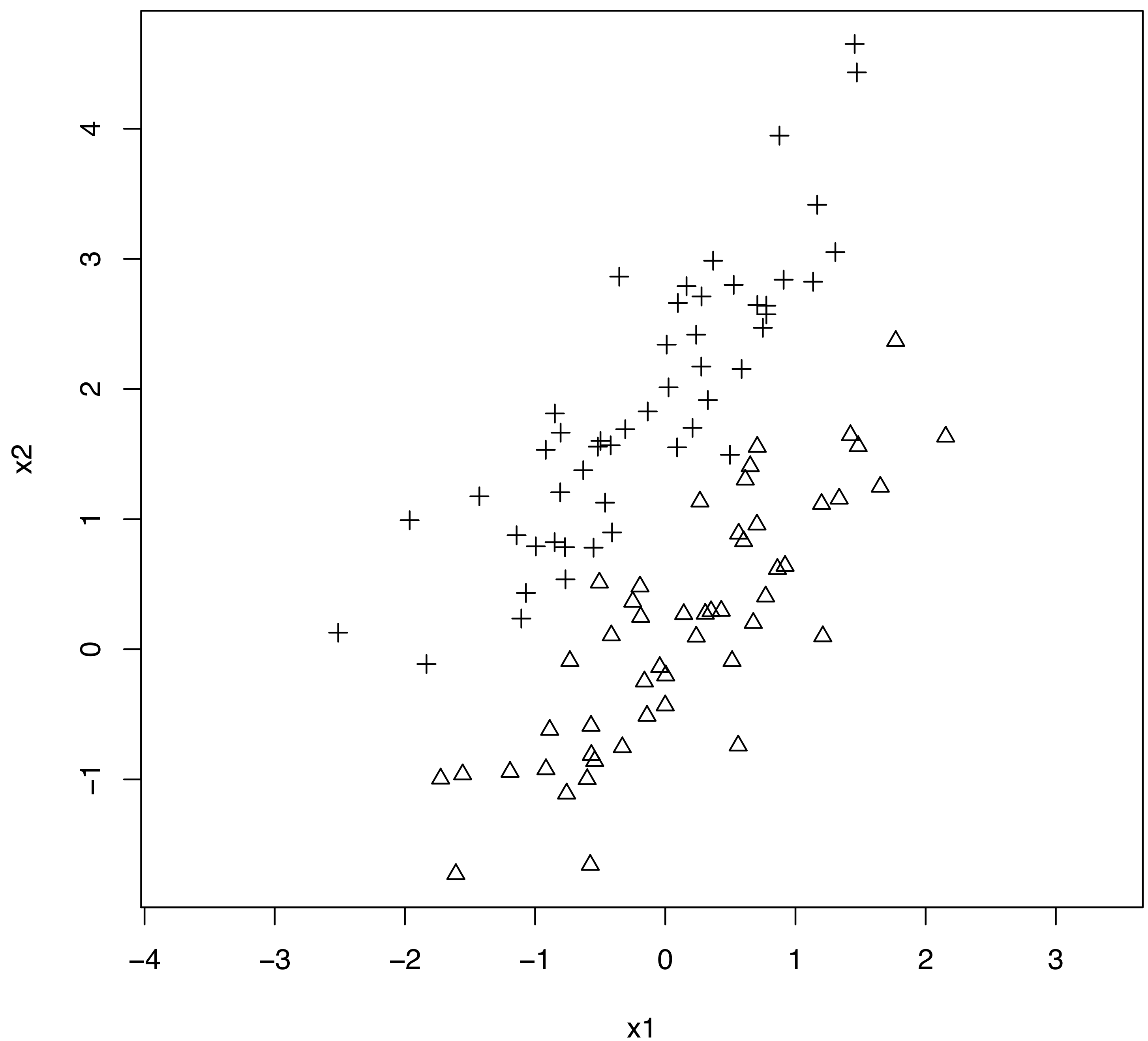
PCA:

- Uncorrelated over the whole sample
- orthogonal transformation from the original variates, $\boldsymbol{x}$, to the new variates $\boldsymbol{y}$. PC axes at right angles to each other in the space of the original variables.

CVA:

- Canonical variates are uncorrelated both *within* and *between* groups
- Canonical variates have equal variance *within* groups, but in decreasing order *between* groups
- non-orthogonal transformation, CV axes *not* at right angle to each other in the original frame of reference.

PCA vs CVA: A Motivating Example



What is the direction of PC1? What is the direction of CVI?

Are any of the groups significantly different in the canonical variate space?

To test:

- $H_0 : \mu_1 = \mu_2 = \ldots = \mu_3$
- H_1: at least one μ_i differs from the rest

A couple of approaches:

- Compare the largest eigenvalue, l_1, of $\boldsymbol{W}^{-1}\boldsymbol{B}$ to critical values in a F-table. H_0 is rejected for large values (> 1).
- Likelihood approach:
  - Wilks' lambda, $\Lambda = |\boldsymbol{W}|/|\boldsymbol{B} + \boldsymbol{W}| = \prod_{i=1}^{p}(1 + l_i)^{-1}$
  - there is an approximation that has a χ^2 distribution.

Both boil down to a consideration of eigenvalues of $\boldsymbol{W}^{-1}\boldsymbol{B}$.

Which groups are different? Where does an unassigned observation belong?

Within groups the canonical variates are:

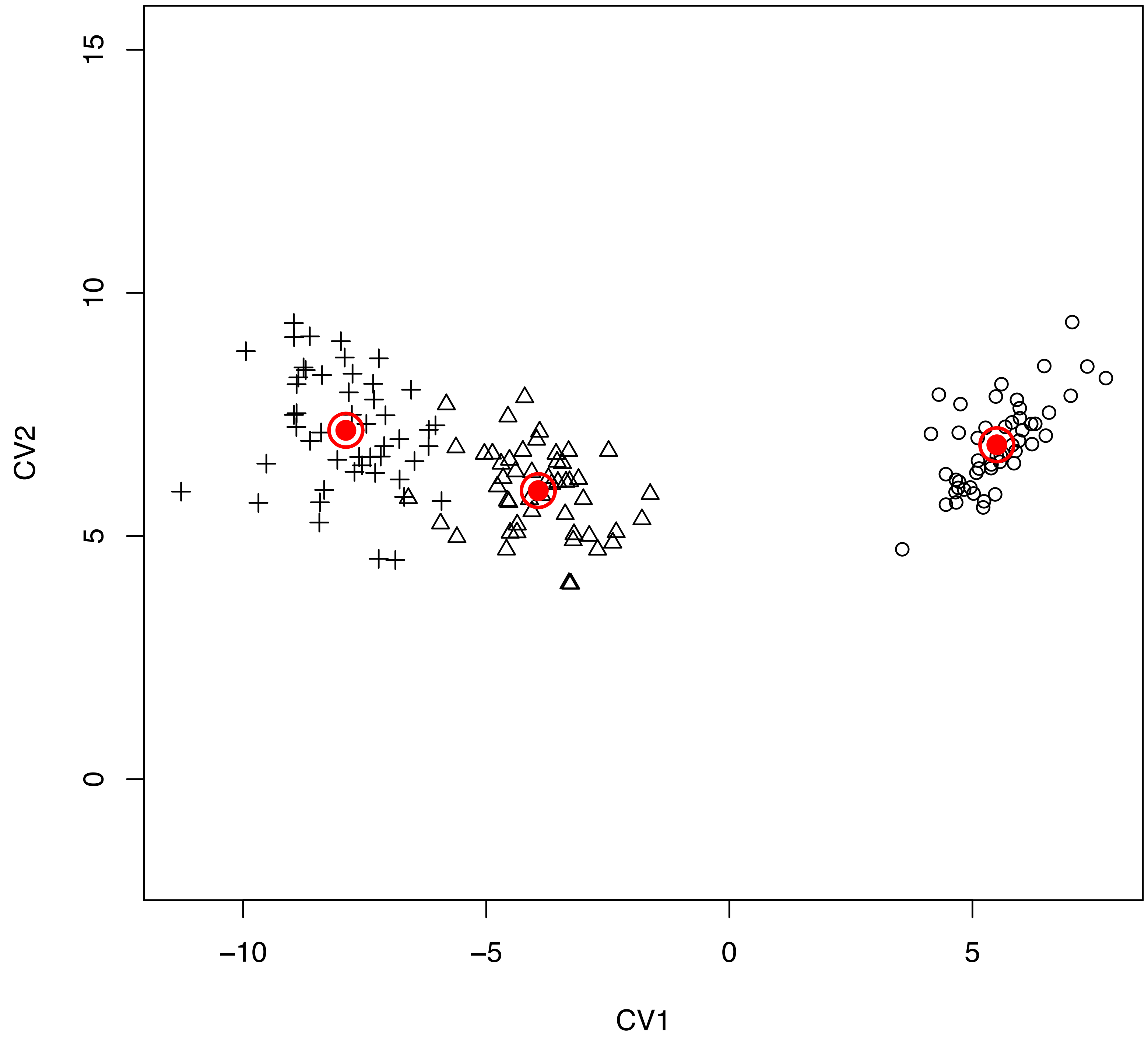
- uncorrelated
- have unit variance

If we assume multivariate normality of the data then we can exploit this to draw confidence intervals around the group means in the canonical variate space.

A 100(1-α) percent confidence region for the true mean $\boldsymbol{\nu}_i$ is given by:

- hypersphere centered at $\bar{\boldsymbol{y}}_i$
- with radius $(\chi^2_{\alpha,r}/n_i)^{1/2}$ where r is the number of canonical variate dimensions considered

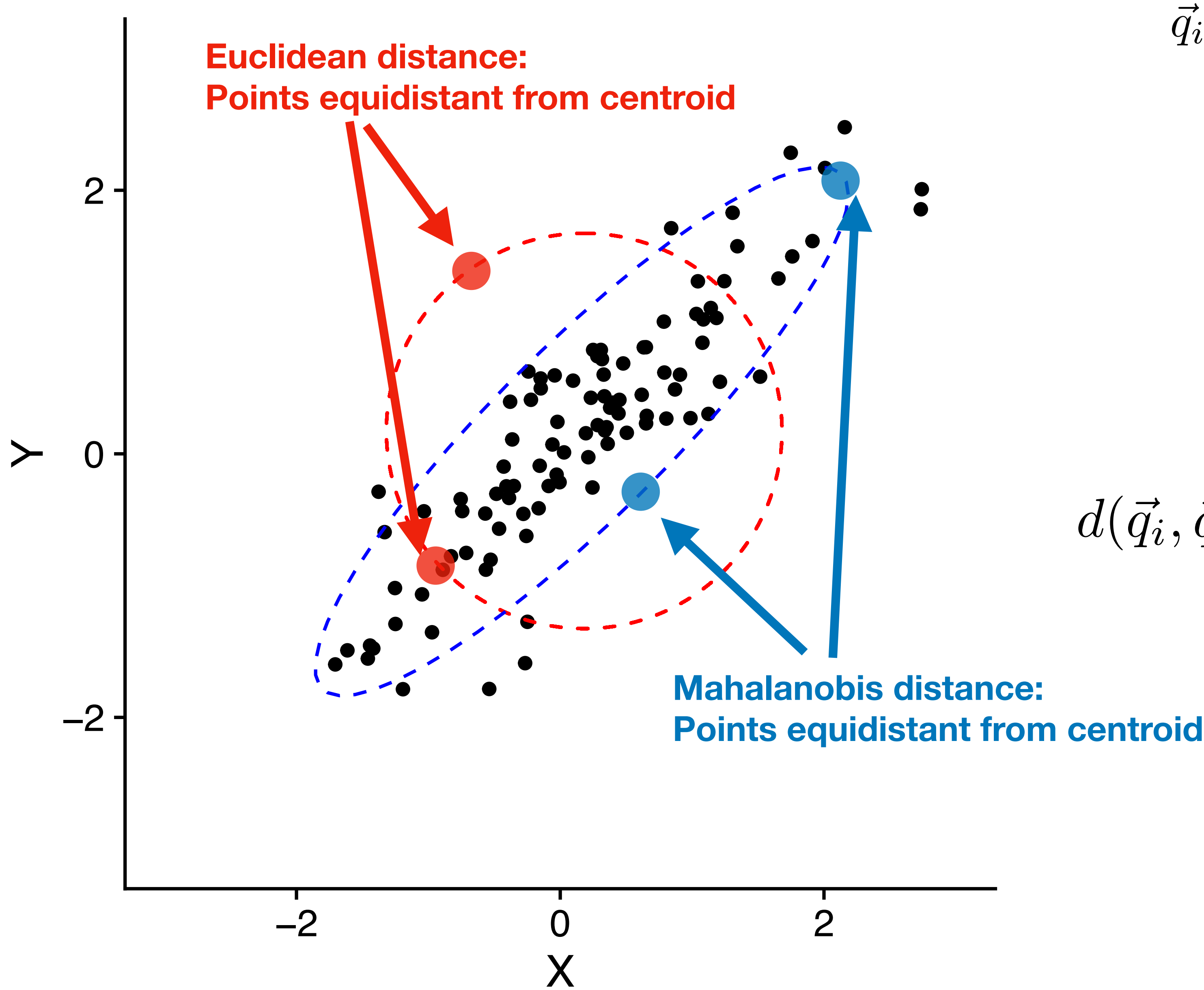
Illustration of group means and tolerance regions



Mahalanobis distance

Mahalanobis distance takes into account the covariance structure of the data.

- Deviations in the directions of greatest variance are "downweighted"



$\vec{q_i}, \vec{q_j}$: points i and j

$\mathbf{S}$: covariance matrix

$$\vec{q_i} = (\mathbf{X}_{i,1}, \mathbf{X}_{i,2}, \ldots, \mathbf{X}_{i,p})$$
$$\vec{q_j} = (\mathbf{X}_{j,1}, \mathbf{X}_{j,2}, \ldots, \mathbf{X}_{j,p})$$

$$d(\vec{q_i}, \vec{q_j}) = \sqrt{(\vec{q_i} - \vec{q_j})^T S^{-1} (\vec{q_i} - \vec{q_j})}$$