# Algebra of Principal Component Analysis

Data: $\mathbf{Y} = \begin{bmatrix} 2 & 1 \\ 3 & 4 \\ 5 & 0 \\ 7 & 6 \\ 9 & 2 \end{bmatrix}$ Centre each column on its mean: $\mathbf{Y}_c = [y - \bar{y}] = \begin{bmatrix} -3.2 & -1.6 \\ -2.2 & 1.4 \\ -0.2 & -2.6 \\ 1.8 & 3.4 \\ 3.8 & -0.6 \end{bmatrix}$

Covariance matrix (2 variables): $\mathbf{S} = \frac{1}{n-1} \mathbf{Y}_c' \, \mathbf{Y}_c = \begin{bmatrix} 8.2 & 1.6 \\ 1.6 & 5.8 \end{bmatrix}$

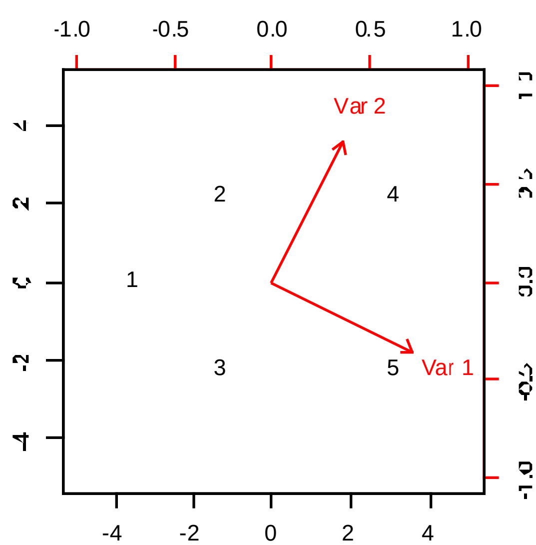
Equation for eigenvalues and eigenvectors of $\mathbf{S}$ : $(\mathbf{S} - \lambda_k \mathbf{I}) \, \mathbf{u}_k = \mathbf{0}$

Eigenvalues: $\lambda_1 = 9$, $\lambda_2 = 5$ Matrix of eigenvalues: $\Lambda = \begin{bmatrix} 9 & 0 \\ 0 & 5 \end{bmatrix}$

Matrix of eigenvectors: $\mathbf{U} = \begin{bmatrix} 0.8944 & -0.4472 \\ 0.4472 & 0.8944 \end{bmatrix}$

Positions of the 5 objects in ordination space: $\mathbf{F} = [y - \bar{y}] \, \mathbf{U}$

$$\mathbf{F} = \begin{bmatrix} -3.2 & -1.6 \\ -2.2 & 1.4 \\ -0.2 & -2.6 \\ 1.8 & 3.4 \\ 3.8 & -0.6 \end{bmatrix} \begin{bmatrix} 0.8944 & -0.4472 \\ 0.4472 & 0.8944 \end{bmatrix} = \begin{bmatrix} -3.578 & 0 \\ -1.342 & 2.236 \\ -1.342 & -2.236 \\ 3.130 & 2.236 \\ 3.130 & -2.236 \end{bmatrix}$$



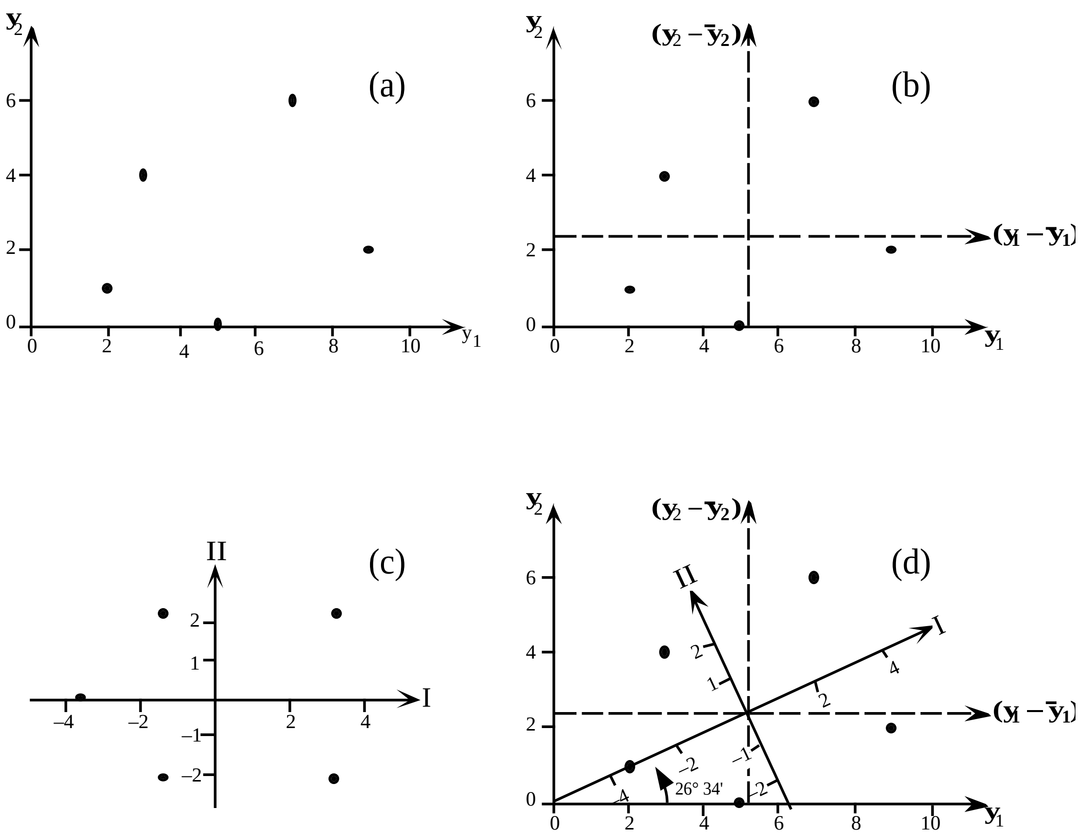



**Figure 9.2** Numerical example of principal component analysis. (a) Five objects are plotted with respect to descriptors $\mathbf{y}_1$ and $\mathbf{y}_2$. (b) After centring the data, the objects are now plotted with respect to $(\mathbf{y}_1 - \bar{\mathbf{y}}_1)$ and $(\mathbf{y}_2 - \bar{\mathbf{y}}_2)$, represented by dashed axes. (c) The objects are plotted with reference to principal axes I and II, which are centred with respect to the scatter of points. (d) The two systems of axes (b and c) can be superimposed after a rotation of 26°34'.

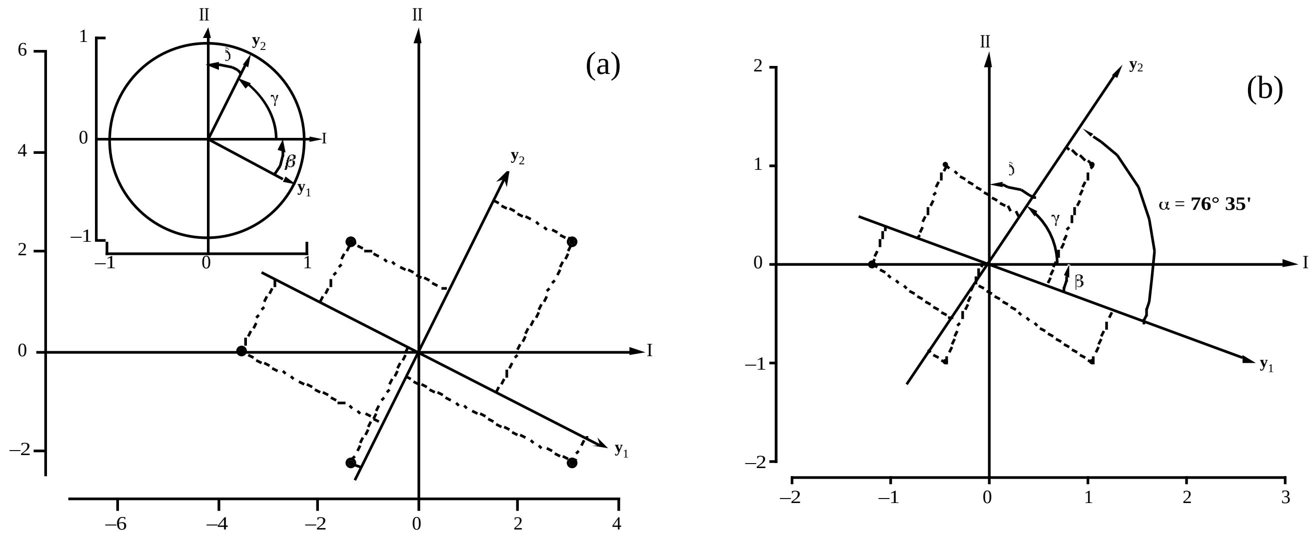



Fig. 9.3 Numerical example from Fig. 9.2. Distance and correlation biplots are discussed in Subsection 9.1.4. **(a) Distance biplot.** The eigenvectors are scaled to lengths 1. Inset: descriptors (matrix **U**). Main graph: descriptors (matrix **U**; arrows) and objects (matrix **F**; dots). The interpretation of the object-descriptor relationships is not based on their proximity, but on orthogonal projections (dashed lines) of the objects on the descriptor-axes or their extensions. **(b) Correlation biplot.** Descriptors (matrix $\mathbf{U}\Lambda^{1/2}$; arrows) with a covariance angle of 76°35'. Objects (matrix **G**; dots). Projecting the objects orthogonally on a descriptor (dashed lines) reconstructs the values of the objects along that descriptors, to within a multiplicative constant.

## Use the following matrices to draw biplots

*Distance biplot* (scaling 1): objects = **F**, variables = **U**

*Correlation biplot* (scaling 2): objects = $\mathbf{G} = \mathbf{F}\boldsymbol{\Lambda}^{-1/2}$, variables = $\mathbf{U}_{sc2} = \mathbf{U}\boldsymbol{\Lambda}^{1/2}$

These two projections respect the biplot rule, that the product of the two projected matrices reconstruct the data **Y**:

Distance biplot: $\mathbf{FU' = Y}$ Correlation biplot: $\mathbf{G(U\boldsymbol{\Lambda}^{1/2})' = Y}$

# PCA example, three variables

# Create the data matrix
```
data.3 <- matrix(c(2,3,5,7,9,10,1,4,0,6,2,5,0,1,-1,-1,1,0),6,3)
data.3
     [,1] [,2] [,3]
[1,]    2    1    0
[2,]    3    4    1
[3,]    5    0   -1
[4,]    7    6   -1
[5,]    9    2    1
[6,]   10    5    0
```

# Centre the variables
```
data.cent <- scale(data.3, center=TRUE, scale=FALSE)
data.cent
     [,1] [,2] [,3]
[1,]   -4   -2    0
[2,]   -3    1    1
[3,]   -1   -3   -1
[4,]    1    3   -1
[5,]    3   -1    1
[6,]    4    2    0
```

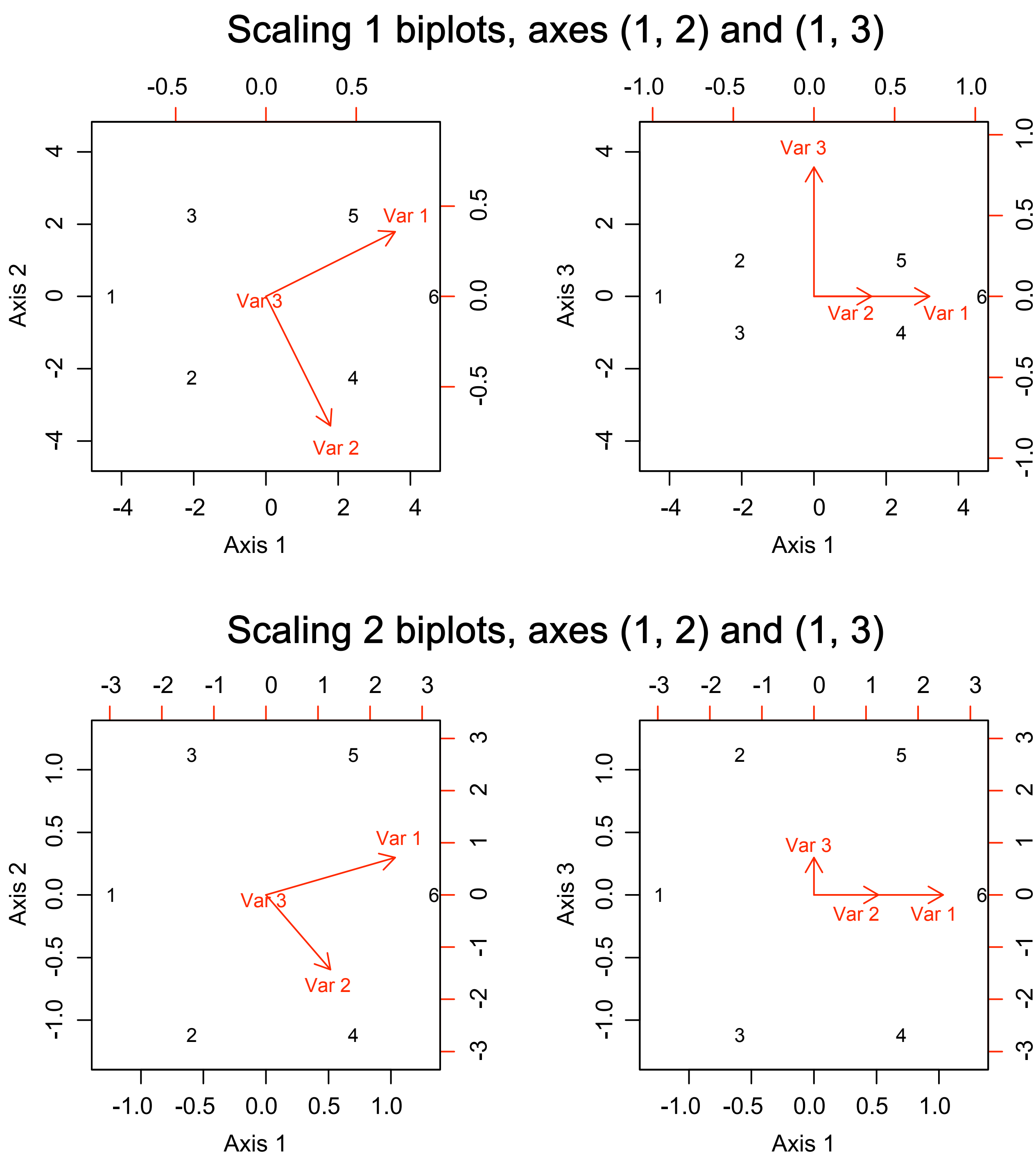
# Compute the covariance matrix
```
data.cov <- cov(data.cent) # or, because the data are not standardized:  cov(data.3)
     [,1] [,2] [,3]
[1,] 10.4  3.2  0.0
[2,]  3.2  5.6  0.0
[3,]  0.0  0.0  0.8
```

# Compute the eigenvalues and eigenvectors
```
data.eig <- eigen(data.cov)
data.eig

$values
[1] 12.0  4.0  0.8

$vectors
          [,1]       [,2] [,3]
[1,] 0.8944272  0.4472136    0
[2,] 0.4472136 -0.8944272    0
[3,] 0.0000000  0.0000000    1
```

# Compute the output matrices for scaling 1
```
U <- data.eig$vectors
F.mat <- data.cent %*% U
```

# Compute the output matrices for scaling 2
```
U.sc2 <- U %*% diag(data.eig$values^(0.5))
G.mat <- F.mat %*% diag(data.eig$values^(-0.5))
```

```
# Draw the scaling 1 and 2 biplots
par(mfrow=c(2,2))
biplot(F.mat[,c(1,2)], U[,c(1,2)])
biplot(F.mat[,c(1,3)], U[,c(1,3)])
biplot(G.mat[,c(1,2)], U.sc2[,c(1,2)])
biplot(G.mat[,c(1,3)], U.sc2[,c(1,3)])
```



**Data transformations**

**<u>Transform physical variables (*Ecology*) or characters (*Taxonomy*)</u>**

- Univariate distributions are not symmetrical

  ⇒ Apply skewness-reduction transformation

- Variables are not in the same physical units

  ⇒ Apply standardization $z_i = \frac{y_i - \bar{y}}{s_y}$ or ranging $y'_i = \frac{y_i - y_{min}}{y_{max} - y_{min}}$

**<u>Transform community composition data (*Ecology*)</u>**

**(species presence-absence or abundance)**

- Reduce asymmetry of distributions

  ⇒ Apply log($y$ + $c$) transformation

- Make community composition data suitable for Euclidean-based ordination methods (PCA, RDA)

  ⇒ Use the chord, chi-square, profile, or Hellinger transformations (Legendre & Gallagher 2001)

## Some uses of principal component analysis (PCA)

- Two-dimensional ordination of the *objects*:

  - Sampling sites in ecology

  - Individuals or taxa in taxonomy

  A 2-dimensional ordination diagram is an interesting graphical support for representing other properties of multivariate data, e.g., clusters.

- Detect outliers or erroneous data in data tables

- Find groups of *variables* that behave in the same way:

  - Species in ecology

  - Morphological/behavioural/molecular variables in taxonomy

- Simplify (collinear) data; remove noise

- Remove an identifiable component of variation

  e.g., size factor in log-transformed morphological data

# Algebra of Correspondence Analysis

$$\text{Frequency data table } \mathbf{Y} = \left[ f_{ij} \right] = \begin{bmatrix} 10 & 10 & 20 \\ 10 & 15 & 10 \\ 15 & 5 & 5 \end{bmatrix} \quad \overset{\left[ f_{i+} \right]}{\begin{bmatrix} 40 \\ 35 \\ 25 \end{bmatrix}}$$

$$\left[ f_{+j} \right] = \begin{bmatrix} 35 & 30 & 35 \end{bmatrix} \quad 100 = f_{++}$$

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

$$\text{Matrix } \bar{\mathbf{Q}} = [\bar{q}_{ij}] = \left[ \frac{p_{ij} - p_{i+}p_{+j}}{\sqrt{p_{i+}p_{+j}}} \right] = \frac{(O_{ij} - E_{ij}) / \sqrt{E_{ij}}}{\sqrt{f_{++}}}$$

$$\text{Matrix } \bar{\mathbf{Q}} = \begin{bmatrix} -0.10690 & -0.05774 & 0.16036 \\ -0.06429 & 0.13887 & -0.06429 \\ 0.21129 & -0.09129 & -0.12667 \end{bmatrix}$$

Cross-product matrix:

$$\bar{\mathbf{Q}}'\bar{\mathbf{Q}} = \begin{bmatrix} 0.06020 & -0.02204 & -0.03980 \\ -0.02204 & 0.03095 & -0.00661 \\ -0.03980 & -0.00661 & 0.04592 \end{bmatrix}$$

Compute eigenvalues and eigenvectors of $\bar{\mathbf{Q}}'\bar{\mathbf{Q}}$ : $(\bar{\mathbf{Q}}'\bar{\mathbf{Q}} - \lambda_k \mathbf{I})\, \mathbf{u}_k = \mathbf{0}$

Eigenvalues: $\lambda_1 = 0.096$, $\lambda_2 = 0.041$ Matrix of eigenvalues: $\Lambda = \begin{bmatrix} 0.096 & 0 \\ 0 & 0.041 \end{bmatrix}$

*There are never more than k = min(r – 1, c – 1) eigenvalues > 0 in CA*

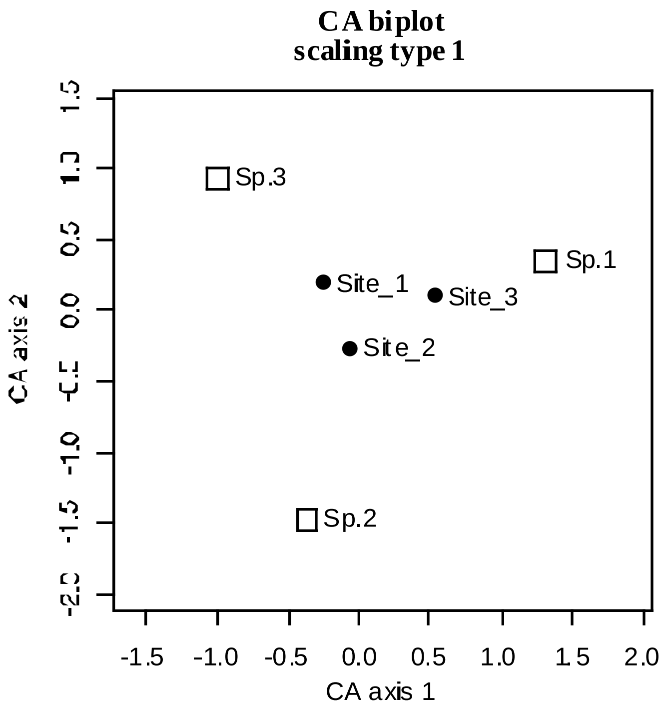
Matrix of eigenvectors of $\bar{\mathbf{Q}}'\bar{\mathbf{Q}}_{(c \times c)}$ :

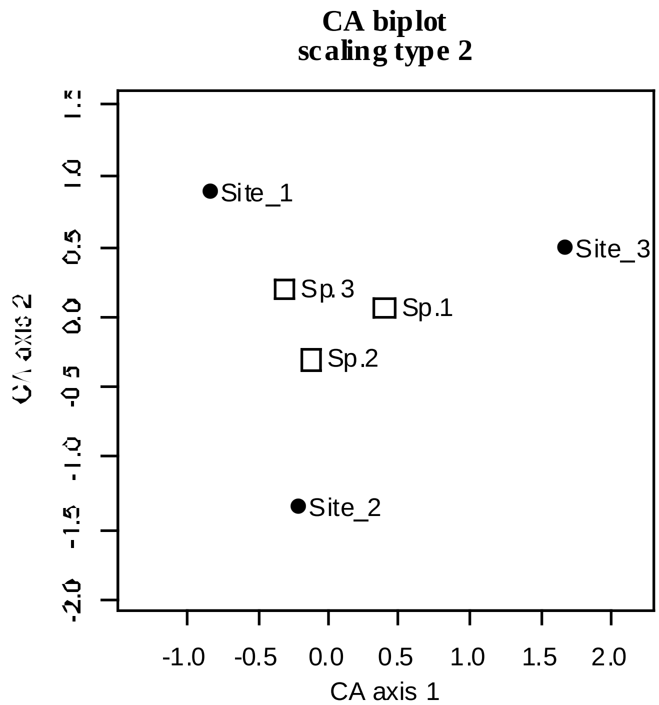
$$\mathbf{U}_{(c \times k)} = \begin{bmatrix} 0.78016 & 0.20336 \\ -0.20383 & -0.81145 \\ -0.59144 & 0.54790 \end{bmatrix}$$

Matrix of eigenvectors of $\bar{\mathbf{Q}}\bar{\mathbf{Q}}'_{(r \times r)}$ :

$$\hat{\mathbf{U}}_{(r \times k)} = \bar{\mathbf{Q}}\mathbf{U}\boldsymbol{\Lambda}^{-1/2} = \begin{bmatrix} -0.53693 & 0.55831 \\ -0.13043 & -0.79561 \\ 0.83349 & 0.23516 \end{bmatrix}$$

Compute matrices **F** and **V** for scaling 1 biplot, and $\hat{\mathbf{V}}$ and $\hat{\mathbf{F}}$ for scaling 2 biplot:




## Calculation details

Compute matrices **V**, $\hat{\mathbf{V}}$, **F**, and $\hat{\mathbf{F}}$ used in the ordination biplots:

$$\mathbf{V}_{(c\times k)} = \mathbf{D}(p_{+j})^{-1/2}\,\mathbf{U} \qquad \text{where } p_{+j} = f_{+j}/f_{++}$$

$$\hat{\mathbf{V}}_{(r\times k)} = \mathbf{D}(p_{i+})^{-1/2}\,\hat{\mathbf{U}} \qquad \text{where } p_{i+} = f_{i+}/f_{++}$$

$$\mathbf{F}_{(r\times k)} = \hat{\mathbf{V}}\boldsymbol{\Lambda}^{1/2}$$

$$\hat{\mathbf{F}}_{(c\times k)} = \mathbf{V}\boldsymbol{\Lambda}^{1/2}$$

Biplot, scaling type 1: plot **F** for sites, **V** for species:

- This projection preserves the chi-square distance among the sites.
- The sites are at the centroids (barycentres) of the species.

Biplot, scaling type 2: plot $\hat{\mathbf{V}}$ for sites, $\hat{\mathbf{F}}$ for species:

- This projection preserves the chi-square distance among the species.
- The species are at the centroids (barycentres) of the sites.

# Principal coordinate analysis (PCoA)

Example: a Euclidean distance matrix computed from the data of the PCA example.

$$\mathbf{D} = \begin{bmatrix} 0.00000 & 3.16228 & 3.16228 & 7.07107 & 7.07107 \\ 3.16228 & 0.00000 & 4.47214 & 4.47214 & 6.32456 \\ 3.16228 & 4.47214 & 0.00000 & 6.32456 & 4.47214 \\ 7.07107 & 4.47214 & 6.32456 & 0.00000 & 4.47214 \\ 7.07107 & 6.32456 & 4.47214 & 4.47214 & 0.00000 \end{bmatrix}$$

Transform **D** to a new matrix $\mathbf{A} = [a_{hi}]$: $a_{hi} = -0.5D_{hi}^2$

Centre matrix **A** to produce matrix $\boldsymbol{\Delta}$ with sums of the rows and columns equal to 0:

$$\boldsymbol{\Delta} = [\delta_{hi}] = [a_{hi} - \bar{a}_h - \bar{a}_i + \bar{\bar{a}}]$$

$$\boldsymbol{\Delta} = \begin{bmatrix} 12.8 & 4.8 & 4.8 & -11.2 & -11.2 \\ 4.8 & 6.8 & -3.2 & 0.8 & -9.2 \\ 4.8 & -3.2 & 6.8 & -9.2 & 0.8 \\ -11.2 & 0.8 & -9.2 & 14.8 & 4.8 \\ -11.2 & -9.2 & 0.8 & 4.8 & 14.8 \end{bmatrix}$$

Compute the eigenvalues and eigenvectors of matrix $\boldsymbol{\Delta}$. Scale the eigenvectors to lengths equal to the square roots of their respective eigenvalues, $\sqrt{\mathbf{u}'_k \mathbf{u}_k} = \sqrt{\lambda_k}$.

| | | |
|---|---|---|
| Eigenvalues: | $\lambda_1 = 36$ | $\lambda_2 = 20$ |
| Objects | Eigenvectors | |
| $\mathbf{x}_1$ | –3.578 | 0.000 |
| $\mathbf{x}_1$ | –1.342 | –2.236 |
| $\mathbf{x}_1$ | –1.342 | 2.236 |
| $\mathbf{x}_1$ | 3.130 | –2.236 |
| $\mathbf{x}_1$ | 3.130 | 2.236 |
| Eigenvector length | $\sqrt{36} = 6.000$ | $\sqrt{20} = 4.472$ |
| PCoA eigenvalues / ($n$–1) | 9 | 5 |

Compare the PCoA eigenvalues and eigenvectors to the PCA eigenvalues and matrix **F**.

PCoA is used for ordination of **D** matrices produced by functions other than the Euclidean.