Correspondence analysis

Recapitulation PCA

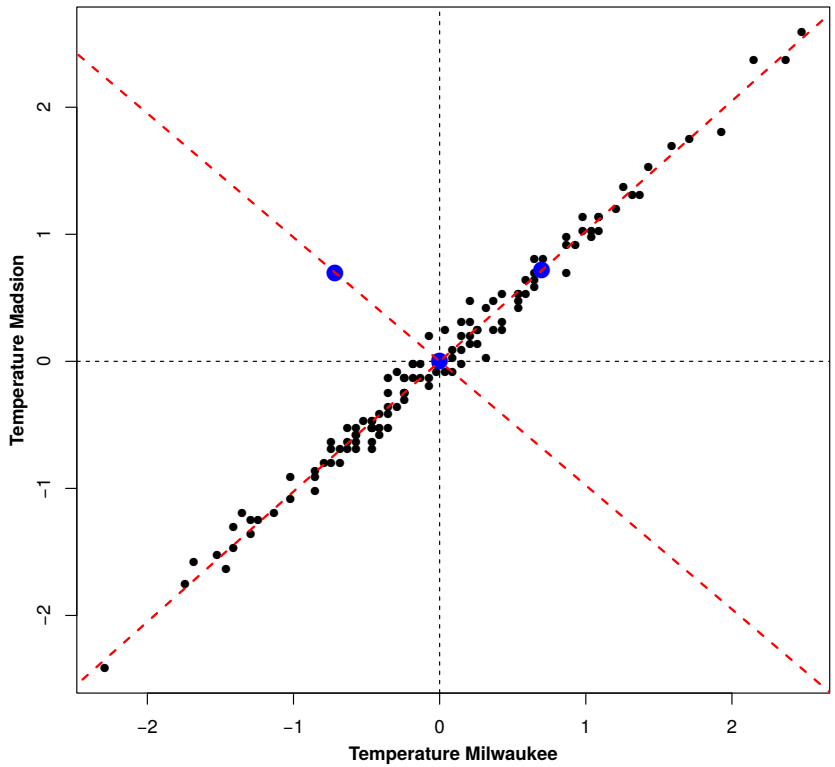
Recapitulation PCA

- Find most relevant patterns in a dataset
- Summarize a dataset in a simple two dimensional scatterplot
  - relation among variables
  - distance among samples

PCA: Geometric representation

New **coordinate system** so that:

Axes go in the direction of maximum elongation of dataset (data cloud)



Direction of new coordinates in old coordinate space: **Eigenvector** (PC loadings, species scores)

PCA: Mathematics

...	Variable 1	Variable 2	...	Variable i
time 1	$X1_1$	$X2_1$	...	Xi_1
time 2	$X1_2$	$X2_2$	...	Xi_2
...	...	...	...	...
time j	$X1_j$	$X2_j$	...	Xi_j

Correlation or covariance matrix

...	Variable 1	Variable 2	...	Variable i
Variable 1	1	r_{12}	...	r_{1i}
Variable 2	r_{12}	1	...	r_{2i}
...	...	...	...	...
Variable i	r_{1j}	r_{2i}	...	1

PCA: Mathematics

Eigenvalue decomposition of correlation or covariance matrix

...	Variable 1	Variable 2	...	Variable i
Variable 1	1	r_{12}	...	r_{1i}
Variable 2	r_{12}	1	...	r_{2i}
...	...	...	...	...
Variable i	r_{1j}	r_{2i}	...	1

Eigenvectors: new coordinate system

...	ev1	ev2	...	ev i
species 1	ev_{11}	ev_{12}	...	ev_{1i}
species 2	ev_{21}	ev_{22}	...	ev_{2i}
...	...	...	...	...
species i	ev_{i1}	ev_{i2}	...	ev_{ii}

PCA: Geometric representation

Position in new coordinate system: **Principal component** (site scores)

...	Var1	Var2	...	Var i	...	PC1	PC2	...	PC i
time 1	$z1_1$	$z2_1$	...	zl_1	...	$pc1_1$	$pc2_1$	...	pcl_1
time 2	$z1_2$	$z2_2$	...	zl_2	...	$pc1_2$	$pc2_2$	...	pcl_2
...	...	...	...	...	...	...	...	...	...
time j	$z1_j$	$z2_j$	...	zl_j	...	$pc1_j$	$pc2_j$	...	pcl_j

Principal components: linear combination of initial variables and eigenvectors

$$pc1_1 = ev1_1 z_{11} + ev1_2 z_{12} + ...ev1_i z_{1i}$$
$$pc1_2 = ev1_1 z_{21} + ev1_2 z_{22} + ...ev1_i z_{2i}$$

PCA as extension of linear regression

Gradient analysis

Some important physical gradient (e.g. altitude) determines occurrences of biological species

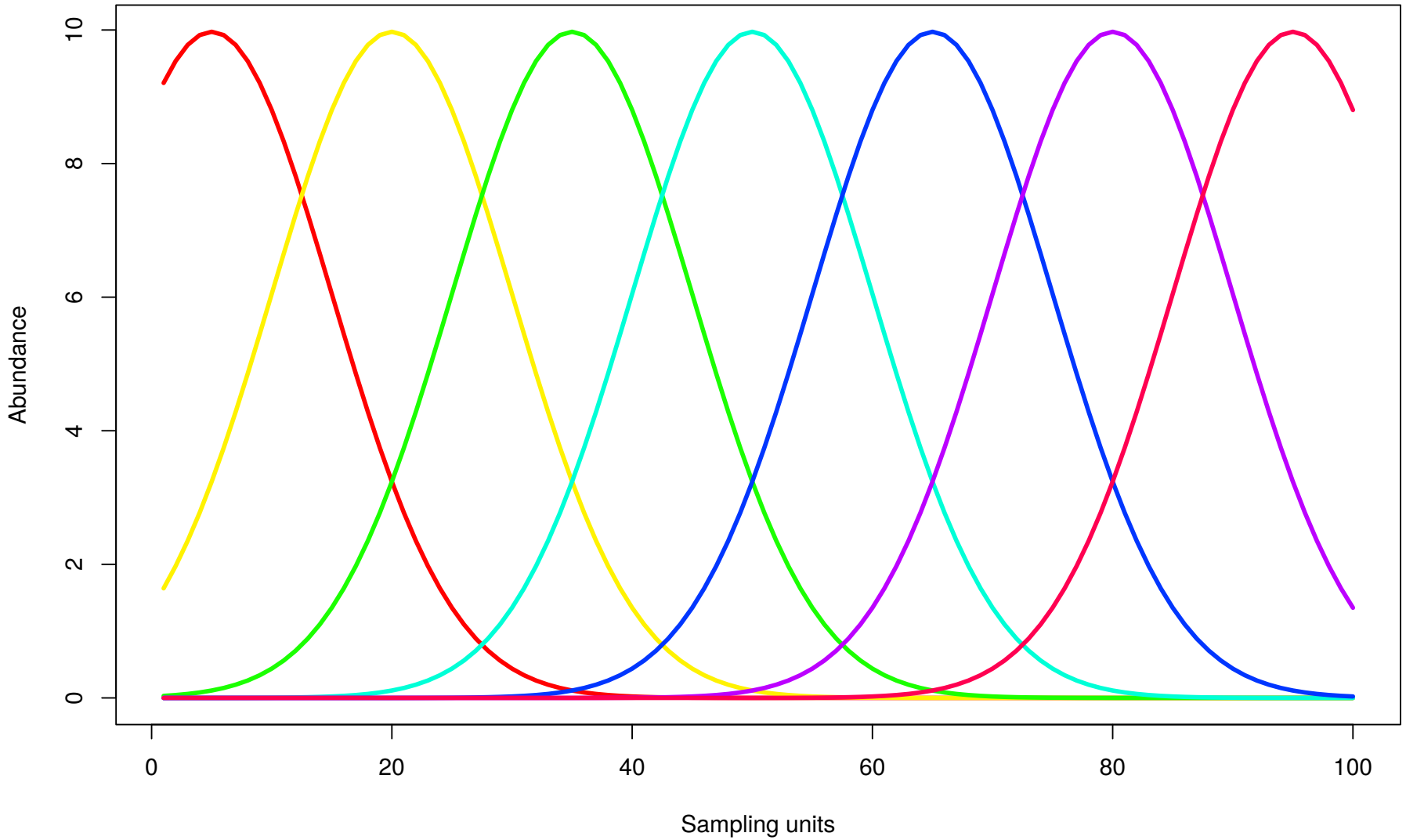
PCA:

- assume linear response of species to gradient (i.e. value of a species is low at one end of the gradient and high at the other end of the gradient)

Do biological species respond linearly to an environmental or latent gradient?

Plant species: Unimodal response

Niche theory: plants have a unimodal response



Gradient analysis:

There is some latent (unobserved) variable underlying that gradient

...	species 1	species 2	...	species i	Σ
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}
...	...	...	...	...	...
site j	p_{j1}	p_{j2}	...	p_{ji}	p_{j+}
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}

The method of gradient analysis is to take some well-marked gradient and to assign scores to the species according to their altitudinal preferences. Sites are then ordinated by taking averages of the scores of the species which occur in them. Hill, 1973

Gradient analysis: Reciprocal averaging

...	species 1	species 2	...	species i	Σ
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}
...	...	...	...	...	...
site j	p_{j1}	p_{j2}	...	p_{ji}	p_{j+}
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}

Site scores: x

Species scores: y

Start with random site scores (assign a random env. variable)

$$scores_{species} = \frac{p_{11}}{p_{+1}} score_{site,1} + \frac{p_{21}}{p_{+1}} score_{site,2} + ... + \frac{p_{j1}}{p_{+1}} score_{site,j}$$

$$y_1 = \frac{p_{11}}{p_{+1}} x_1 + \frac{p_{21}}{p_{+1}} x_2 + ... + \frac{p_{j1}}{p_{+1}} x_j$$

Simpler notation

$$y_1 = w_{11}x_1 + w_{21}x_2 + ... + w_{j1}x_j$$

...	species 1	species 2	species i
site_1	$w_{11} = \frac{p_{11}}{p_{+1}}$	$w_{12} = \frac{p_{12}}{p_{+2}}$	$w_{1i} = \frac{p_{1i}}{p_{+i}}$
site_2	$w_{21} = \frac{p_{21}}{p_{+2}}$	$w_{22} = \frac{p_{22}}{p_{+2}}$	$w_{2i} = \frac{p_{2i}}{p_{+i}}$
site_j	$w_{j2} = \frac{p_{j1}}{p_{+j}}$	$w_{j2} = \frac{p_{j2}}{p_{+2}}$	$w_{2i} = \frac{p_{ji}}{p_{+i}}$

$$scores_{species} = y_i = \sum_{j=1}^{j=m} w_{ji}x_j = weighted - average$$

$$\overline{z} = \sum_{j=1}^{j=m} \frac{1}{m}a = \frac{1}{m}\sum_{j=1}^{j=m} a = normal - average$$

New site scores

...	species 1	species 2	...	species i	Σ
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}
...	...	...	...	...	...
site j	p_{j1}	p_{j2}	...	p_{ji}	p_{j+}
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}

$$scores_{site} = \frac{p_{11}}{p_{1+}} scores_{spec,1} + \frac{p_{12}}{p_{1+}} scores_{spec,2} + ... + \frac{p_{1i}}{p_{1+}} scores_{spec,i}$$

$$x_1 = \frac{p_{11}}{p_{1+}} y_1 + \frac{p_{12}}{p_{1+}} y_2 + ... + \frac{p_{1i}}{p_{1+}} y_i$$

Simpler notation

$$x_1 = v_{11}y_1 + v_{21}y_2 + ... + v_{j1}y_j$$

...	species 1	species 2	species i
site 1	$v_{11} = \frac{p_{11}}{p_{1+}}$	$v_{12} = \frac{p_{12}}{p_{1+}}$	$v_{1i} = \frac{p_{1i}}{p_{1+}}$
site 2	$v_{21} = \frac{p_{21}}{p_{2+}}$	$v_{22} = \frac{p_{22}}{p_{2+}}$	$v_{2i} = \frac{p_{2i}}{p_{2+}}$
site j	$v_{j2} = \frac{p_{j1}}{p_{j+}}$	$v_{j2} = \frac{p_{j2}}{p_{j+}}$	$v_{2i} = \frac{p_{ji}}{p_{j+}}$

$scores_{site,j} = x_j = \sum_{i=1}^{i=n} v_{ij}y_i$

$\overline{z} = \sum_{j=1}^{j=m} \frac{1}{m}a = \frac{1}{m}\sum_{j=1}^{j=m} a = normal - average$

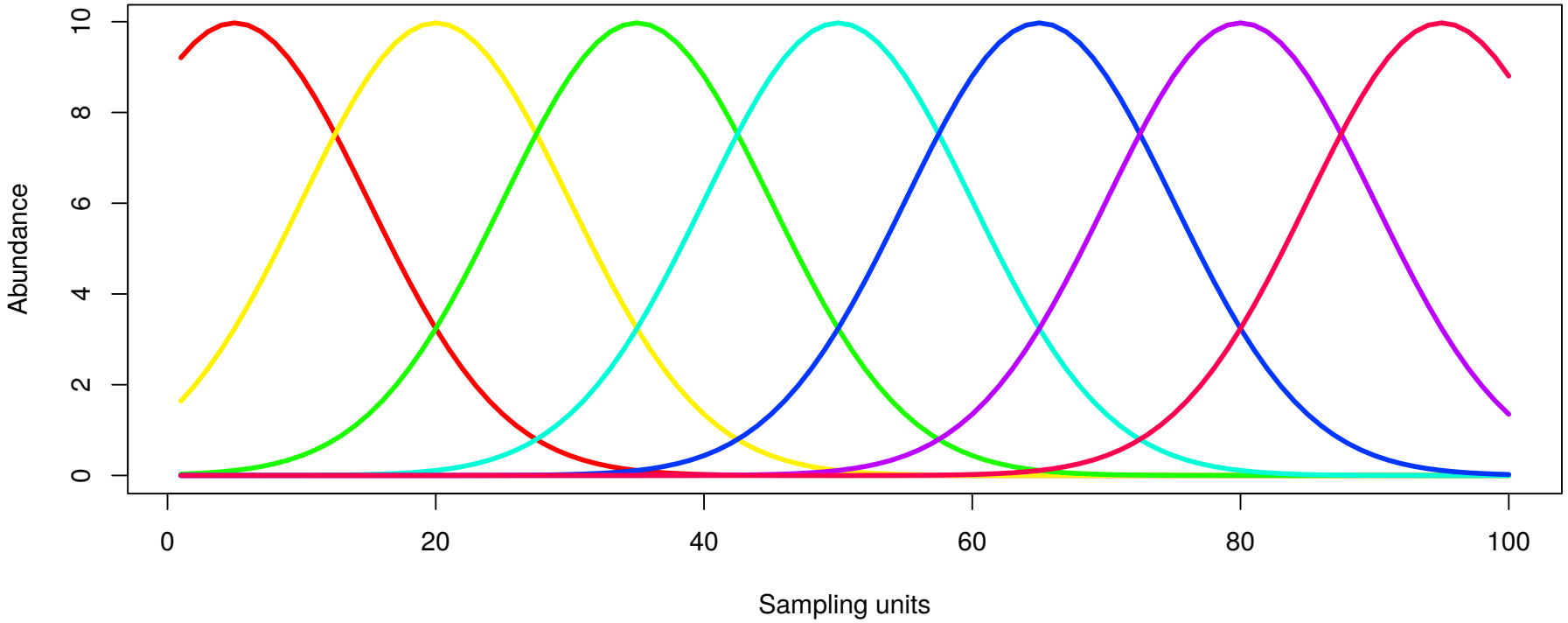
Reciprocal averaging

Repeat until site and species scores converged (remain constant)

Built a latent (unobserved) variable that best discriminates between species scores

Weighted averaging representation of CA:

Consider a set of species with unimodal distributions arranged along an environmental gradient



The explanatory power of the gradient is measured by the degree of separation of the species

CA finds the theoretical (latent) variable that maximizes the separation of species - that is, best explains the species data in terms of a unimodal weighted averaging model

Relation to PCA

CA is a PCA on transformed data

...	species 1	species 2	...	species i	Σ
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}
...	...	...	...	...	...
site j	p_{j1}	p_{j2}	...	p_{ji}	p_{j+}
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}

Matrix $\overline{Q}$

...	species 1	species 2	species i
*site*1	$q_{11} = \frac{p_{11}-p_{1+}p_{+1}}{\sqrt{p_{1+}p_{+1}}}$	$q_{12} = \frac{p_{12}-p_{1+}p_{+2}}{\sqrt{p_{1+}p_{+2}}}$	$q_{1i} = \frac{p_{1i}-p_{1+}p_{+i}}{\sqrt{p_{1+}p_{+i}}}$
*site*2	$q_{21} = \frac{p_{21}-p_{2+}p_{+1}}{\sqrt{p_{2+}p_{+1}}}$	$q_{22} = \frac{p_{22}-p_{2+}p_{+2}}{\sqrt{p_{2+}p_{+2}}}$	$q_{2i} = \frac{p_{2i}-p_{2+}p_{+i}}{\sqrt{p_{2+}p_{+i}}}$
sitej	$q_{j1} = \frac{p_{j1}-p_{j+}p_{+1}}{\sqrt{p_{j+}p_{+1}}}$	$q_{j2} = \frac{p_{j2}-p_{j+}p_{+2}}{\sqrt{p_{j+}p_{+2}}}$	$q_{ji} = \frac{p_{ji}-p_{j+}p_{+i}}{\sqrt{p_{j+}p_{+i}}}$

PCA on $\overline{Q}$

- Site scores (Principal components, linear combinations)

...	PC1	PC2	...	PC i
site 1	pc_{11}	pc_{12}	...	pc_{1i}
site 2	pc_{21}	pc_{22}	...	pc_{2i}
...	...	...	...	...
site j	pc_{j1}	pc_{j2}	...	pc_{jci}

- Species scores (Loadings, Eigenvector)

...	ev1	ev2	...	ev i
species 1	ev_{11}	ev_{12}	...	ev_{1i}
species 2	ev_{21}	ev_{22}	...	ev_{2i}
...	...	...	...	...
species i	ev_{i1}	ev_{i2}	...	ev_{ii}

CA site scores

...	species 1	species 2	...	species i	Σ
site 1	q_{11}	q_{12}	...	q_{1i}	q_{1+}
site 2	q_{21}	q_{22}	...	q_{2i}	q_{2+}
site j	q_{j1}	q_{j2}	...	q_{ji}	q_{j+}
Σ	q_{+1}	q_{+2}	...	q_{+i}	q_{++}

CA site scores: weighted averages of PC site scores (Principal component)

...	CA1	CA2	...	CA i
*site*1	$\frac{pc1_1}{\sqrt{\frac{q_{1+}}{q_{++}}}}$	$\frac{pc2_1}{\sqrt{\frac{q_{1+}}{q_{++}}}}$	...	$\frac{pcl_1}{\sqrt{\frac{q_{1+}}{q_{++}}}}$
*site*2	$\frac{pc1_2}{\sqrt{\frac{q_{2+}}{q_{++}}}}$	$\frac{pc2_2}{\sqrt{\frac{q_{2+}}{q_{++}}}}$	...	$\frac{pcl_2}{\sqrt{\frac{q_{2+}}{q_{++}}}}$
sitej	$\frac{pc1_j}{\sqrt{\frac{q_{j+}}{q_{++}}}}$	$\frac{pc2_j}{\sqrt{\frac{q_{j+}}{q_{++}}}}$	...	$\frac{pcl_{jc}}{\sqrt{\frac{q_{j+}}{q_{++}}}}$

CA species scores

...	species 1	species 2	...	species i	Σ
site 1	q_{11}	q_{12}	...	q_{1i}	q_{1+}
site 2	q_{21}	q_{22}	...	q_{2i}	q_{2+}
site j	q_{j1}	q_{j2}	...	q_{ji}	q_{j+}
Σ	q_{+1}	q_{+2}	...	q_{+i}	q_{++}

CA species scores: weighted averages of PC species scores (eigenvector)

...	CA axis 1	CA axis 2	...	CA axis i
*species*1	$\frac{ev1_1}{\sqrt{\frac{q_{+1}}{q_{++}}}}$	$\frac{ev2_1}{\sqrt{\frac{q_{+1}}{q_{++}}}}$	...	$\frac{evl_1}{\sqrt{\frac{q_{+1}}{q_{++}}}}$
*species*2	$\frac{ev1_2}{\sqrt{\frac{q_{+2}}{q_{++}}}}$	$\frac{ev2_2}{\sqrt{\frac{q_{+2}}{q_{++}}}}$	...	$\frac{evl_2}{\sqrt{\frac{q_{+2}}{q_{++}}}}$
speciesl	$\frac{ev1_i}{\sqrt{\frac{q_{+i}}{q_{++}}}}$	$\frac{ev2_i}{\sqrt{\frac{q_{+i}}{q_{++}}}}$	...	$\frac{evl_i}{\sqrt{\frac{q_{+i}}{q_{++}}}}$

Correspondence analysis

Pre transform data

Run PCA

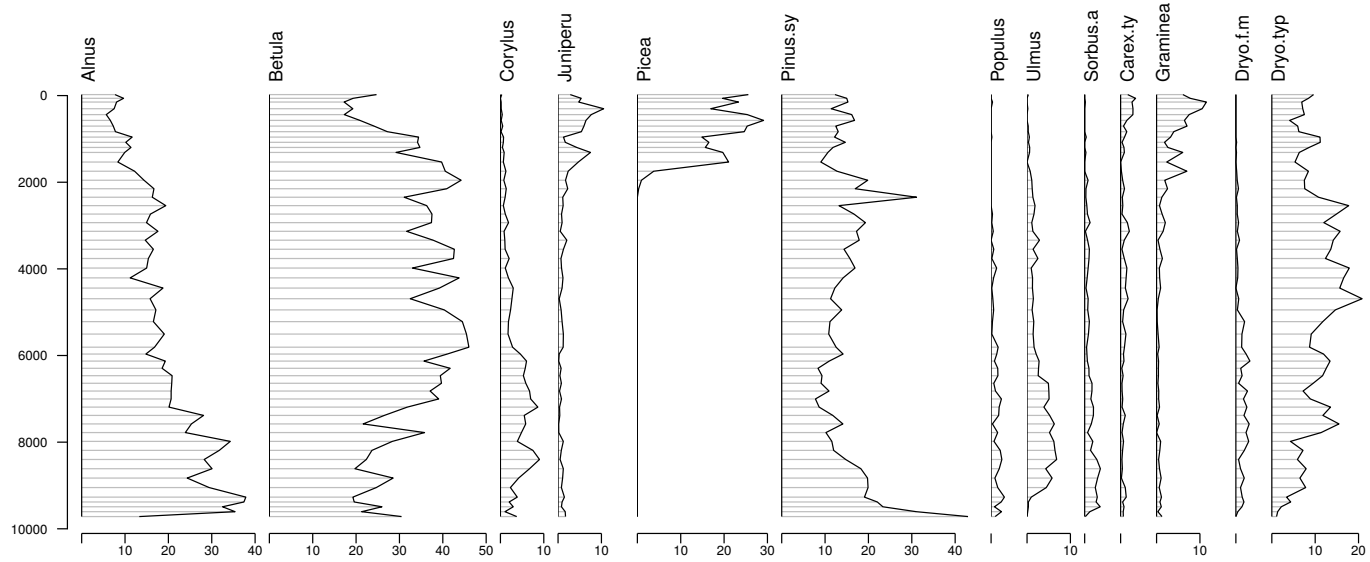
Post transform site and species scores (weighted average)

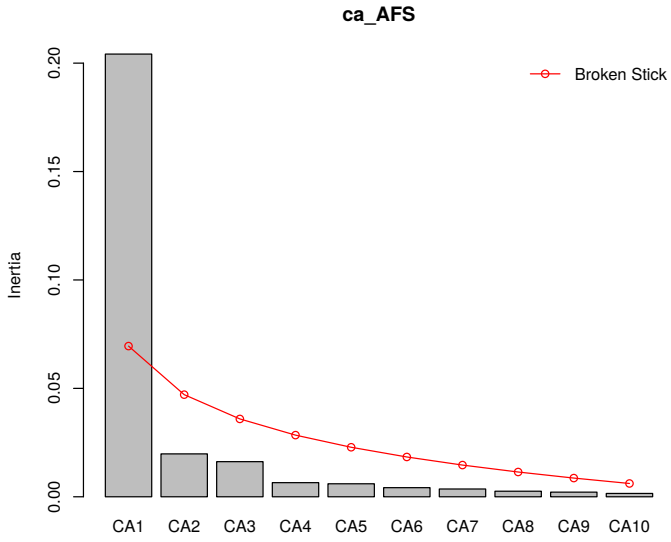
Unimodal response: Inertia instead of variance

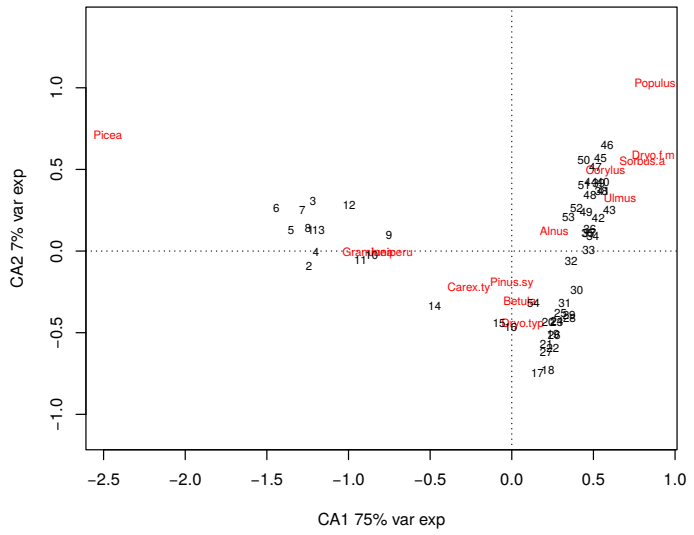
Inertia of one axis divided by total inertia = variance explained by this axis

Distances among samples preserved in CA χ^2 distance

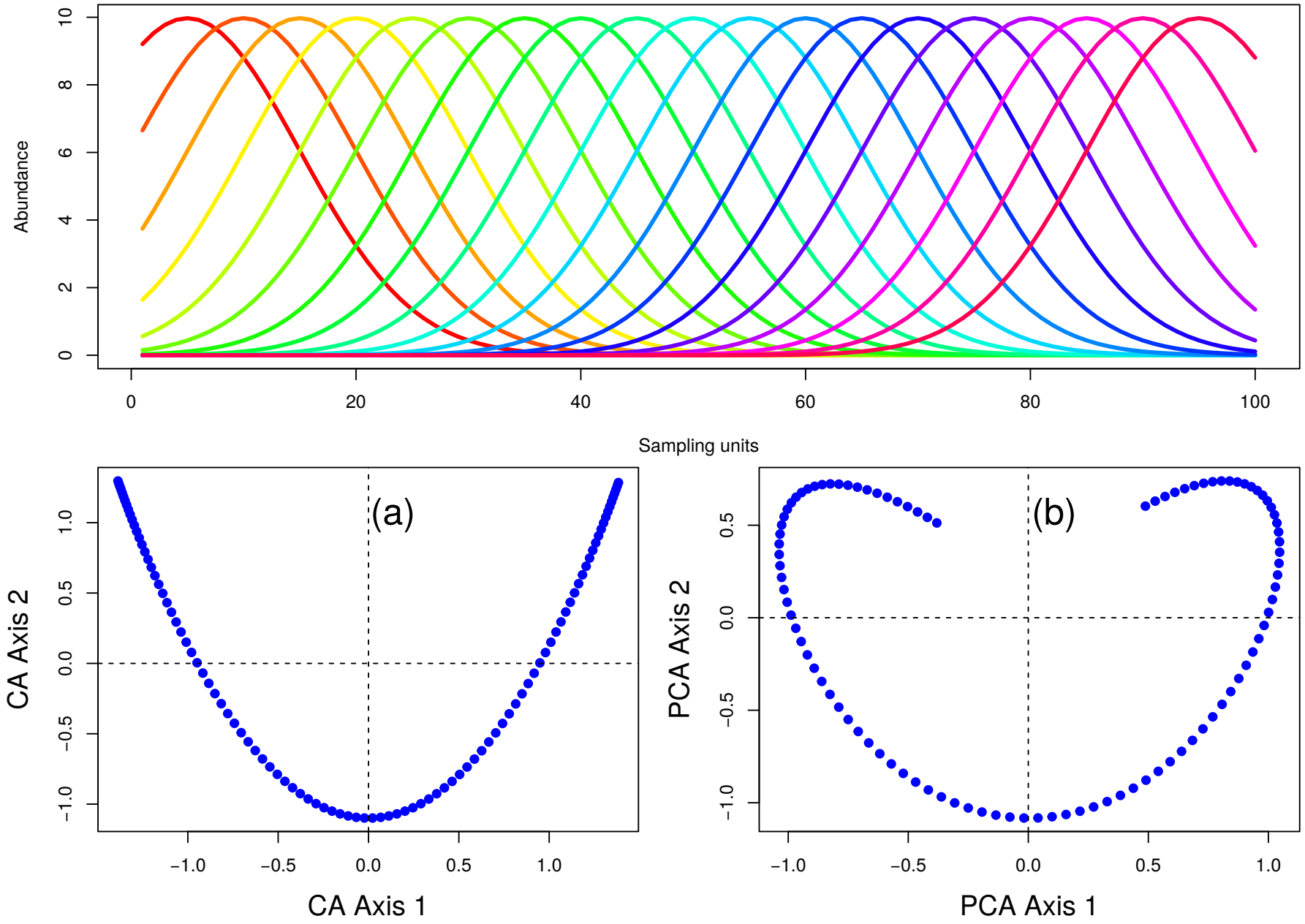
CA example: Kinnshaugen southern Norway







CA arch effect - PCA horse shoe effect



CA arch effect

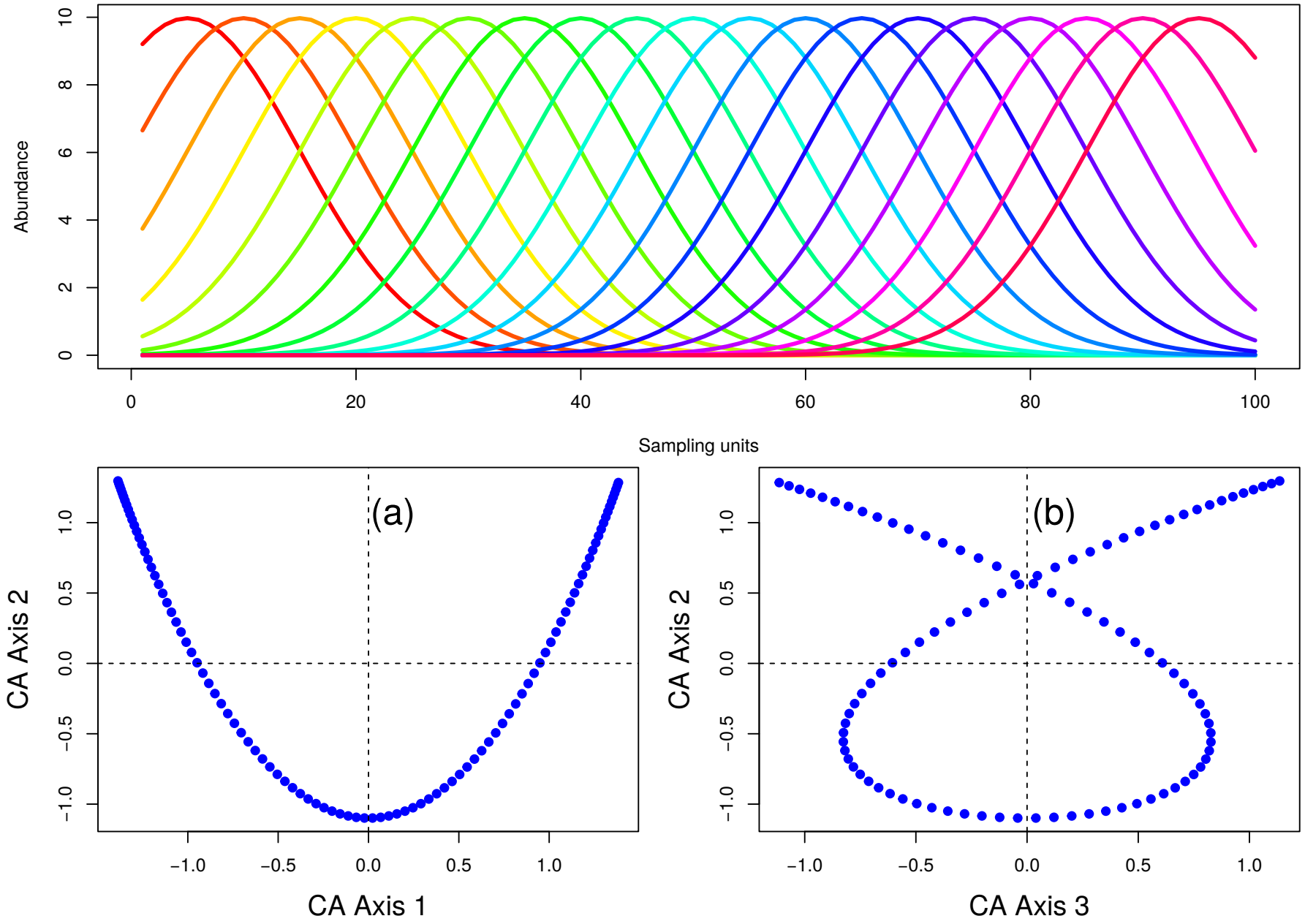
Long environmental gradient:

- species at either end of the gradient do not co-occur
- correlation between those species r $= 0$
- angle between species scores: 90° and not 180°

Ninety degree angle in 3 dimensions:

- lower (upper) end of the gradient:
  - negative (positive) on axis 1
  - positive on axis 2
  - negative (positive) on axis 3

CA Arch effect



CA arch effect - PCA horse shoe effect

Arch effect: only interpret axis one

Horse shoe effect: find a recycling bin...

Alternatives: Detrended correspondence analysis

- axis 1 is virtually unchanged from CA
- not possible to interpret axis 2

Non metric multidimensional scaling (NMDS)

Principal curves (flexible response model instead of WA)

In our crafted example: DCA $>$ CA $>$ NMDS $>>>>>>>>>$
Principal curve (unimodal responses favor DCA and CA)

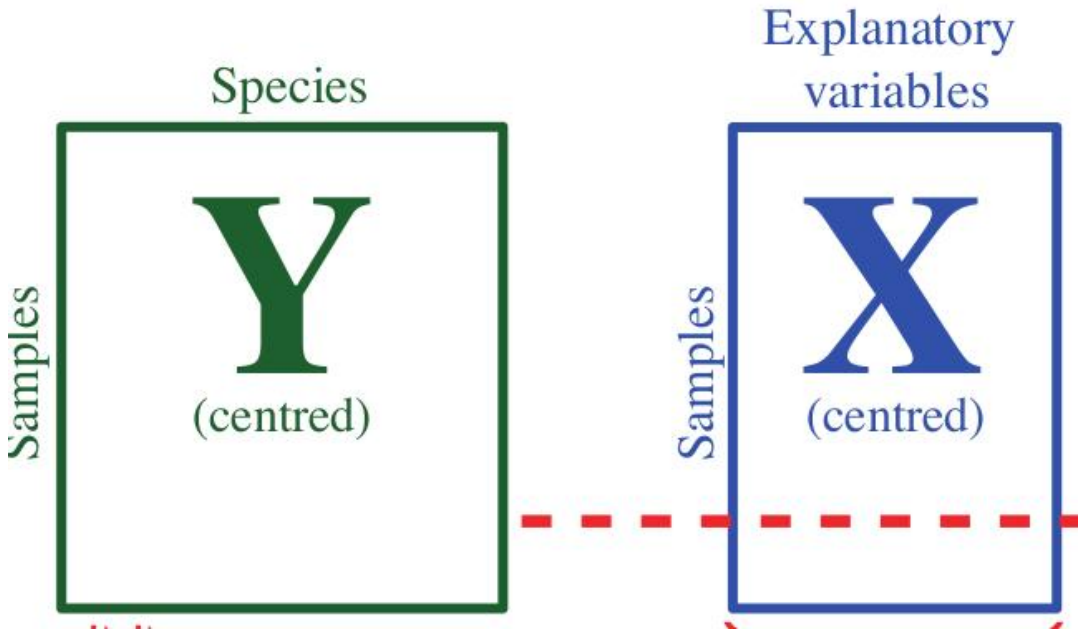
Constrained ordination

Goal: explain dependent variables (usually species data) as function of independent variables (usually environemntal variables)

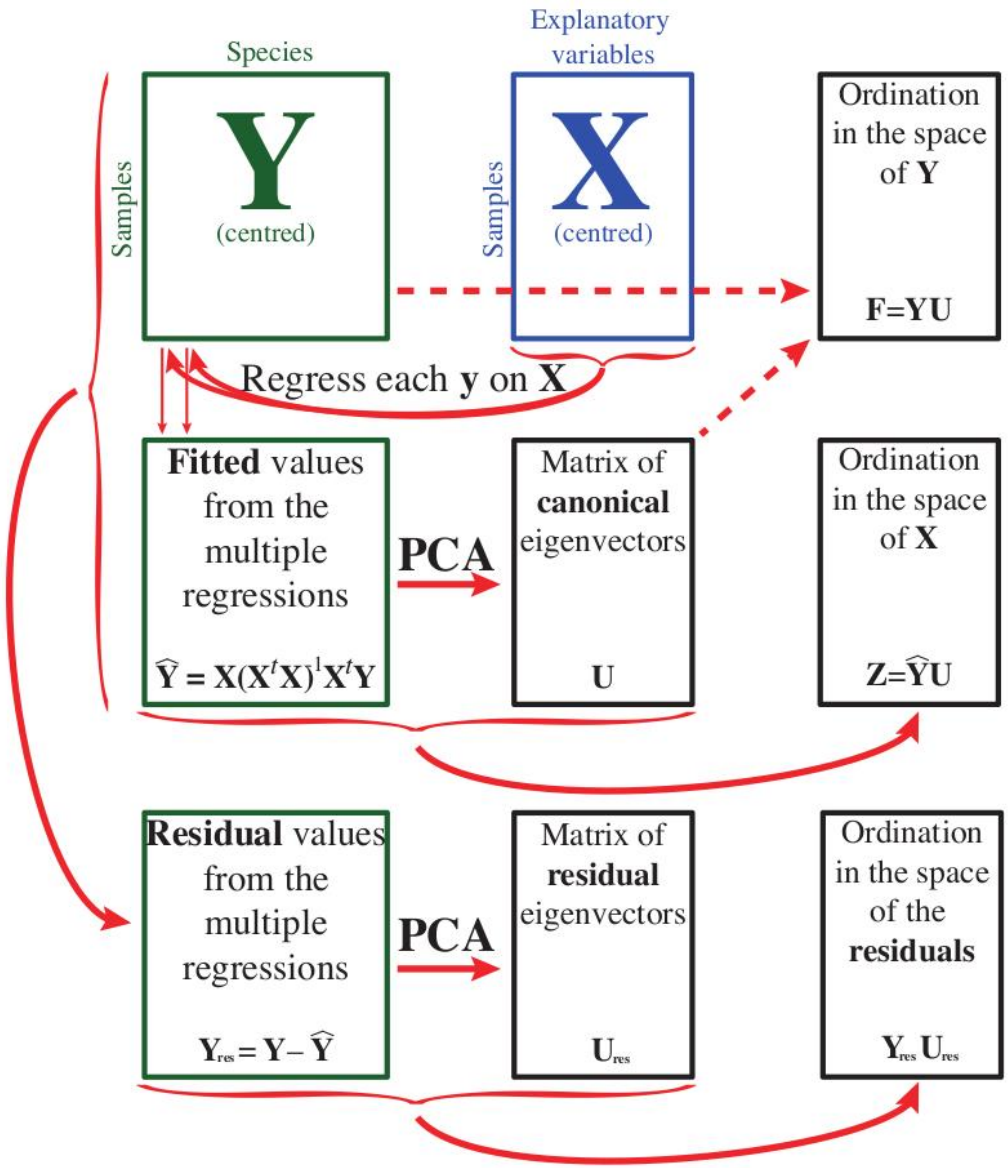
PCA and CA: axes chosen freely

Constrained ordination:

- ordination axes are linear combinations of independent variables
- allows assessment of influence of environemntal variables on species assemblages



Redundancy analysis



Redundancy analysis

Two datasets:

- explanatory data set (e.g. environmental data): **X**
- response data set (e.g. species assemblages): **Y**

Two steps:

- Regression
- Ordination

Redundancy analysis: One environmental variable

Regression

Fitted values

$\hat{y}_1 = a + bx$

$\hat{y}_2 = a + bx$

...

$\hat{y}_i = a + bx$

Reminder: $b = \frac{s_{xy}^2}{s_x} = r_{xy} s_y$

Residuals

$y_{1,res} = y_1 - \hat{y}_1$

$y_{2,res} = y_2 - \hat{y}_2$

...

$y_{i,res} = y_i - \hat{y}_i$

Redundancy analysis: Ordination

One constraining variable

PCA on $\widehat{\mathbf{Y}}$: RDA axis 1

PCA on $\mathbf{Y_{res}}$: PCA axes 1 to (n-1)

RDA site scores: rescaled environmental variable

RDA species scores: rescaled regression coefficients

Redundancy analysis

Total variance: Sum of variances of individual variables in y

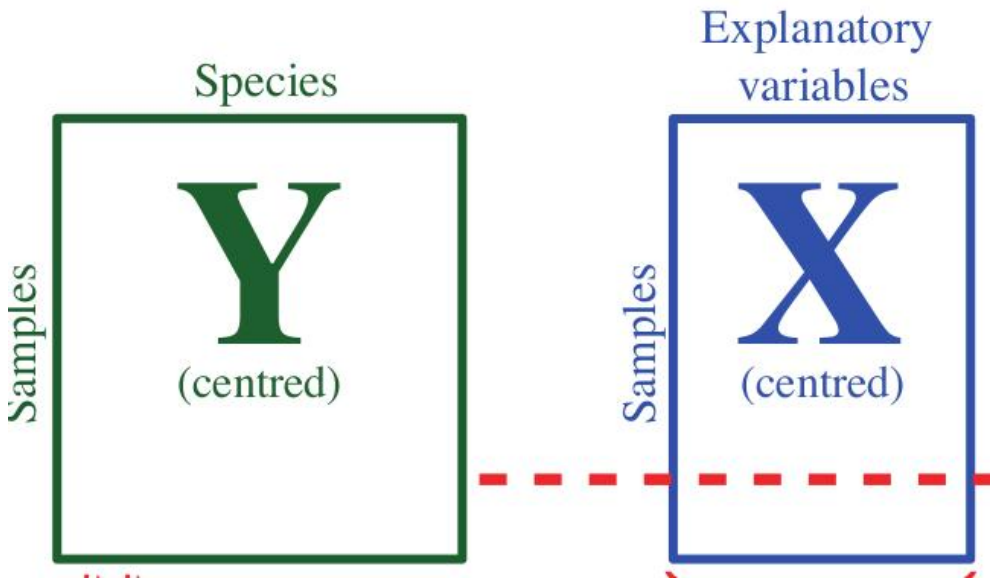
Variance explained by RDA: Variance of all variables in $\hat{Y}$

Variance explained by PCA: Variance of all variables in Y_{res}

Quantity of interest:

- Variance explained by RDA axis 1 divided by variance explained by PCA 1
- Is the first constrained gradient more important than the first unconstrained gradient?
- Ideally: $\frac{\lambda_{RDA1}}{\lambda_{PCA1}} >> 1$

Redundancy Analysis: Regression and Ordination



fitted values $\hat{y}_1 = a + b_1 x_1 + b_2 x_2 + \ldots b_l x_l$

residuals $y_{1,res} = y_1 - \hat{y}_1$

matrix of fitted values $\widehat{\mathbf{Y}} = \mathbf{X}b$

matrix of residuals $\mathbf{Y_{res}} = \mathbf{Y} - \widehat{\mathbf{Y}}$

PCA on $\widehat{\mathbf{Y}}$: RDA axes 1 to l

PCA on $\mathbf{Y_{res}}$: PCA axes 1 to (n-l)

RDA example: Diatoms Round Loch of Glenhead and pH