This presentation contains material by Steve Juggins, Guillaume Blanchet and Richard Telford

Jack Williams did not contribute to this presentation

Canonical correspondence analysis and weighted averaging

Types of ordinations:

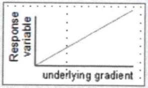
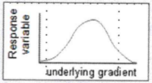
We talked about two types of ordinations and about two types of response models:

What is the main difference between the two ordination types?

What is the main difference between the two response models?

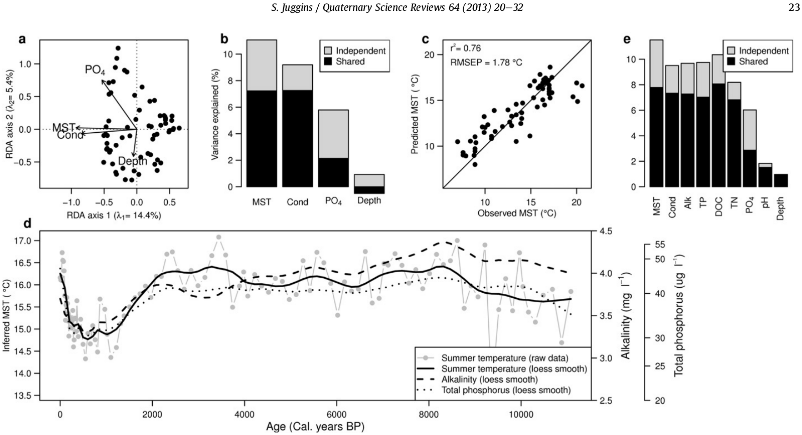
Ordination types:

Classification of ordination methods

		Linear	Unimodal	Complex (Unimodal, linear, skewed)
Response model				
Distance measure		Euclidean	Chi-square	Many to choose from
Role of explanatory variables in analysis	Indirect	Principal Components Analysis (PCA)	Correspondence Analysis (CA) & Detrended Correspondence Analysis (DCA)	non-Metric Multidimensional Scaling (nMDS)
	Direct	Redundancy Analysis (RDA)	Canonical Correspondence Analysis (CCA)	Non-Euclidean RDA

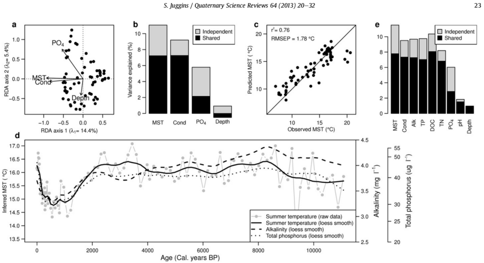
Juggins (2012)

Application of ordinations and reconstructions



Juggins (2013)

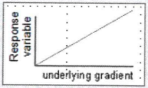
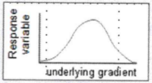
Application of ordinations and reconstructions



- Constrained ordination
- Independent and shared variance
- Transfer function
- Reconstructions
- Variable selection

Ordination types:

Classification of ordination methods

		Linear	Unimodal	Complex (Unimodal, linear, skewed)
Response model				
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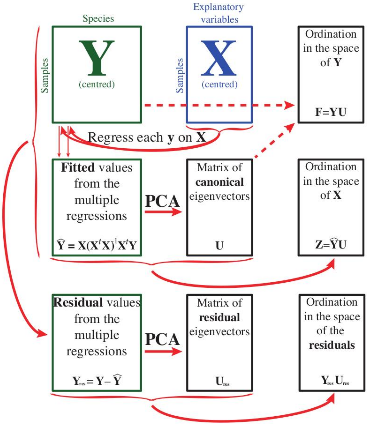
Juggins (2012)

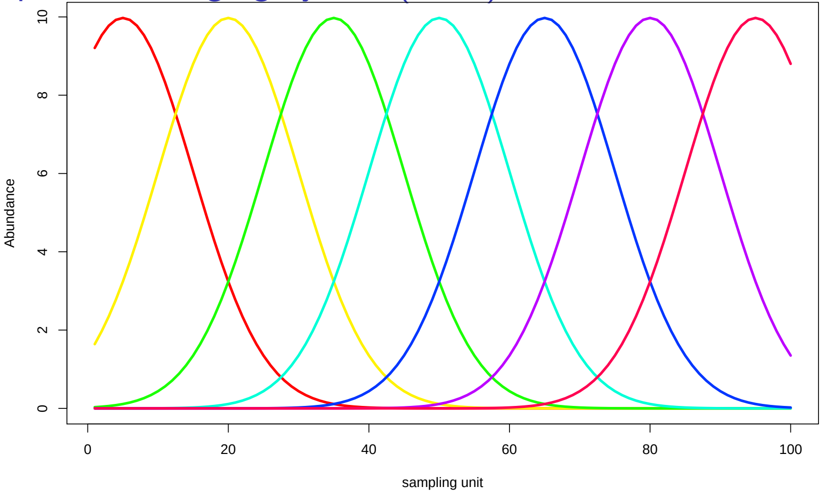
Canonical correspondence analysis

Same principle as redundancy analysis:

- **regression:** weighted regression
- **ordination:** correspondence analysis



Reciprocal averaging by Hill (1973):



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

Gradient analysis: Reciprocal averaging

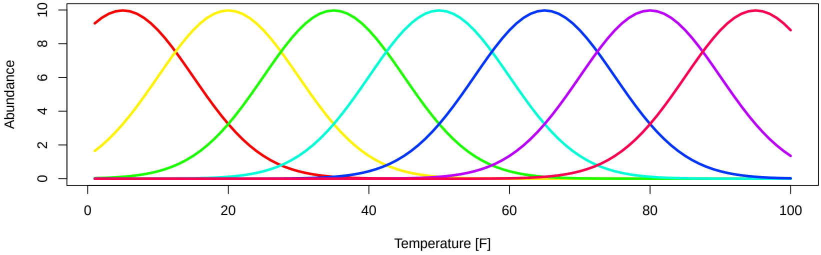
...	species 1	species 2	...	species i	Σ
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}
...	...	...	...	...	...
site M	p_{M1}	p_{M2}	...	p_{Mi}	p_{M+}
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}

Site scores: x

Species scores: y

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

Canonical correspondence analysis



...	species 1	species 2	...	species i	Σ	Env. var.
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}	$env1_1$
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}	$env1_2$
...	...	...	...	...	...	...
site M	p_{M1}	p_{M2}	...	p_{Mi}	p_{M+}	$env1_M$
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}	

Environmental variable: env

Canonical correspondence analysis

...	species 1	species 2	...	species i	Σ	Env. var.
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}	$env1_1$
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}	$env1_2$
...	...	...	...	...	...	...
site M	p_{M1}	p_{M2}	...	p_{Mi}	p_{M+}	$env1_M$
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}	

Environmental variable: env

Start with environmental variable to calculate species scores

Species score: environmental preference of a species

$$scores_{species} = \frac{p_{11}}{p_{+1}} env1_1 + \frac{p_{21}}{p_{+1}} env1_2 + ... + \frac{p_{M1}}{p_{+1}} env1_M$$

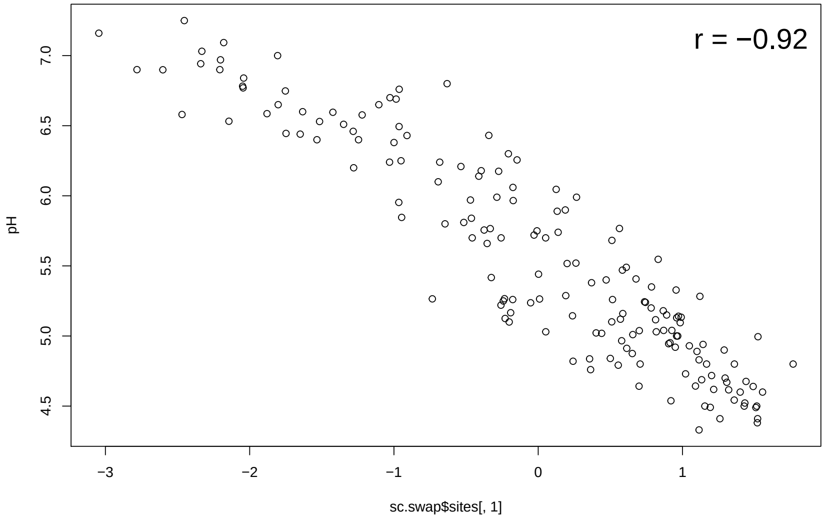
Canonical correspondence analysis: site scores

...	species 1	species 2	...	species i	Σ	Env. var.
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}	$env1_1$
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}	$env1_2$
...	...	...	...	...	...	...
site M	p_{M1}	p_{M2}	...	p_{Mi}	p_{M+}	$env1_M$
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}	

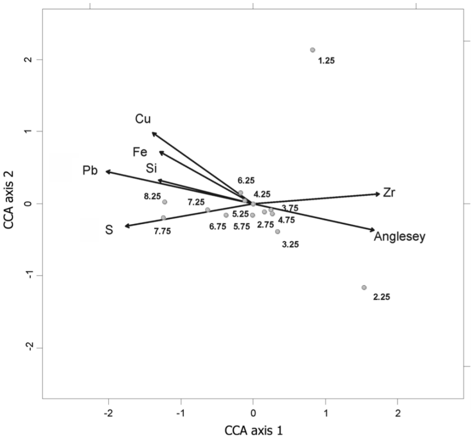
Site scores: environmental conditions at a site as determined by the environmental preferences of species found at that site

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

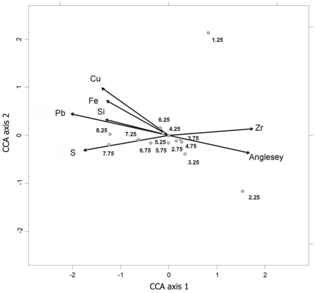
Compare site scores to environmental variable; Diatoms and pH



CCA: bi or triplot



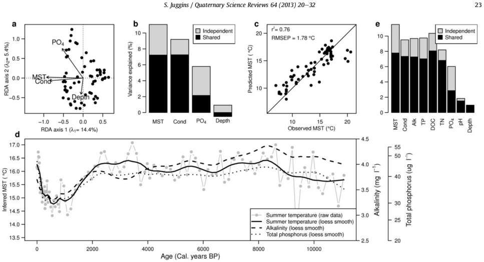
Variable selection:



Issues:

- many, highly correlated variables
- 7 variables for 14 samples
  - which variables are really important?
  - how do we select them?

Variable selection:

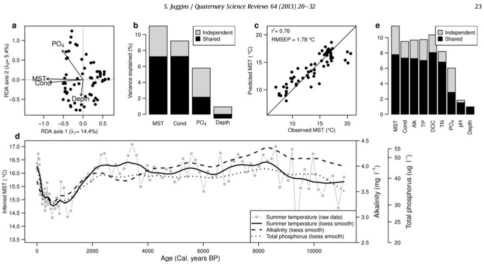


Different selection and inclusion criteria

- forward selection
- backward elimination
- Reviewed in Borcard et al. (2011, see github repository)
- **Always use your ecological knowledge**

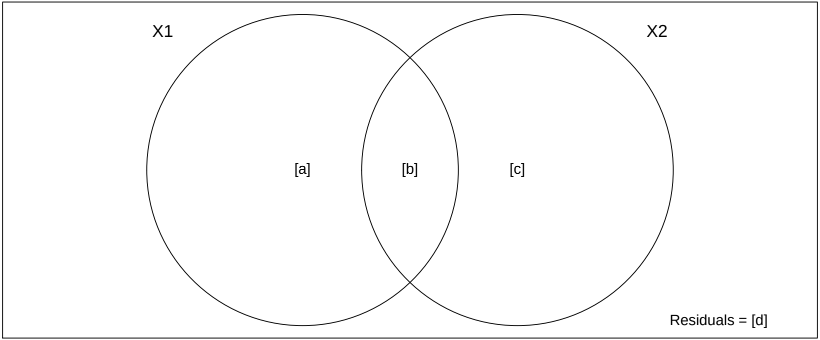
Correlated environmental variables:

Part of the variance explained is shared between the variables



Correlated environmental variables:

Part of the variance explained is shared between variables

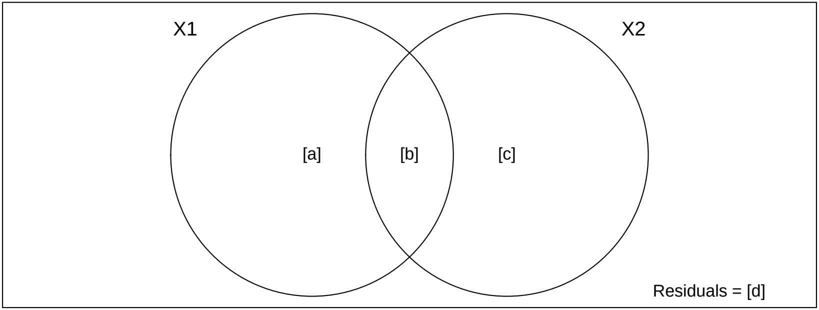


a: variance exclusively explained by X1

c: variance exclusively explained by X2

b: variance shared between X1 and X2

Variance partitioning:



Step1: Remove influence of one environmental variable (**X1**) on species assemblage

- fit model with env variable you want to condition on (**[a]** + **[b]**) and then take residuals

Step2: Constrain residuals using second environmental variable (**X2**) (**[c]**)

Variance partitioning: RDA

varpart in **vegan** package

```
##                     Df R.squared Adj.R.squared Testable
## [a+b] = X1           1 0.2289742     0.2280408     TRUE
## [b+c] = X2           1 0.1482025     0.1471713     TRUE
## [a+b+c] = X1+X2  2 0.2895756     0.2878534     TRUE
```

```
##                     Df R.squared Adj.R.squared Testable
## [a] = X1|X2          1        NA     0.1406821     TRUE
## [b]                  0        NA     0.0873587    FALSE
## [c] = X2|X1          1        NA     0.0598126     TRUE
## [d] = Residuals     NA        NA     0.7121466    FALSE
```

Variance partitioning: CCA

cca in **vegan**

cca.cond.tjul <- cca(sqrt(arctic.pollen) ~ taug + Condition(tjul), data= arctic.env)

cca.cond.taug <- cca(sqrt(arctic.pollen) ~ tjul + Condition(taug), data= arctic.env)

Conditional: [a] + [b] or [b]+[c]

Constrained: [c] or [a]

Unconstrained: residuals [d]

Conditional + **Constrained** = [a] + [b] + [c]

No adjusted R^2

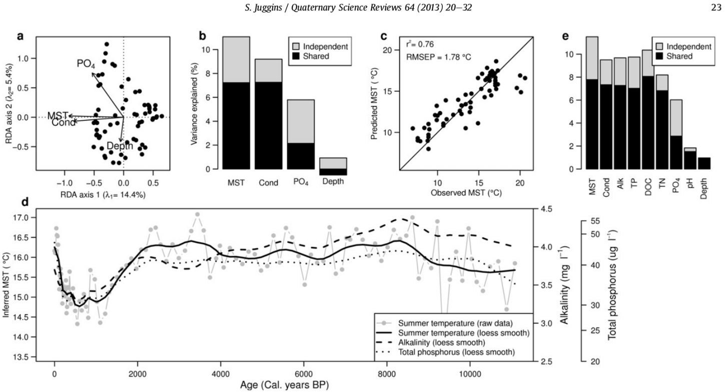
Variance partitioning:

Transform data following Legendre and Gallagher (2001) and then run rda

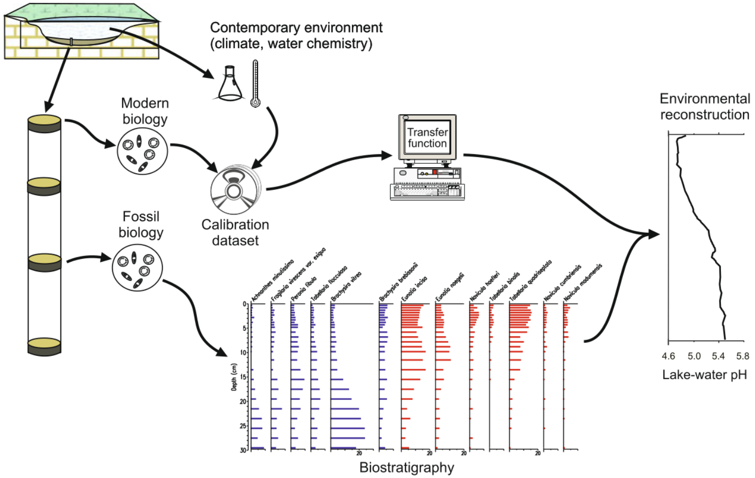
decostand() in vegan

varpart

Environmental reconstructions

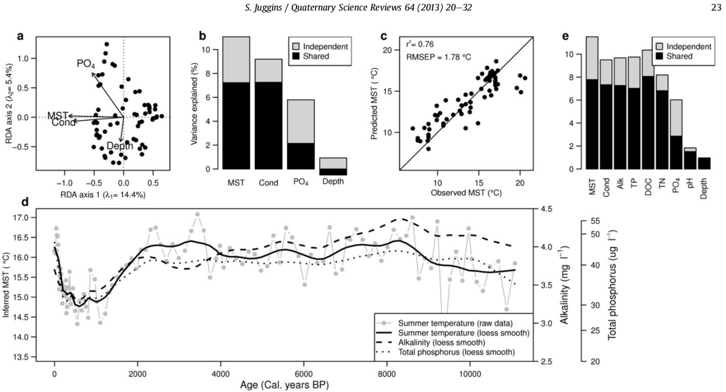


Environmental reconstructions



Juggins and Birks (2012)

Environmental reconstructions



Modern analogue technique vs weighted averaging

MAT: local solution (use k closest analogues and average environment of these analogues)

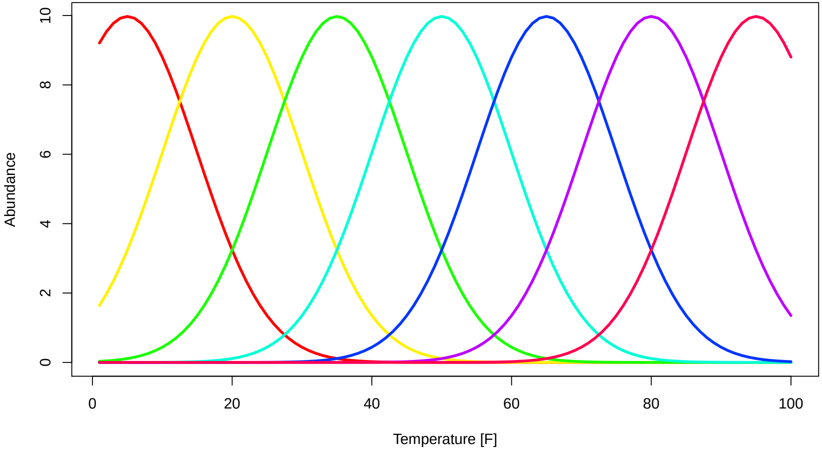
k: number of analogues (usually a few)

WA: global solution estimating optimal environmental conditions for species/taxa

From optimal conditions for species estimate past environment based on species composition

Have we encountered this procedure before?

WA: unimodal response



Estimate species optimum

Using species optima, estimate environmental conditions at a site

WA and CCA: Optima and species scores

...	species 1	species 2	...	species i	Σ	Env. var.
site 1	p_{11}	p_{12}	...	p_{1i}	p_{1+}	env_1
site 2	p_{21}	p_{22}	...	p_{2i}	p_{2+}	env_2
...	...	...	...	...	...	...
site M	p_{M1}	p_{M2}	...	p_{Mi}	p_{M+}	env_M
Σ	p_{+1}	p_{+2}	...	p_{+i}	p_{++}	

Optimum: environmental preference of a species

Environmental variable: env

$$Optimum_{species1} = \frac{p_{11}}{p_{+1}} env_1 + \frac{p_{21}}{p_{+1}} env_2 + ... + \frac{p_{M1}}{p_{+1}} env_M$$

Optimum = CCA species scores

WA and CCA: Predicted value and site scores

...	species 1	species 2	...	species N	Σ	Env. var.
site 1	p_{11}	p_{12}	...	p_{1N}	p_{1+}	$env1_1$
site 2	p_{21}	p_{22}	...	p_{2N}	p_{2+}	$env1_2$
...	...	...	...	...	...	...
site M	p_{M1}	p_{M2}	...	p_{MN}	p_{M+}	$env1_M$
Σ	p_{+1}	p_{+2}	...	p_{+N}	p_{++}	

Predicted values: environmental conditions at a site as determined by the environmental preferences of species found at that site

$Pred_{site} = \frac{p_{11}}{p_{1+}} Opt_{spec1} + \frac{p_{12}}{p_{1+}} Opt_{spec2} + ... + \frac{p_{1N}}{p_{1+}} Opt_{specN}$

Predicted values = CCA site scores

Deshrinking

max(Optima) $<=$ max(env)

min(Optima) $>=$ min(env)

max(predicted value) $<=$ max(Optima)

min(predicted value) $>=$ min(Optima)

Reconstructed values have less variance than environmental variables

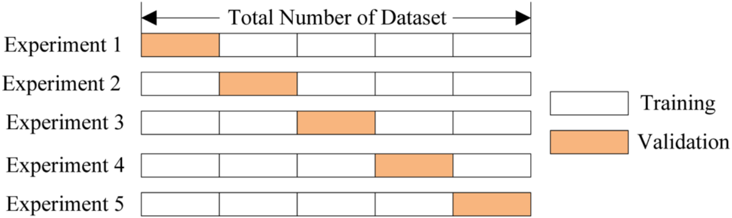
Deshrinking: increase variance of reconstructed values

- inverse
- classical
- monotonic (predicted values no longer equal to CCA site scores but still monotonically related)

Cross-validation

CCA and apparent WA: method knows environmental conditions it is supposed to estimate

Should test model on (hopefully) independent data: **calibration** and **validation**



Cross-validation

- Divide data set in two parts
  - construct model (calibrate) on part one
  - test model (validate) on part two

Leave-one-out:

- Use all except one sample to calibrate model, predict omitted sample (validate)

k-fold:

- Divide data set into k-parts (e.g. $k = 10$)
- Use k-1 parts to calibrate and one part to validate
- repeat k times

Outlook

- Weighted averaging partial least squares (WA-PLS)
- Validate predictions/reconstructions
- Cautionary notes