Model-based ordination

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Outline

What should I cover in this workshop

- Model-based ordination
- Rotation (and post-hoc rotation)
- Variation explained
- Adding row-effects (and what role it plays)
- Conditioning
- Compositional data (or rather, different data types)
- Double-zero problem

Questions so far?

Outline

...

Ordination

Goodall (1954) introduced the word “ordination”

1) Ordination summarizes data
2) Ordination **embeds** in a low-dimensional space
3) Ordination **orders** samples and species

Ordination

Goal: to explore co-occurrence patterns
Problem: data forms high-dimensional space

- Why do species co-occur?
  - Similar environmental preferences
  - Similar history in the environment
  - Might results in *Interactions*
- But sometimes we lack measurements of the environment
- Thus cannot test anything

Figure 1: NIBIO

The ecological process

Ecological gradient theory informs us about the process

- Type of response curve
- Measured and/or unmeasured components
- Spatial and/or temporal components
- Functional traits or Phylogeny
- Et cetera.

In contrast to traditional ordination methods, we have a more process-based view (sampling process and ecological process)

Gradients

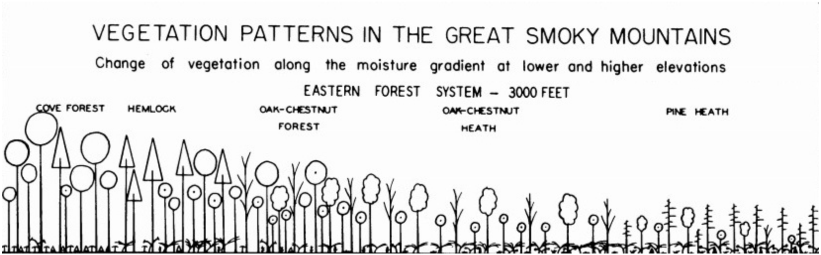


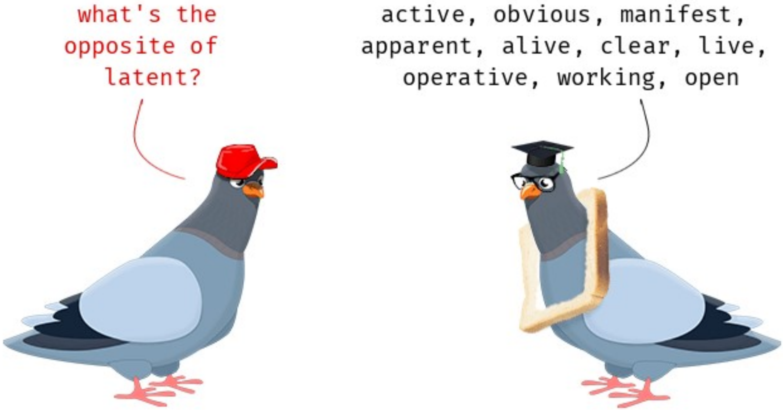
Figure 2: Whittaker 1956

There are different types of gradient, for example:

- Environmental gradient
- Complex ecological gradient
- Coenoclines

Ordination axes

"Ordination axis" has become synonymous to "latent variable"



In essence: an unobserved gradient

Ecological gradients

"Few major complex ecological gradients normally account for most of the variation in species composition." (Halvorsen, 2012)

Ecological gradients

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Which is synonymous to saying "we can probably get a way with fitting a JSDM using only a few dimensions"

Ordination as latent variable model

Many ordination methods are thought of as implementing a latent variable model

- ter Braak (1985)
- Jongman et al. (1995)
- van der Veen et al. (2022, section 3 chapter 1)

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They approximately implement:

$$y_{ij} = \beta_{0j} + \mathbf{u}_i^\top \boldsymbol{\gamma}_j \tag{1}$$

This makes GLLVMs a framework for many types of ordination, with foundations in existing methods.

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The main issue? We do not know how approximate it is! We cannot validate!

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Classical ordination

Traditionally the go-to method for multivariate analysis

From p columns to $d << m$ dimensions

- Principal Component Analysis (PCA; Pearson 1901)
- Factor Analysis (FA; Spearman 1904)
- Correspondence Analysis (CA; Hirschfeld 1935)
- Non-metric Multidimensional Scaling (NMDS; Kruskal 1964a,b)
- Principal Coordinate Analysis (PCoA; Gower 1967)
- Detrended Correspondence Analysis (DCA; Hill and Gauch 1980)

Main benefits of these methods

1) Easy to use
2) Loads of resources
3) Isuess, artefacts, usecases are all well known
4) Permutation testing is readily available
5) Variance partitioning is straightforward

Problems with classical methods

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Forum | Open Access

The central role of mean-variance relationships in the analysis of multivariate abundance data: a response to Roberts (2017)

David I. Warton, Francis K. C. Hui

First published: 26 July 2017 | https://doi.org/10.1111/2041-210X.12843 | Citations: 16

Methods in Ecology and Evolution BRITISH ECOLOGICAL SOCIETY

| Free Access

Distance-based multivariate analyses confound location and dispersion effects

David I. Warton, Stephen T. Wright, Yi Wang

First published: 06 June 2011 | https://doi.org/10.1111/j.2041-210X.2011.00127.x | Citations: 627

Correspondence site: http://www.respond2articles.com/MEE/

Validation

A "bad" looking ordination plot has often been used as indicator that the ordination method does not do well.

- PCA: horseshoe effect
- CA: arch effect
- DCA: tongue effect (and very heuristic)
- PCoA: similar to PCA
- NMDS: no species effects, no variation explained, no hypothesis testing, I can go on

Small eigenvalues: also bad.

Model-based ordination

Suggested to use Generalized Linear Latent Variable Models for unconstrained ordination

Methods in Ecology and Evolution BRITISH ECOLOGICAL SOCIETY

Special Feature: New Opportunities at the Interface Between Ecology and Statistics | Free Access

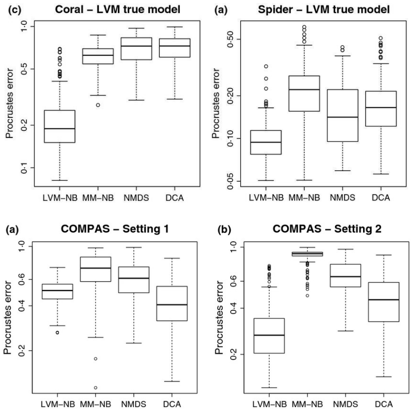
Model-based approaches to unconstrained ordination

Francis K.C. Hui, Sara Taskinen, Shirley Pledger, Scott D. Foster, David I. Warton

First published:23 July 2014 | https://doi.org/10.1111/2041-210X.12236 | Citations: 57

Building on a long history of using latent variables in ecology (e.g., ter Braak 1985)

Unconstrained ordination



Figures from **Hui et al. 2015**

Generalised Linear Latent Variable Model

Unlike in the JSDM, model-based ordination has a focus on the latent variables. The model is:

$$\eta_{ij} = \beta_{0j} + \mathbf{u}_i^\top \boldsymbol{\gamma}_j \qquad (2)$$

but now, we have a much stronger focus on the lower dimensions. And the ordination axis can be treated as fixed or random effect (but usually random).

Conditioning

In classical method, we can use `Condition` to remove variation due to a covariate from the ordination. Here, we add an effect outside of the ordination:

$$\eta_{ij} = \beta_{0j} + \boxed{\ldots} + \mathbf{u}_i^\top \boldsymbol{\gamma}_j \tag{3}$$

Which can be a fixed or random effect (fixed in classical ordination)

So how is this different from JSDM

1. Ordination and JSDM use the same statistical framework (GLLVMs)
2. The models take a different angle (associations versus latent variables)
3. JSDM **can** be an LVM, ordination **is** an LVM

JSDM vs. ordination

JSDMs build more heavily on SDMs than on traditional multivariate analysis

Ordination methods have been criticised for being too descriptive rather than predictive nature

Ovaskainen and Abrego 2021

JSDM vs. ordination

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Ordination methods have been criticised for being too descriptive rather than predictive nature

Ovaskainen and Abrego 2021

ordination did it first Walker and Jackson 2011

JSDM vs. ordination

The differences is in how we think of the model:

- Do we formulate on the basis of latent variables or associations
- Do we look at patterns in the ordination, or patterns on a map?
- Do we believe the “axes” have meaning, or not?
- The scale at which we operate: local or macroecological
- Is the **the sampling process** considered?

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Both of the angles have a lot to teach us about community ecology

A new approach!..or is it?

- Community ecology has been doing it for a hundred years
- e.g. Forbes (1907) or Goodall (1954)
- Walker and Jackson (2011): Random-effects ordination!
- Hui et al. (2015): Model-based unconstrained ordination

BIOMETRICS 41, 859–873
December 1985

Correspondence Analysis of Incidence and Abundance Data: Properties in Terms of a Unimodal Response Model

Cajo J. F. ter Braak

TNO Institute of Mathematics, Information Processing and Statistics,
P. O. Box 100, 6700 AC Wageningen, The Netherlands

GLLVMs vs. classical ordination: main differences

1) GLLVMs have a real model
2) GLLVMs incorporate distributions, not distances
3) There are no eigenvalues (but there is variance)
4) Number of dimensions are set a-priori as in NMDS
5) Latent variables are found by "best fit"
6) You might not get the same solution every time
7) Forget about permutation testing
8) We do not care much about rotation
9) $\longrightarrow$

Rotation and orthogonality

Ordination methods are defined by their rotation (except NMDS?), here:

- Latent variables are orthogonal **a-priori**
- The latent variables are **not** maximum variance-rotated
- **A-posteriori** the latent variables are not orthogonal

We can rotate them afterwards in whatever manner we want, with the `GPArotation` package

When to use ordination

Mostly when we want to do dimension reduction. But also when:

1. We want to determine latent variables
   - Especially when we have not measured the environment
2. **We have too sparse data to estimate species effects**
3. We want to make pretty pictures

Classifying ordination

There are many ways to group ordination methods

- Indirect or direct
- Linear or unimodal
- Unconstrained or constrained
- Simple-method or distance-based

Gradient analysis

Indirect gradient analysis: patterns in species composition that may be due to environment, but without studying environmental variables

Direct gradient analysis: estimate how species are affected by environmental variables

Both are used to analyze patterns in ecological communities

Unconstrained ordination

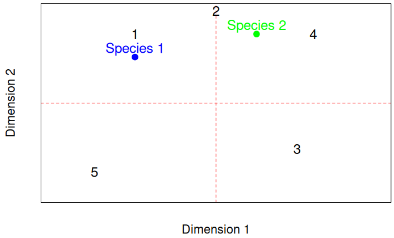
Used to:

- Visualize patterns in data
- Draw 2D plots
- Generate hypotheses
- Explore drivers of community composition

To infer environmental conditions from species relationships

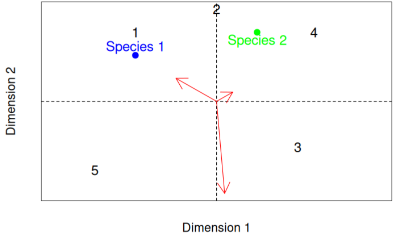
Reading an Ordination plot

- Ordination plots capture the main patterns in the data
- Two coordinates close together are similar
- Close sites have similar community composition
- Close species have similar niches
- Distance in the ordination plot is analogous to correlation of JSDM
- We usually assume the environment drives patterns in an ordination



Ordination plot

- We interpret sites relative to sites, and species to species (so not usually species to sites)
- Coordinates are interpreted relative to the axes (LVs)
- In constrained ordination, arrows represent the axes-environment association
- Long arrows have a (relative) stronger effect
- The angle of arrows to the axes represent the association (orthogonal with no association)
- So, covariates help interpret the ordination



Example: Dutch Dune data

Achimill	Agrostol	Airaprae	Alopgeni	Anthodor	Bellpere	Bromhord	Chenal
1	0	0	0	0	0	0	
3	0	0	2	0	3	4	
0	4	0	7	0	2	0	
0	8	0	2	0	2	3	
2	0	0	0	4	2	2	
2	0	0	0	3	0	0	
2	0	0	0	2	0	2	
0	4	0	5	0	0	0	
0	3	0	3	0	0	0	
4	0	0	0	4	2	4	

- A classic dataset, originally by Jongman et al. (1995)
- Ordinal classes for 30 plant species at 20 sites
- 5 covariates; A1, Moisture, Management, Use, Manure

The ordinal model: proportional odds

More commonly, the categories are ordered.

$$\text{pr}(y_{ij} \leq k) = \Phi(\tau_{jk} - \eta_{ij}) \tag{4}$$

and

$$\text{pr}(y_{ij} = k) = \Phi(\tau_{jk} - \eta_{ij}) - \Phi(\tau_{jk-1} - \eta_{ij}) \tag{5}$$

- τ_{jk} are cut-off parameters that induce ordering
- τ_{jk} requires having at least one observation in every category
- If we have missing classes, we can re-order and skip some
- Alternatively, we can assume $\tau_{jk} = \tau_k$; same cut-offs for all species
- Controlled with `zeta.struc = common` but defaults to `species`

Called "proportional odds" because the effects η_{ij} are the same for all

Example: unconstrained ordination

```
model1 <- gllvm(Y, num.lv = 2, family = "ordinal")
```

```
## Warning in gllvm.iter(y = y, X = X, xr = xr, lv.X = lv.X.design, for
## formula, : Can't fit ordinal model if there are species with missing
## Setting 'zeta.struc = `common`'.

## Warning in nlminb(objr$par, objr$fn, objr$gr, control = list(rel.tol
## : NA/NaN function evaluation
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```
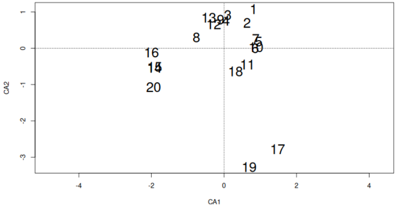
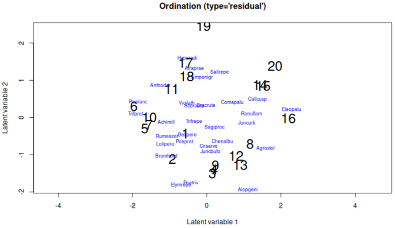

Example: making an ordination plot

```
gllvm::ordiplot(model1, biplot = TRUE, s.cex = 2)
```

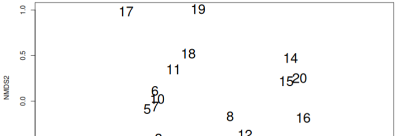
CA



GLLVM



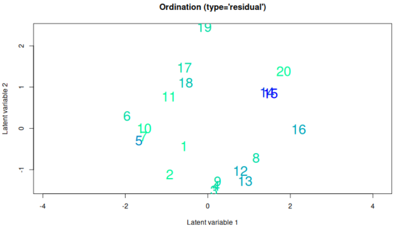
NMDS



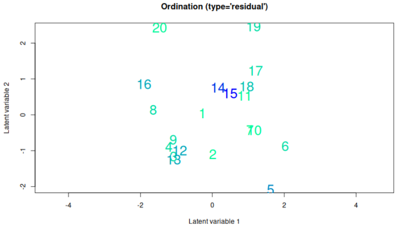
Example: conditioning or “residual” ordination

```
model2 <- gllvm(Y, X = X, formula = ~scale(A1), num.lv = 2, family = "ordi
```

Without A1 covariate



With A1 covariate



Example: conditioning or "residual" ordiantion

```
cor(getLV(model1), X$A1)
```

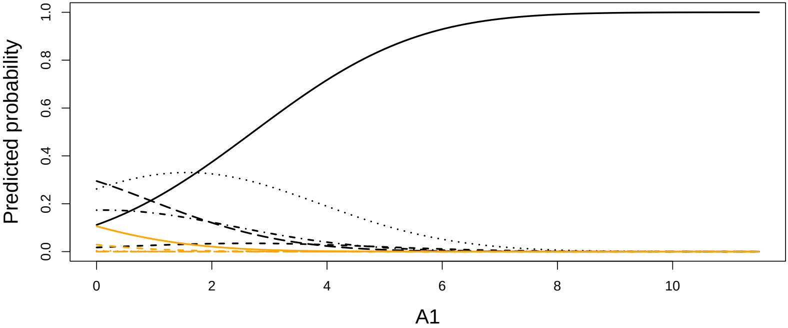
```
##             [,1]
## LV1 -0.4934432
## LV2 -0.0642982
```

```
cor(getLV(model2), X$A1)
```

```
##                [,1]
## LV1 -1.727955e-05
## LV2 -4.724424e-06
```

The ordination of the model including the covariate is uncorrelated with the covariate.

Example: prediction



Note that ordering has introduces some shapes.
Class 1-5: black with linetype 1-5
Class 6-10: orange with linetype 6-10

What makes for a good ordination method?

Michael Palmer:

1. It recovers gradients without distortion.
2. If clusters exist in nature, this should be obvious in the ordination.
3. It does not produce clusters which do not exist.
4. It gives the same result every time for a given data set.
5. There is a unique solution.
6. Ecological similarity is related to proximity in ordination space.
7. Scaling of axes is related to beta diversity.
8. "Signal" and "Noise" are easily separated.
9. You do not need to pre-specify number of axes.
10. The solution is the same, no matter how many dimensions one chooses to look at.
11. Unless by choice, all sites/stands/quadrats are treated equally.
12. The solution does not take much computer time.
13. The method is robust: it works well for short and for long gradients, for low and high noise, for sparse and full matrices, for big and for small data sets, for species-rich and species-poor systems.

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4. It gives the same result every time for a given data set.
5. There is a unique solution.
6. Ecological similarity is related to proximity in ordination space.
7. Scaling of axes is related to beta diversity.
8. "Signal" and "Noise" are easily separated.
9. You do not need to pre-specify number of axes.
10. The solution is the same, no matter how many dimensions one chooses to look at.
11. Unless by choice, all sites/stands/quadrats are treated equally.
12. The solution does not take much computer time.
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What makes for a good ordination method? a shorter list

Gauch (1982):

Three criteria are basic for ordination techniques.

(1) Effective (realistic in assumptions, suitably convey information)
(2) Robust (to real data)
(3) Practical (computer time)

1) Effective

- realistic in assumptions
- suitably conveys information

We can test assumptions in GLLVMs, or adjust the method to relax them.

2) Robust

Classical methods have artefacts, in model-based ordination they can crop-up: but we adjust the model (non-linearity)

Example 2

In 1987, Minchin concluded that NMDS was the “most robust” ordination method, as it allowed deviation from a parametric response model.

- 56 “Species”
- 48 “Sites”
- Simulated from COMPAS with a skewed response model

Vegetatio 69: 89–107, 1987

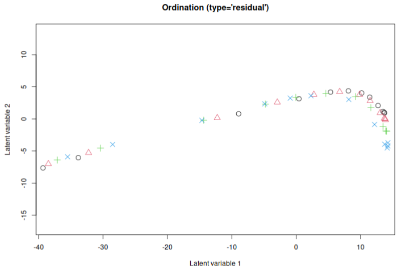
89

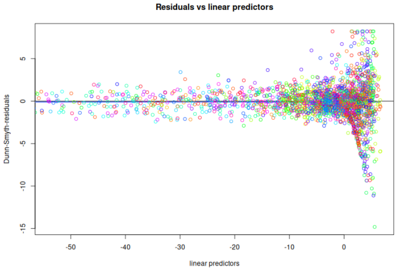
An evaluation of the relative robustness of techniques for ecological ordination

Peter R. Minchin*
CSIRO Division of Water and Land Resources, G.P.O. Box 1666, Canberra, 2601, Australia

Example 2: fitting the model

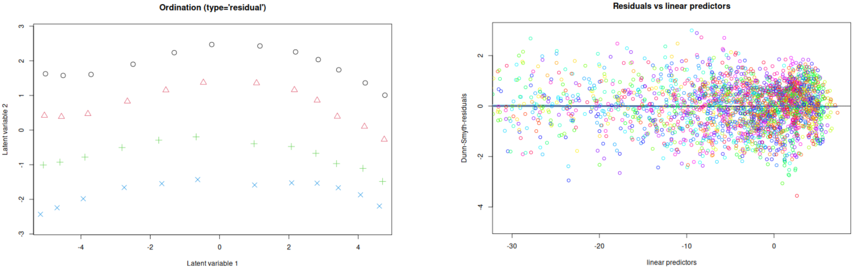
```
model3 <- gllvm(Y, num.lv = 2, family = "poisson", sd.errors = FALSE, maxi
```



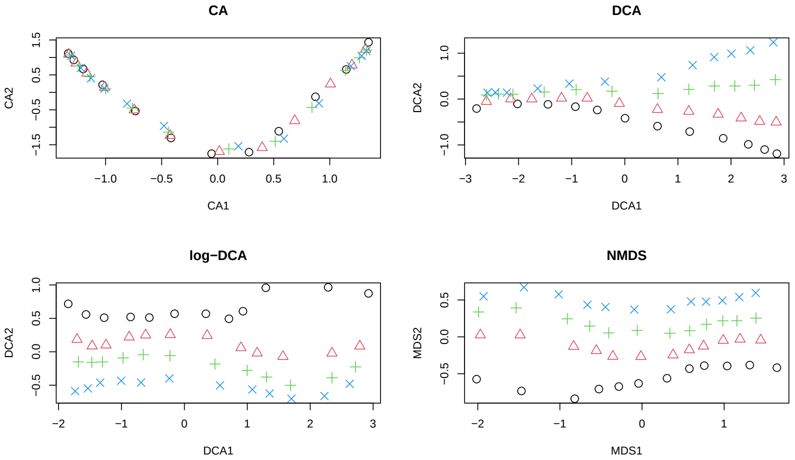


Example 2: we "just" change the model!

```
gllvm::ordiplot(model4, rotate = FALSE, s.col=rep(1:4,each=12), pch=rep(1:
```



Example 2: the competition



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- Have an arh(-like) effect
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- Have data type ...?
- Have double-zeros
- Have compositional data

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You adjust to model to acommodate whatever property of the data

Unconstrained or constrained

a) Unconstrained ordination: explore main drivers of variation (i.e., indirect gradient analysis)
b) Constrained ordination: filter variation due to covariates (i.e., gradient analysis)
c) (Concurrent ordination)

Unconstrained is mostly descriptive, constrained can also be used for hypothesis testing.
Both can be understood as estimating latent variables.

Model-based ordination

Group-level ordination

Not covered, but use `lvCor` or `num.RR` (more later)