Concepts in model-based clustering

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Summer School on model-based multivariate analysis for ecologists

Outline

- Clustering sites and/or species
- Clustering incoporating covariates

Questions so far?

The models so far

Throughout the course of the summer school, many of the models we have studied so far can be written in the generic form:

$$\eta_{ij} = \beta_{0j} + \alpha_i + \delta_{ij},$$

where:

- β_{0j} are species-specific intercepts (column standardization);
- α_i are (optional) row effects (row standardization);
- δ_{ij} is "stuff" e.g., effects of measured covariates, latent variables, traits and phylogeny etc. . .

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For the next little bit, we will assume α_i is always included i.e., both rows and columns are standardized.

By doing so, we can focus on the δ_{ij} part of the model i.e., what is left over after adjusting for heterogeneity in recorded species prevalence and site sampling effort.

What to do about δ_{ij}?

On Wednesday, we covered the idea of model-based ordination or some variation thereof, where $\delta_{ij} = \mathbf{u}_i^\top \gamma_j$. Provided the number of latent variables is small, then the $\mathbf{u}_i$'s and/or γ_j's can be plotted in some way to give a low-dimensional representation of patterns in species composition/indicator species etc. . .

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In this lecture, we will talk about another way to model the δ_{ij}'s using ideas from clustering...

What to do about δ_{ij}?

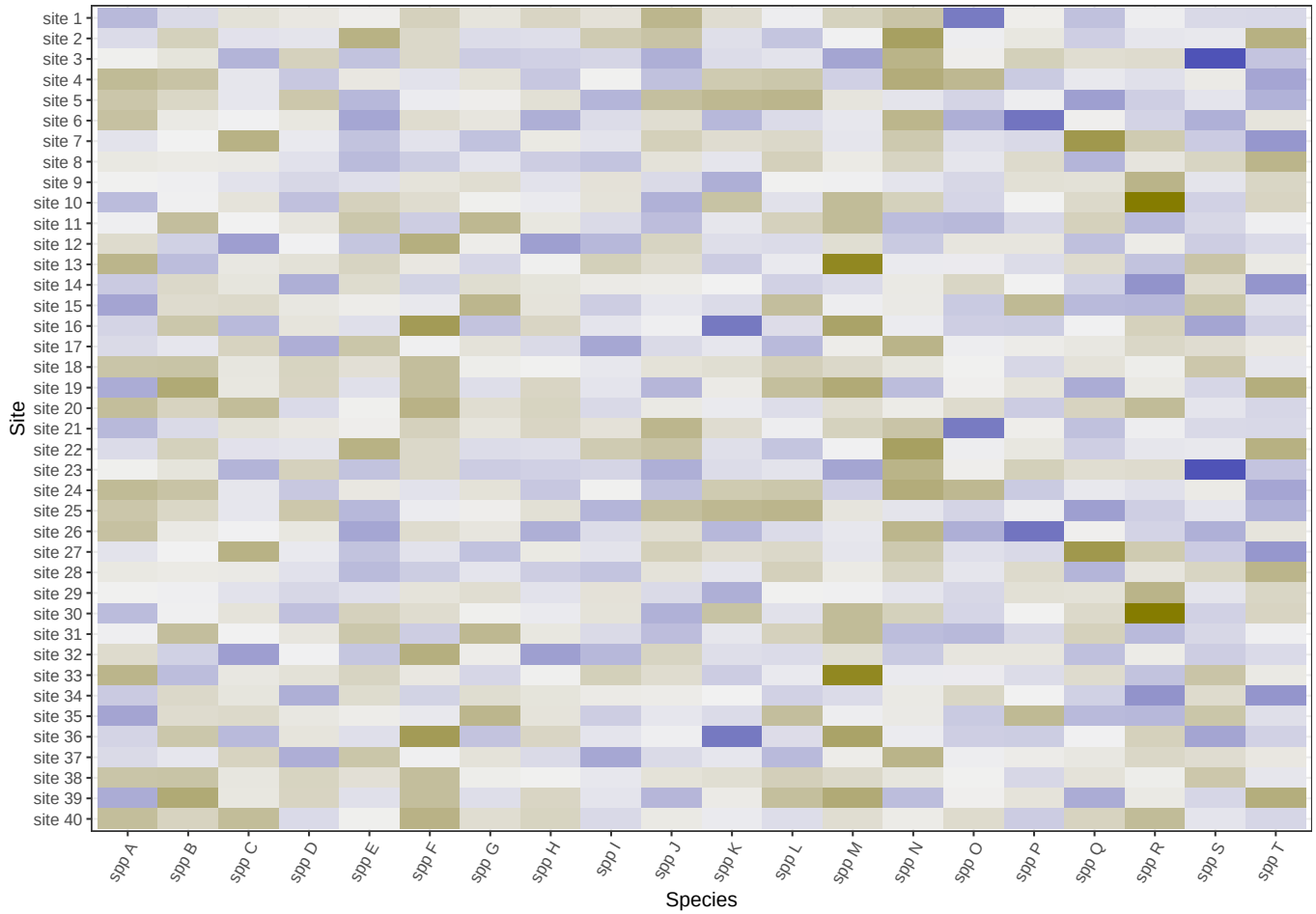
Consider again the model

$$\eta_{ij} = \beta_{0j} + \alpha_i + \delta_{ij},$$

and suppose now the δ_{ij}'s are just directly estimated as fixed effects, alongside the β_{0j}'s and α_i. We will refer this as the **saturated** model, since:

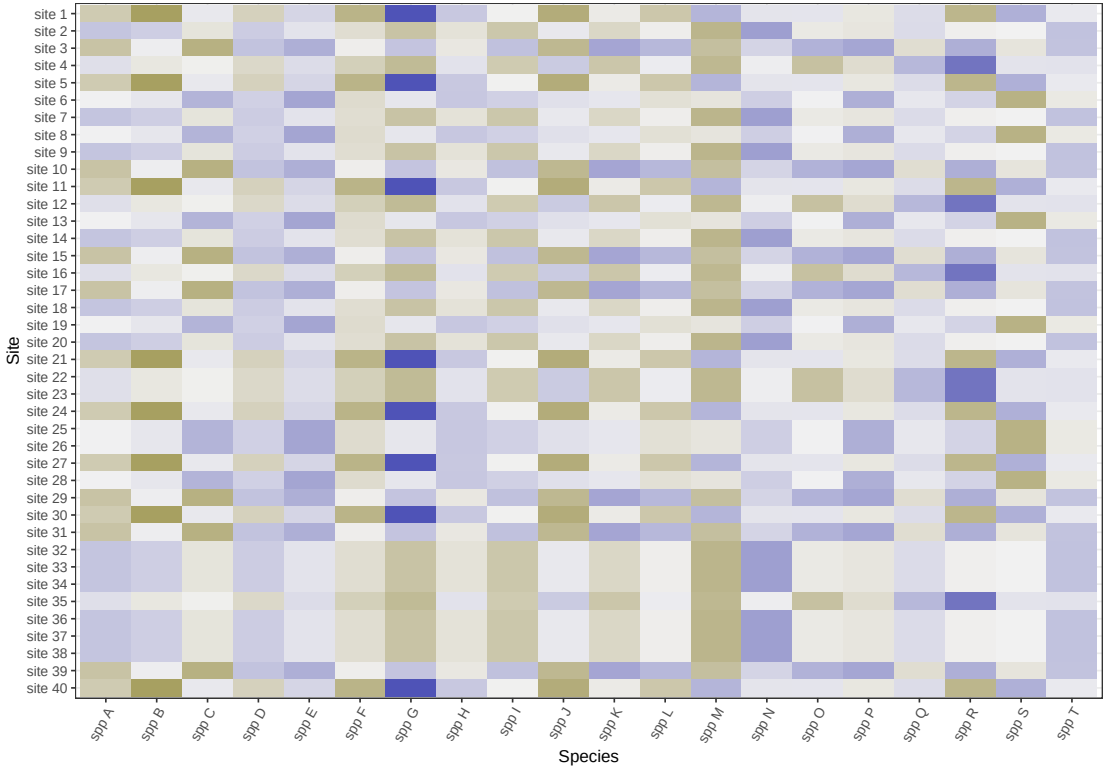
- it estimates a unique "interaction" for every combination of sites and species;
- the number of parameters is basically the same as the number of observations.

What to do about δ_{ij}?



Simplifying the δ_{ij}'s

The above may be overly complex for many multivariate abundance datasets however, as in practice there may be **row patterns**



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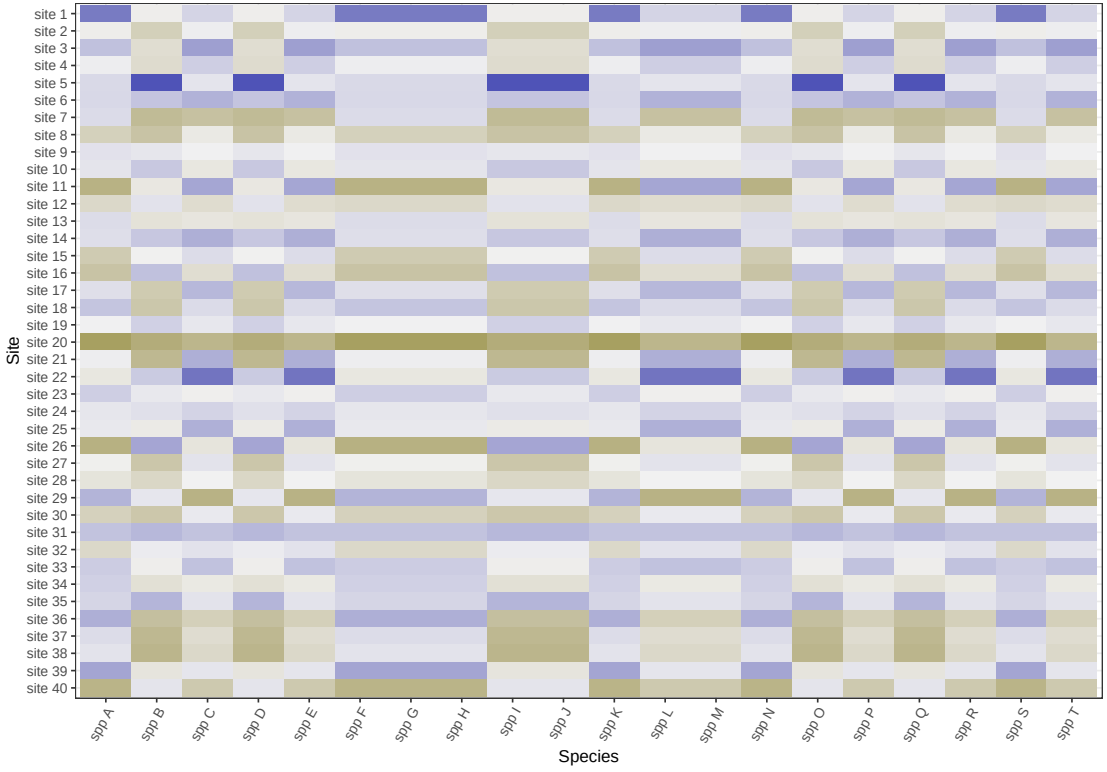

Simplifying the δ_{ij}'s

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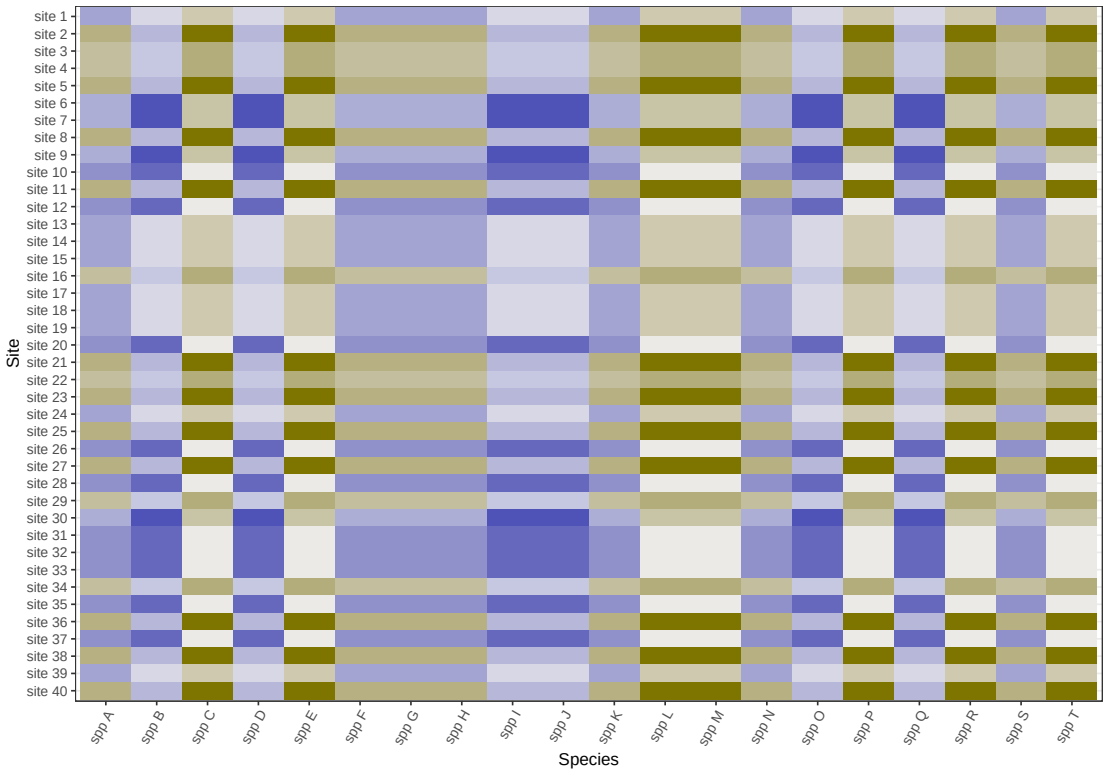

Clustering the δ_{ij}'s

The above motivates a way of simplifying the saturated model, namely by clustering the interaction terms δ_{ij}'s based on the row and/or column indices:

- **Row/site clustering**: δ_{rj} where $r = 1, \ldots, R < n$;
- **Column/species clustering**: δ_{ic} where $c = 1, \ldots, C < m$;
- **Biclustering**: δ_{rc}.

Row pattern detection model

Assume the patterns of site relative abundance can be in clustered into one of $R < n$ groups:

$$\eta_{ij} = \beta_{0j} + \alpha_i + \delta_{rj}.$$

Intuition: The assemblage is comprised of only a small number of "species profiles". Two sites i and i' in the same species profile have the same relative abundance and only differ in their α_i's e.g., site total abundance, sampling effort, and so on.

Column pattern detection model

Assume the species can be in clustered into one of $C < m$ groups:

$$\eta_{ij} = \beta_{0j} + \alpha_i + \delta_{ic}.$$

Intuition: The species in the assemblage can be classified into a small number of "archetypes" (or guilds?). Two species j and j' in the same guild have the same distribution across sites, and only differ in their β_{0j}'s e.g., overall prevalence.

Biclustering pattern detection model

Assume the species can be in clustered into one of $C < m$ groups:

$$\eta_{ij} = \beta_{0j} + \alpha_i + \delta_{ic}.$$

Intuition: Combine the ideas of species profiles and guilds.

We will talk briefly about the stats behind these models a bit later. . .

Pattern detection models

Like model-based unconstrained ordination, clustering/pattern detection offer a parsimonious way of understanding the species community. But their goals are different:

- Is your goal a low-dimensional representation of how species composition varies over sites, or wanting to find sites with the same/similar species composition?
- Is your goal a low-dimensional representation of which species primarily drive composition across sites, or wanting to find species with the same/similar distributions?

Can read more a bit more about the differing characteristics of ordination versus clustering in Section 10.1 of Legendre and Legendre, 2012 and Section 3.1 of McGarigal et al., 2000.

Pattern detection models

Note environmental covariates and species traits are not utilized in the PD models discussed so far, analogous to model-based unconstrained ordination. We will discuss more about how to incorporate covariates later.

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What about doing both unconstrained ordination and clustering simultaneously?

You can! We won't talk about it in this lecture, but see Hui, 2017 and Stratton et al., 2024 for some ideas.

Pattern detection models – A bit of statistics

To fit something like the row pattern detection model with $R < n$,

$$\eta_{ij} = \beta_{0j} + \alpha_i + \delta_{rj},$$

we can assume:

1. The prior probability for site i to belong to cluster r is given by π_r (to be estimated);
2. The species are independent of each conditional on belong to the same cluster (big assumption!);
3. Species responses y_{ij} come from some distribution with mean given by $\mu_{ij} = g^{-1}(\eta_{ij})$ plus some species-specific dispersion/nuisance parameters as required

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Things to think about:

- What distribution to assume for y_{ij} e.g., presence-absence, counts, biomass, percent cover etc. . .
- What to choose for R and/or C
- Do you need the row effects α_i? Depends on the interpretation. . .

Pattern detection models

Brief live demonstration using the `R` package clustglm and the `aviurba` dataset in ade4.

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Brief live demonstration using the `R` package clustglm and the `aviurba` dataset in ade4.

- Can use AICs and BICs to choose the number of row/column clusters. Can also use it to decide what kind of PD model you want, but really that should be governed by the question of interest!
- Model diagnostics are possible like with other models introduced previously;
- Profile plots as a way of visualizing the uncovered cluster profiles i.e., species profiles, archetypes of guilds;
- The more mathematically-curious can visit Pledger and Arnold, 2014

The state of play with `clustglm`

Unfortunately, clustglm is not actively maintained, and has lots of limitations:

- Handles only a very limited number of response types;
- Standard errors are not done properly;
- Slow;
- Was an attempt to, but at the moment does not really work with replace distance-based clustering

The state of play with `clustglm`

Clustering incorporating covariates