Models for the Analysis of Discrete Compositional Data

An Application of Random Effects Graphical Models

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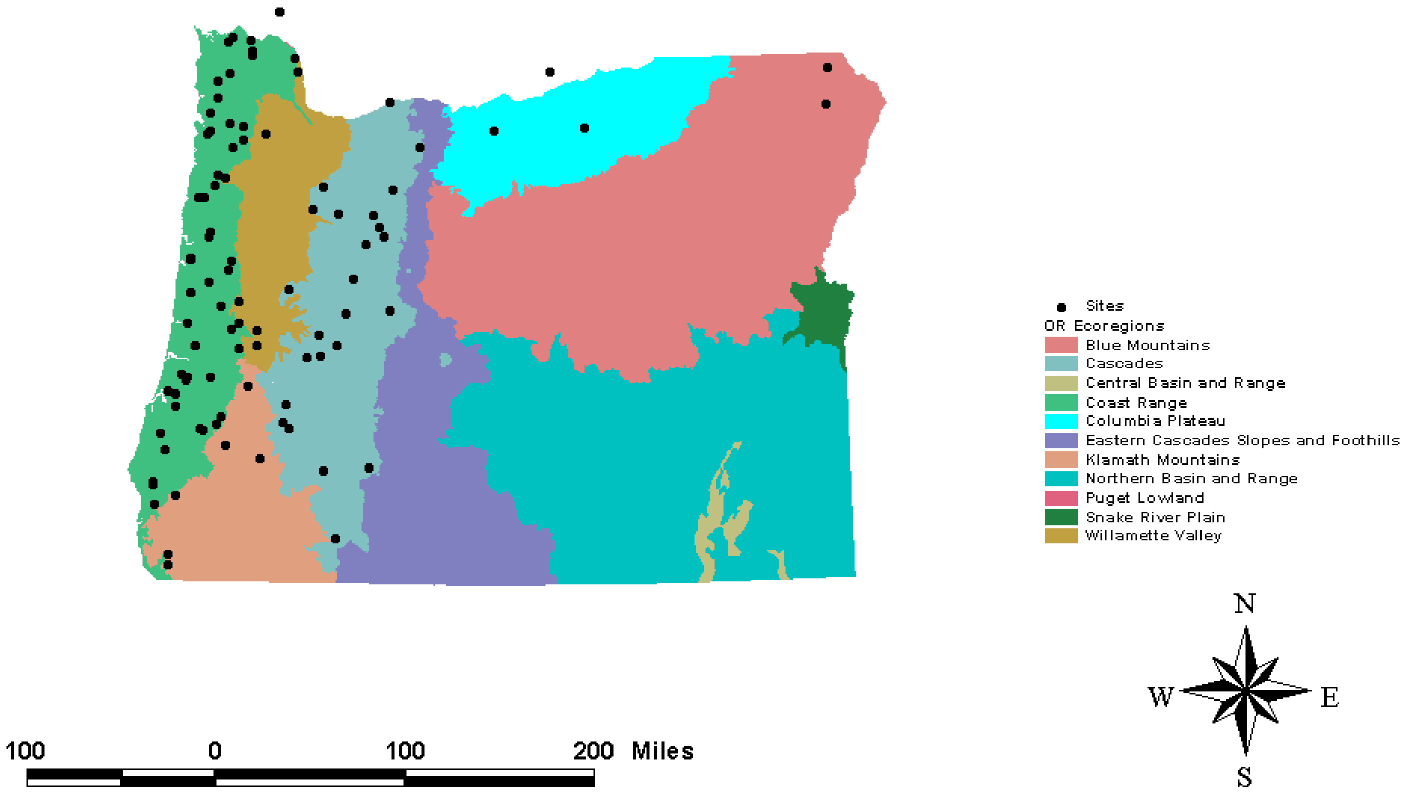
Motivating Problem

- Various stream sites in Oregon were visited.
  - Benthic invertebrates collected at each site and cross categorized according to several traits (e.g. feeding type, body shape,…)
  - Environmental variables are also measured at each site (e.g. precipitation, % woody material in substrate, …)
- Total number in each category is not interesting.
- Relative proportions are more informative.
- How can we determine if collected environmental variables affect the relative proportions (which ones)?

1994-1996 REMAP and 1997 EMAP Sites in Oregon



Outline

- Motivation
  - Compositional data
  - Probability models
- Overview of graphical chain models
  - Description
  - Markov properties
- Discrete Response models
  - Modeling individual probabilities
  - Random effects DR models
- Analysis of discrete compositional data
- Conclusions and Future Research

Discrete Compositions and Probability Models

- Compositional data are multivariate observations $Z = (Z_1,\ldots,Z_D)$ subject to the constraints that $\Sigma_i Z_i = 1$ and $Z_i \geq 0$. (measures relative size of each category)

- Compositional data are usually modeled with the *Logistic-Normal* distribution (Aitchison 1986).
  - Scale and location parameters provide a large amount of flexibility
  - LN model defined for positive compositions only

- Problem: With discrete counts one has a non-trivial probability of observing 0 individuals in a particular category

Existing Compositional Data Models

- Billhiemer and Guttorp (2001) proposed using a multinomial state-space model for a single composition,

$$\left(Y_{i1},\ldots,Y_{iD}\right) \sim \text{Multinomial}\left(N_i, Z_{i1},\ldots,Z_{iD}\right)$$

$$\left(Z_{i1},\ldots,Z_{iD}\right) \sim \text{LN}\left(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\right),$$

  where Y_{ij} is the number of individuals belonging to category $j = 1,\ldots,D$ at site i = 1,…,S.

  Limitations:

  - Models proportions of a single categorical variable.
  - Abstract interpretation of included covariate effects

Graphical Models

- Graph model theory (see Lauritzen 1996) has been used for many years to
  - model cell probabilities for high dimensional contingency tables
  - determine dependence relationships among categorical and continuous variables

  Limitation:
  - Graphical models are designed for a single sample (or site in the case of the Oregon stream data). Compositional data may arise at many sites

New Improvements for Compositional Data Models

- The BG state-space model can be generalized by the application of graphical model theory.
  - Generalized models can be applied to cross-classified compositions
  - Simple interpretation of covariate effects as dependence in probability

- Conversely, the class of graphical models can be expanded to include models for multiple site sampling schemes

Graphical Chain Models

- Mathematical graphs are used to illustrate complex dependence relationships in a multivariate distribution

- A random vector is represented as a set of vertices, V.

  Ex. $V = \{\alpha$ = Precipitation, β = Stream velocity,

  γ = Amount of large rock in substrate$\}$

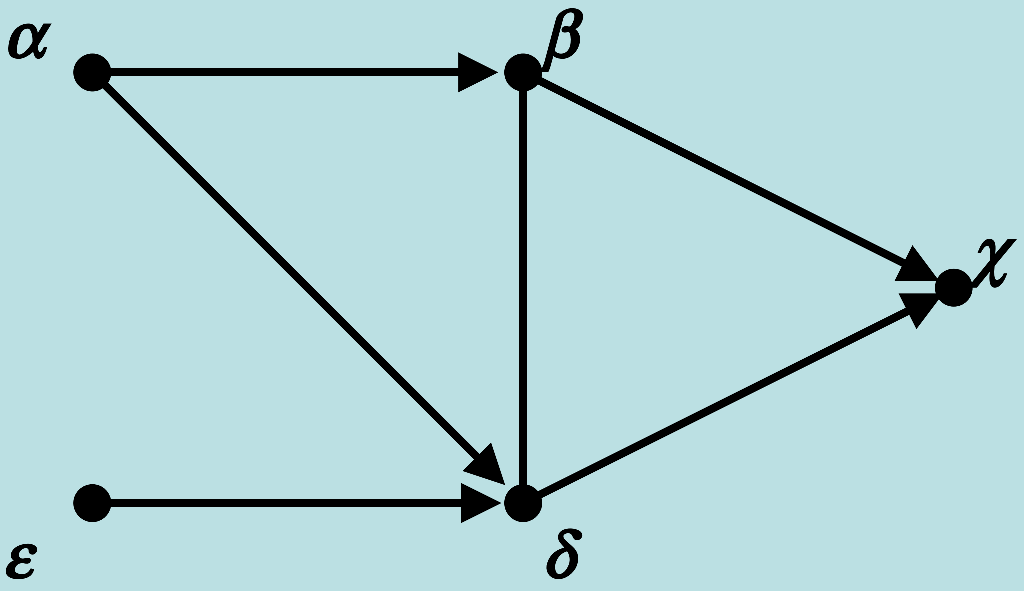
- Pairs of vertices are connected by directed or undirected edges depending on the nature of each pair's association

  Relationships are determined by a "causal" ordering

  If $\alpha < \beta$ in causal ordering, then $\alpha \rightarrow \beta$

  If $\beta = \gamma$, then $\beta - \gamma$

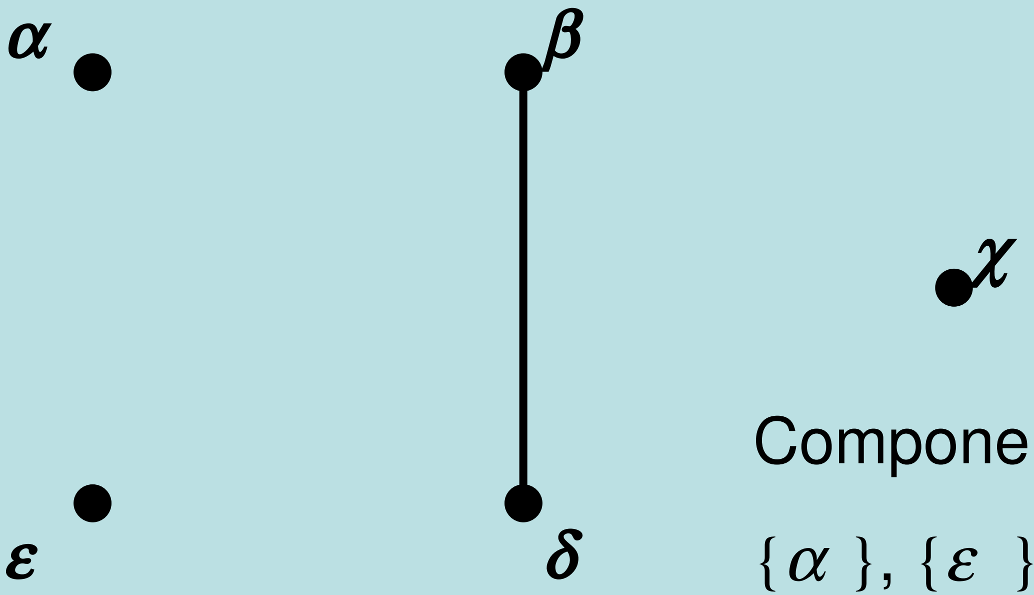
Example Chain Graph



Concepts

- **Causal ordering** $(\alpha , \varepsilon) < \beta = \delta < \chi$
- **Chain components** Sets of vertices whose elements are connected by undirected edges only

Example Chain Graph



Components

$\{\alpha\}, \{\varepsilon\}, \{\beta, \delta\}, \{\chi\}$

<u>Concepts</u>

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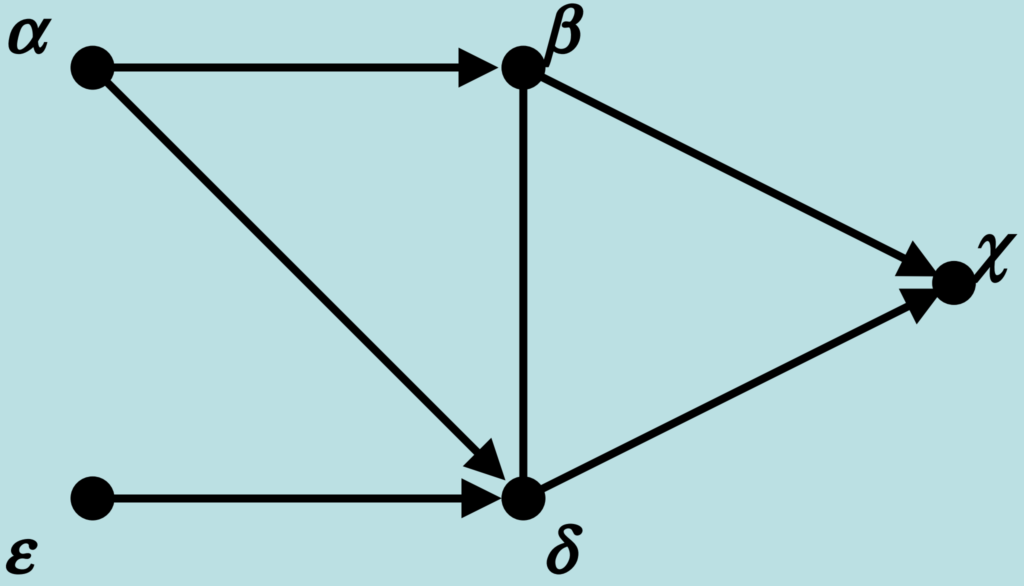
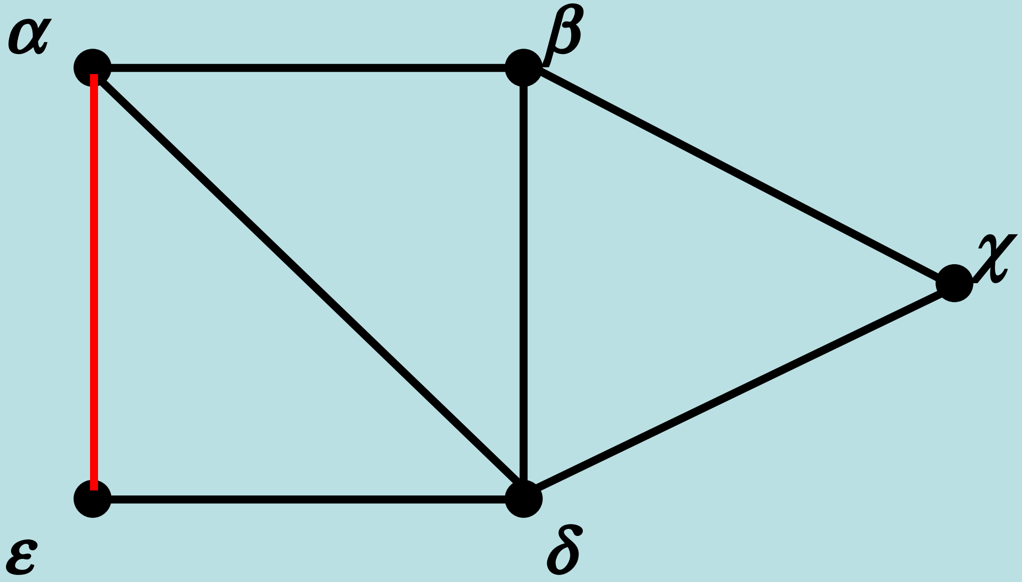


Concepts

- **Moral Graph** (G^m)**:** Graph induced by making all edges undirected and connecting parents of chain components

  Basis for determining dependence relationships between variables

Example Chain Graph



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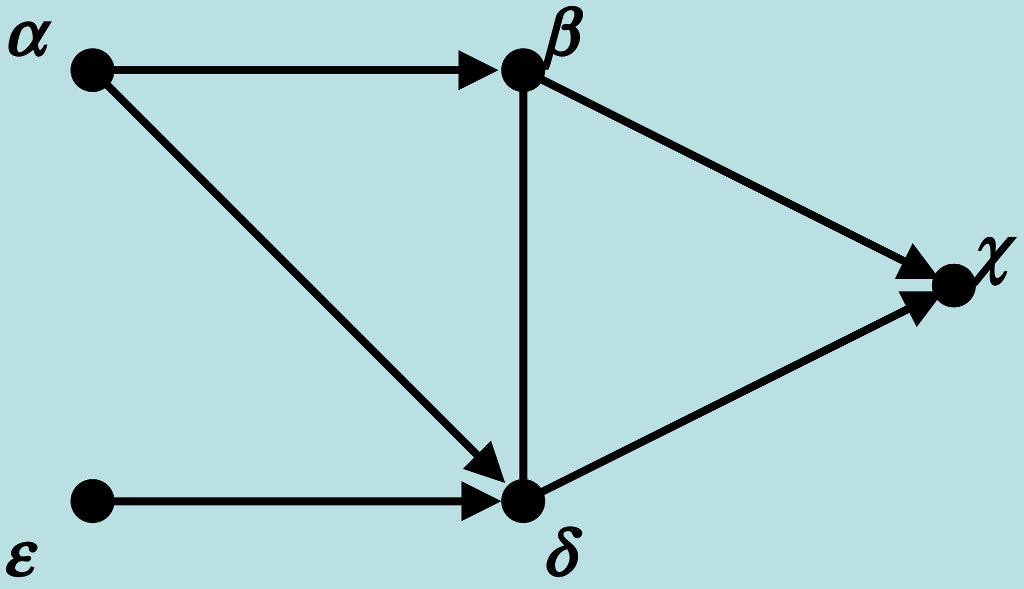


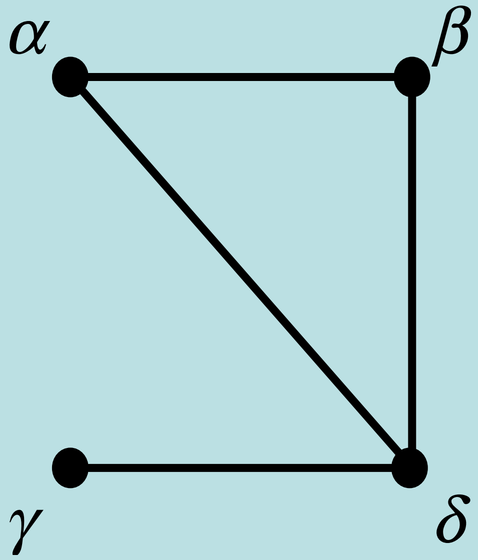
Concepts

- **Distribution models**: Joint distribution modeled as a product of conditional distributions.

  Ex. $f(\alpha , \beta , \delta , \gamma , \varepsilon) = f(\alpha) f(\varepsilon) f(\beta , \delta \mid \alpha , \varepsilon) f(\chi \mid \alpha , \varepsilon , \beta , \delta)$

Markov Properties of Undirected Graphs

- Let P denote a probability measure on the product space $X = X_\alpha \times X_\beta \times X_\gamma \times X_\delta$, and $V = \{\alpha, \beta, \gamma, \delta\}$



- Markov properties (w.r.t. P).
  - **Pairwise** Markovian $\alpha \perp \gamma \mid V \setminus \{\alpha, \gamma\}$.
  - **Local** Markovian $\beta \perp \gamma \mid (\alpha, \delta)$
  - **Global** Markovian $(\alpha, \beta) \perp \gamma \mid \delta$

Markov Properties and Factorization

- Markov relationships are related to the factorization of the joint density

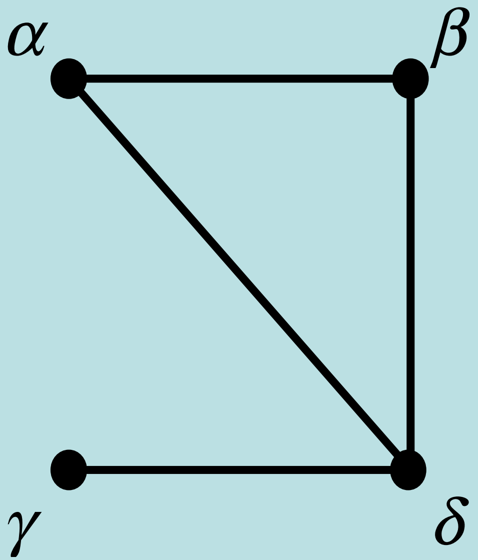
- **Theorem (Hammersley-Clifford)**.
  - G is an undirected graph
  - P has a positive and continuous density f with respect to a product measure μ .

  All three Markov properties are equivalent if and only if f factors as

$$f(\mathbf{x}) = \prod_{C \text{ complete}} h_C(\mathbf{x}_C)$$

- A **complete** set is one where all vertices in the set are connected to one another.

Factorization Example



$$
\begin{aligned}
f(\alpha,\beta,\delta,\gamma) &= f(\alpha \mid \beta,\delta,\gamma)\; f(\beta \mid \delta,\gamma)\; f(\delta \mid \gamma)\; f(\gamma) \\
&= f(\alpha \mid \beta,\delta)\; f(\beta \mid \delta)\; f(\delta \mid \gamma)\; f(\gamma) \\
&= h_{\{\alpha,\beta,\delta\}}(\alpha,\beta,\delta) \times h_{\{\delta,\gamma\}}(\delta,\gamma)
\end{aligned}
$$

Discrete Regression (DR) Chain Model

- **Response variables** (terminal chain component)
  - Set Δ of discrete categorical variables
  - Notation: $\mathbf{y}$ is a specific cell
- **Explanatory variables**
  - Set $\Gamma = \Gamma_D \cup \Gamma_C$ of categorical (Γ_D) or continuous (Γ_C) variables
  - Notation: $\mathbf{x}$ refers to a specific explanatory observation
- DR Joint distribution: $f(\mathbf{x})\, p(\mathbf{y}|\mathbf{x})$
- DR distribution is an example of a mixed variable graphical model (Lauritzen and Wermuth, 1989)

Discrete Regression Model (Response)

Model for conditional response:

$$p(\mathbf{y} \mid \mathbf{x}) = \exp \overset{\rightarrow}{} \alpha_{\Delta}(\mathbf{x}) + \underset{d\,\text{�}\,\Delta}{\text{�}} \underset{c\,\text{�}\,\Gamma}{\text{�}} \beta_{dc} \underset{\gamma \rightarrow c}{\longrightarrow} x_{\gamma}$$

$$+ \underset{d\,\text{�}\,\Delta}{\text{�}} \underset{c\,\text{�}\,\Gamma_D}{\text{�}} \underset{\gamma\,\text{�}\,\Gamma_C}{\text{�}} \overset{m}{\underset{j=2}{\text{�}}} \omega_{dc\gamma j} x_{\gamma}^{j} \overset{\rightarrow}{\text{�}}$$

- The function $\alpha_{\Delta}(\mathbf{x})$ is a normalizing constant w.r.t. $\mathbf{y}|\mathbf{x}$
- The parameters β_{dc} and $\omega_{dc\gamma\ j}$ are interaction effects that depend on $\mathbf{y}$ through the levels of the variables in d only.
- Certain interaction parameters are set to zero for identifiability of the model (analogous to interaction terms in ANOVA models)

Discrete Regression Model (Predictors)

- Model for explanatory variables (CG distribution):

$$f(\mathbf{x}) = \exp\left[\sum_{c\subseteq\Gamma_D}\lambda_c + \sum_{c\subseteq\Gamma_D}\sum_{\gamma\in\Gamma_C}\eta_{c\gamma}x_\gamma - \frac{1}{2}\sum_{c\subseteq\Gamma_D}\sum_{\mu,\gamma\in\Gamma_C}\psi_{c\mu\gamma}x_\mu x_\gamma\right]$$

- Again, interactions depend on $\mathbf{x}_{\Gamma_c}$ through the levels of the variables in the set c only, and identifiability constraints are imposed.

Markov Properties of Graphical Chain Models

- Frydenburg (1990) extended Hammersley-Clifford theorem for application to chain models
  - Markov properties are based on moral graphs constructed from “past” and “present” chain components (relative to the set of vertices in question).
  - For a distribution P with positive and continuous density f, P is Markovian if and only if f factors as

$$f(\mathbf{x}) = \prod_{\tau \in T} \prod_{C \in C_\tau} h_{C,\tau}(\mathbf{x}_{C,\tau})$$

where C_τ represents a class of complete sets in $(G_{cl(\tau)})^m$ for all chain components.

Markov Properties of the DR Model

Proposition. A DR distribution is Markovian with respect to a chain graph G, with terminal chain component Δ and initial component Γ, if and only if

- $\boldsymbol{\beta}_{dc} \equiv \mathbf{0}$ unless d is complete and $c \subseteq pa(\delta)$ for every δ in d,
- $\boldsymbol{\omega}_{dc\gamma j} \equiv \mathbf{0}$ unless d is complete and $\{\gamma\} \cup c \subseteq pa(\delta)$ for every δ in d,
- $\boldsymbol{\lambda}_{c} \equiv \boldsymbol{\eta}_{c\gamma} \equiv \boldsymbol{\psi}_{c\mu\gamma} \equiv \mathbf{0}$ unless the sets corresponding to the subscripts are complete in G_Γ

Markov Properties of the DR Distribution

Sketch of Proof:

- LW prove conditions concerning the $\boldsymbol{\lambda}$, $\boldsymbol{\eta}$, and $\boldsymbol{\psi}$ parameters for the CG distribution, therefore, we only need look at the $\boldsymbol{\beta}$ and $\boldsymbol{\omega}$ interactions.

- If the $\boldsymbol{\beta}$ and $\boldsymbol{\omega}$ parameters are $\mathbf{0}$ for the specified sets then it is easy to see that the density factorizes on $(G_{cl(\tau\ )})^m$

- A modified version of the proof of the Hammersley-Clifford Theorem shows that if $p(\mathbf{y}|\mathbf{x})$ separates into complete factors, then, the corresponding $\boldsymbol{\beta}$ and $\boldsymbol{\omega}$ vectors for non-complete sets must be $\mathbf{0}$.

Random Effects for DR Models

- Sampling of individuals occurs at many different random sites, $i = 1,\ldots,S,$ where covariates are measured only once per site
- Hierarchical model:

$$p(\mathbf{y}_i \mid \mathbf{x}_i) = \exp \overset{\rightarrow}{\alpha}_\Delta(\mathbf{x}_i, \boldsymbol{\varepsilon}_i) + \underset{d \text{�} \Delta}{\text{�}} \underset{c \text{�} \Gamma}{\text{�}} \beta_{dc} \underset{\gamma \rightarrow c}{\longrightarrow} x_{i\gamma}$$

$$+ \underset{d \text{�} \Delta}{\text{�}} \underset{c \text{�} \Gamma_D}{\text{�}} \underset{\gamma \text{�} \Gamma_C}{\text{�}} \overset{m}{\underset{j=2}{\text{�}}} \omega_{dc\gamma j} x_{i\gamma}^{j} + \underset{d \text{�} \Delta}{\text{�}} \boldsymbol{\varepsilon}_{id} \text{�}$$

$$\boldsymbol{\varepsilon}_{id} \sim \begin{cases} \mathbf{0} & \text{if } d \text{ is not complete in } G \\ MVN\left(\mathbf{0}, \mathbf{T}_d^{-1}\right) & \text{if } d \text{ is complete in } G \end{cases}$$

- Markov properties still hold over the integrated likelihood in some cases.

Graphical Models for Discrete Compositions

- For a set Δ of categorical responses
  - Let D be the number of cross-classified cells
  - Y_{ij} = Number of observations in cell $j=1,\ldots,D$ at site $i=1,\ldots,S$

- **Likelihood**

$$(Y_{i1},\ldots,Y_{iD}) \mid X_\Gamma = x_\Gamma \sim \text{Multinomial}(N_i; p_{i1},\ldots,p_{iD}),$$

where p_{ij} is given by the DR random effects model

- **Covariate distribution**

$$X_\Gamma \sim CG(\boldsymbol{\lambda}, \boldsymbol{\eta}, \boldsymbol{\psi})$$

Parameter Estimation

- A Gibbs sampling approach is used for parameter estimation

- Hierarchical centering
  - Produces Gibbs samplers which converge to the posterior distributions faster
  - Most parameters have standard full conditionals if given conditional conjugate distributions.

- Independent priors imply that covariate and response models can be analyzed with separate MCMC procedures.

Stream Invertebrate Functional Groups

- 94 stream sites in Oregon were visited in an EPA REMAP study
- Response composition: Stream invertebrates were collected at each site and placed into 1 of 6 categories of functional feeding type

1. Collector-gatherer
2. Collector-filterer
3. Scraper
4. Engulfing predator
5. Shredder
6. Other (mostly, benthic herbivores)

Stream Covariates

- Environmental covariates: values were measured at each site for the following covariates

1. % Substrate composed of woody material
2. Alkalinity
3. Watershed area
4. Minimum basin elevation
5. Mean basin precipitation
6. % Barren land in watershed
7. Number of stream road crossings

Stream Invertebrate Model

- Composition Graphical Model:

$$\log p_{ij} = \alpha_{\Delta}\left(\mathbf{x}_i\right) + \beta_{0,j} + \sum_{\gamma=1}^{7}\beta_{\gamma,j}\left(x_{i\gamma} - \bar{x}_{\gamma}\right)s_{\gamma}^{-2} + \varepsilon_{ij}$$

$$\boldsymbol{\varepsilon}_i \sim MVN\left(\mathbf{0},\mathbf{T}_{\Delta}^{-1}\right)$$

and

$$\mathbf{x}_i\boldsymbol{\mu}\,\tilde{}\,\boldsymbol{\Psi}MVN\left(\quad,\quad{}_{\Gamma}^{-1}\right)$$

- Prior distributions

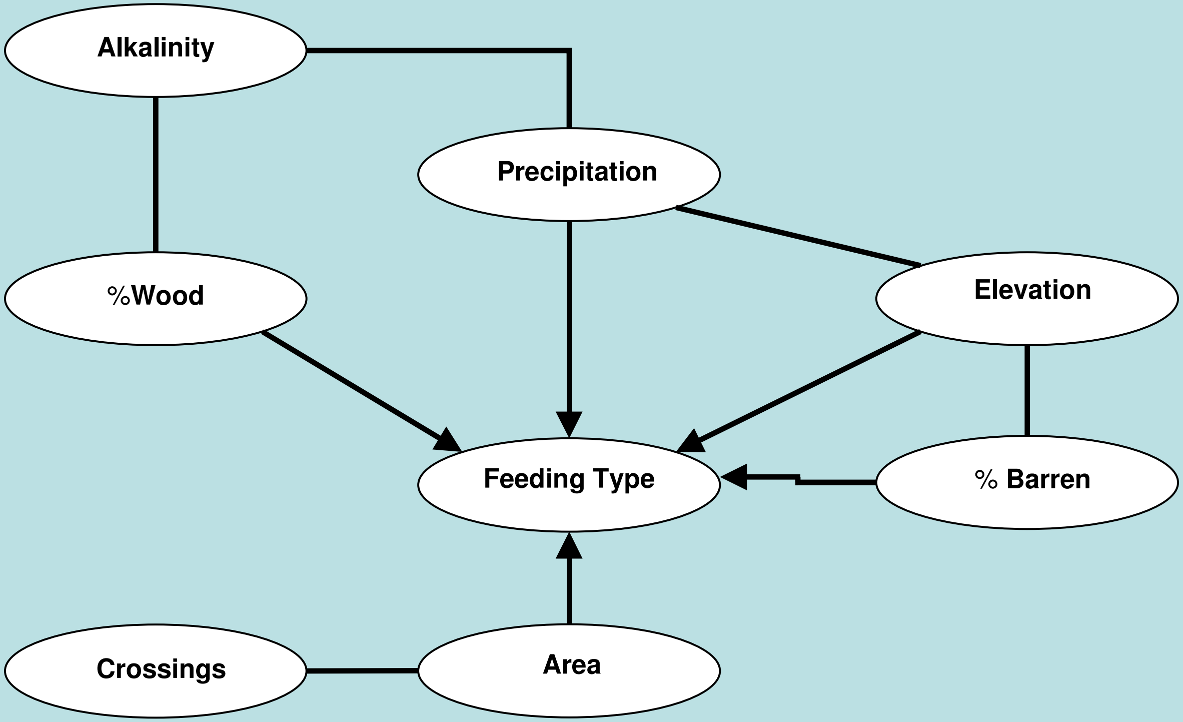
$$\beta_{\gamma,j}\left(x_{\Delta}\right) \sim \text{iid } N\left(0,\boldsymbol{\sigma}_{\gamma,j}^{2}\right),;\ldots,\qquad = 0 \qquad 7$$

$$\mathbf{T}_{\Delta} \sim \text{Wish}\left(6,\mathbf{R}\right)$$

$$\boldsymbol{\Psi}_{\Gamma} \sim \text{Wish}\left(7,\mathbf{R}\right)$$

Stream Invertebrate Functional Groups

Posterior suggested chain graph



Edge exclusion determined from 95% HPD intervals for $\boldsymbol{\beta}$ parameters and off-diagonal elements of $\boldsymbol{\psi}_{\Gamma}$.

Comments and Conclusions

- Using *Discrete Response* model with random effects, the BG model can be generalized
  - Relationships evaluated though a graphical model
  - Multiway compositions can be analyzed with specified dependence structure between cells
  - MVN random effects imply that the cell probabilities have a constrained LN distribution

- DR models also extend the capabilities of graphical models
  - Data can be analyzed from many multiple sites
  - Over dispersion in cell counts can be added

Future Work

- Model determination under a Bayesian framework
  - Models involve regression coefficients as well as many random effects

- Prediction of spatially correlated compositions over a continuous domain
  - Desirable to have a closed form predictor such as a kriging type predictor

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