Bayesian nonparametric dependent model for the study of diversity for species data

Journées jeunes probabilistes et statisticiens

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Project’s bio

Authors

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Status

Chapter of my PhD thesis. Two submitted manuscripts Arbel et al. (2013b) and Arbel et al. (2013a).
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1. Ecological data and diversity
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3. Applications
Series of measurements at different places around Casey Station, permanent base in Antarctica
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At each site: pollution level (total petroleum hydrocarbon (TPH) in mg/kg of soil), and abundance of microbes.

Site 9
Context in ecology

- Series of measurements at different places around Casey Station, permanent base in Antarctica
- At each site: pollution level (total petroleum hydrocarbon (TPH) in mg/kg of soil), and abundance of microbes.
Series of measurements at different places around Casey Station, permanent base in Antarctica.

At each site: pollution level (total petroleum hydrocarbon (TPH) in mg/kg of soil), and abundance of microbes.

Goals: Assess the impact of a pollutant on the soil composition / biodiversity, e.g. compute effective concentration values at level \( x\% \), \( EC_x \).
Soil samples were collected from a range of sites across a fuel contamination gradient at Australia's Casey Station in East Antarctica (110°32' E, 66°17' S). The data comprise counts of a large number (of the order of 1800) of microbial taxa, referred to as OTUs (operational taxonomic units; see Schloss et al., 2009), collected at 60 sites, across a range of hydrocarbon contamination (Siciliano et al., 2014). Genomic DNA extracted from samples was sequenced on a 454 Titanium FLX+ instrument (Roche, Branford, CT, USA) at the Research and Testing facility (Lubbock, TX, USA) using the universal bacterial primers 28F and 519R (Dowd et al., 2008). Pyrosequencing data were processed using the mothur software package (Schloss et al., 2009). This involved removal of short reads (<150bp), excessive homoploymeric reads (>8bp repeats) and denoising with AmpliconNoise (min/max flows 360/720) (Quince et al., 2011). Preclustering at 1% was performed to negate the per base error rate of the 454 platforms. Seed sequences were then aligned to the SILVA 16S rRNA gene database alignment using a NAST alignment algorithm (Pruesse et al., 2007; Caporaso et al., 2010). Reads were then chimaera-checked (Edgar et al., 2011) and clustered into OTUs at 96% sequence similarity to achieve approximately species-level units as derived by Kim et al. (2011). Seed sequences from each OTU were then classified using a Naive Bayesian classifier in mothur against the Greengenes 16S reference database (October 2012 version, see McDonald et al., 2012).
Diversity indices

Shannon index

\[ H_{\text{Shan}}(p) = - \sum p_j \log p_j \]

Simpson index

\[ H_{\text{Simp}}(p) = 1 - \sum p_j^2 \]

Good index

\[ H_{\text{Good},\alpha,\beta}(p) = - \sum p_j^\alpha \log^\beta p_j \]
Diversity indices of microbial data

- Shannon $(\alpha = 1 \; \beta = 1)$
- Simpson $(\alpha = 2 \; \beta = 0)$
- Good $(\alpha = 0.1 \; \beta = 2)$

J. Arbel et al. Dependent model for species data
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1. Ecological data and diversity

2. Dependent model for species data and diversity

3. Applications
Model the distribution of microbes in the soil:

*The nth observation at site i is species j with probability \( p_j(X_i) \)*
Model the distribution of microbes in the soil:

The $n$th observation at site $i$ is species $j$ with probability $p_j(X_i)$

For every site $i$

$$Y_{n,i} | p(X_i), X_i \overset{\text{ind}}{\sim} \sum_{j=1}^{\infty} p_j(X_i)\delta_j$$
Model

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For every site \( i \)

\[
Y_{n,i} \mid p(X_i), X_i \overset{\text{ind}}{\sim} \sum_{j=1}^{\infty} p_j(X_i) \delta_j
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Parameters: \( p = (p(X_1), \ldots, p(X_I)) = (p_j(X_i))_{i,j} \)
Model

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- Holmes et al. (2012): Dirichlet Multinomial Mixtures: Generative Models for Microbial Metagenomics (PloS one)
Model the distribution of microbes in the soil:

*The nth observation at site i is species j with probability $p_j(X_i)$*

For every site $i$

$$\begin{align*}
Y_{n,i} \mid p(X_i), X_i \sim & \text{ind} \sum_{j=1}^{\infty} p_j(X_i)\delta_j \\
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\end{align*}$$

- Holmes et al. (2012): Dirichlet Multinomial Mixtures: Generative Models for Microbial Metagenomics (PloS one)
- Lijoi et al. (2007): Bayesian nonparametric estimation of the probability of discovering new species (Biometrika)
Randomizing the weights $p_j(X_i)$
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- Use the distribution of the weights in a Dirichlet process, obtained by a **stick-breaking** construction.
Randomizing the weights $p_j(X_i)$

- Use the distribution of the weights in a Dirichlet process, obtained by a stick-breaking construction.

**Stick-breaking construction**

$$p_1 = V_1, \quad p_j = V_j \prod_{l<j} (1 - V_l),$$

with $V_j \sim \text{Beta}(1, M)$. 

![Site 9](image-url)
Randomizing the weights $p_j(X_i)$

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**Stick-breaking construction**

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![Site 9](image1)

![M=6](image2)
Randomizing the weights $p_j(X_i)$

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**Stick-breaking construction**

$$p_1 = V_1, \quad p_j = V_j \prod_{l<j} (1 - V_l),$$

with $V_j \overset{iid}{\sim} \text{Beta}(1, M)$.

It is denoted $\mathbf{p} \sim \text{GEM}(M)$. 

Site 9

M=6

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On convergence rates

$\sum_{j=N+1}^{\infty} p_j$ or partial product or partial sum

$\prod_{j=1}^{N} (1 - V_j) = \sum_{j=1}^{N} - \log(1 - V_j)$

which is shown to be $\text{Ga}(N, M)$ when $V_j \text{iid} \sim \text{Beta}(1, M)$

Trickier when $V_j \text{ind} \sim \text{Beta}(a, b + c_j)$, $a \neq 1$

Need a central limit theorem for $\sum_{j=1}^{N} - \log(1 - V_j)$

Limit distribution seems to be Gumbel...
On convergence rates

Need control in probability tail sums

\[ \sum_{j=N+1}^{\infty} p_j \]
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\sum_{j=1}^{N} - \log(1 - V_j)
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Limit distribution seems to be \text{Gumbel}...
On convergence rates

\[
\left\{
\begin{align*}
&\text{Need control in probability tail sums} \\
&\sum_{j=N+1}^{\infty} p_j
\\
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&\prod_{j=1}^{N}(1 - V_j)
\\
&\sum_{j=1}^{N} - \log(1 - V_j)
\\
&\text{which is shown to be Ga}(N, M) \text{ when} \\
&V_j \overset{\text{iid}}{\sim} \text{Beta}(1, M)
\end{align*}
\right.
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\[V_j \overset{\text{ind}}{\sim} \text{Beta}(a, b + cj), \ a \neq 1\]

Need a central limit theorem for

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\sum_{j=1}^{N} - \log(1 - V_j)
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Limit distribution seems to be Gumbel...
Construction of the prior

- With the strick-breaking relation, a Dep - GEM prior is obtained from a Beta process.
Construction of the prior

- With the strick-breaking relation, a Dep – GEM prior is obtained from a **Beta process**.
- Such a dependent Beta process is obtained by a transformed **Gaussian process** (Rasmussen and Williams, 2006)

→ Denote by $Z \sim N(0, \sigma^2)$ a Gaussian random variable, by $\Phi_{\sigma Z}$ its CDF and by $F_M$ a Beta(1, $M$) CDF. Then:

$$\Phi_{\sigma Z}(Z) \sim \text{Unif}(0, 1) \text{ and } V = F_M^{-1} \circ \Phi_{\sigma Z}(Z) \sim \text{Beta}(1, M),$$
Construction of the prior

- With the strick-breaking relation, a Dep − GEM prior is obtained from a Beta process.
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  → Denote by $Z \sim N(0, \sigma^2)$ a Gaussian random variable, by $\Phi_{\sigma_Z}$ its CDF and by $F_M$ a Beta$(1, M)$ CDF. Then:
    \[
    \Phi_{\sigma_Z}(Z) \sim \text{Unif}(0, 1) \quad \text{and} \quad V = F_M^{-1} \circ \Phi_{\sigma_Z}(Z) \sim \text{Beta}(1, M),
    \]

- Dependence specified by covariance function
    \[
    K(X_i, X_j) = \text{Cov}(Z(X_i), Z(X_j)).
    \]

<table>
<thead>
<tr>
<th>Covariance function</th>
<th>$\tilde{K}_\lambda(X_1, X_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Squared Exponential (SE)</td>
<td>$\exp\left(-\frac{(X_1 - X_2)^2}{2\lambda^2}\right)$</td>
</tr>
<tr>
<td>Ornstein-Uhlenbeck (OU)</td>
<td>$\exp\left(-\frac{</td>
</tr>
<tr>
<td>Rational Quadratic (RQ)</td>
<td>$\left(1 + \frac{(X_1 - X_2)^2}{2\lambda^2}\right)^{-1}$</td>
</tr>
</tbody>
</table>
Graphical model representation for the Dep – GEM model

Covariates

Dep-GEM, $\mathcal{Z}$

Observations

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Dependent model for species data
Algorithm: Metropolis within Gibbs

Algorithm 1 Dep – GEM algorithm (Gibbs)

1: Update $Z$ given $(\sigma_Z, \lambda, M)$
2: Update $\sigma_Z$ given $(Z, \lambda, M)$
3: Update $\lambda$ given $(Z, \sigma_Z, M)$
4: Update $M$ given $(Z, \sigma_Z, \lambda)$
Algorithm: Metropolis within Gibbs

Algorithm 3  Dep – GEM algorithm (Gibbs)

1: Update $Z$ given $(\sigma_Z, \lambda, M)$
2: Update $\sigma_Z$ given $(Z, \lambda, M)$
3: Update $\lambda$ given $(Z, \sigma_Z, M)$
4: Update $M$ given $(Z, \sigma_Z, \lambda)$

Algorithm 4  MH algorithm

1: Given $\theta$, propose $\theta' \sim Q_\theta(\cdot \mid \theta)$
2: Compute $\rho_\theta = \frac{P_\theta(\theta')}{P_\theta(\theta)} \frac{Q_\theta(\theta \mid \theta')}{Q_\theta(\theta' \mid \theta)}$
3: Accept $\theta'$ wp $\min(\rho_\theta, 1)$, otherwise keep $\theta$
Predictive distribution

- Predictive distribution of $Z_*$ obtained by integrating out $Z$ in the conditional distribution according to the posterior distribution $\pi(Z|Y, X)$:

$$\pi(Z_* | X_*, Y) = \int \pi(Z_* | X_*, X, Z) \pi(Z|Y, X) dZ.$$  

- No particular computational burden:

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**Algorithm 5** Predictive distribution simulation

1. Sample $Z$ from the posterior distribution $\pi(Z|Y, X)$
2. Given $Z$, sample $Z_*$ from the conditional distribution $\pi(Z_* | X_*, X, Z)$
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Comparison of the Dep – GEM and indep. GEM models

(a) GEM
Comparison of the Dep – GEM and indep. GEM models

(c) GEM

(d) Dep – GEM
Effective concentration estimation $EC_x$
Effective concentration estimation $EC_x$

(g) Bray-Curtis dissimilarity

(h) Illustration of $EC_x$ estimation

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Future work

- Extension to multiple covariates
  - by using Gaussian random fields instead of Gaussian processes
  - model choice
Future work

- Extension to multiple covariates
  - by using Gaussian random fields instead of Gaussian processes
  - model choice

- Use of finer stick-breaking distributions
  - e.g. Beta($a, b$) or Gibbs-type priors instead of Beta(1, $M$)


