Analysis of multi-species point patterns using multivariate log Gaussian Cox processes

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Based on completed work with Abdollah Jalilian, Yongtao Guan, Jorge Mateu
and
ongoing work with Jeff Coeurjolly and Achmad Choiruddin

Tropical rain forest data

Large Spatio-Temporal point pattern data:

- Locations of high number ($\approx$ 300.000) of trees
- Many ($\approx$ 300) different types of trees
- temporal data: trees observed each 5 years

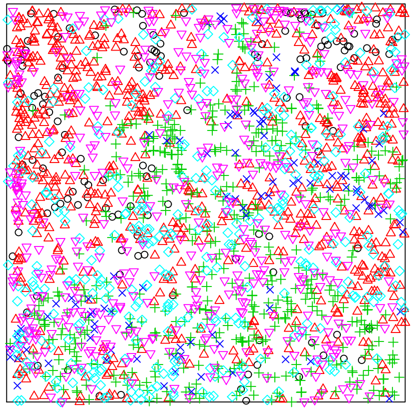
Aim: discuss selected approaches to statistical analysis of multivariate point patterns - and some plans for further development

Outline:

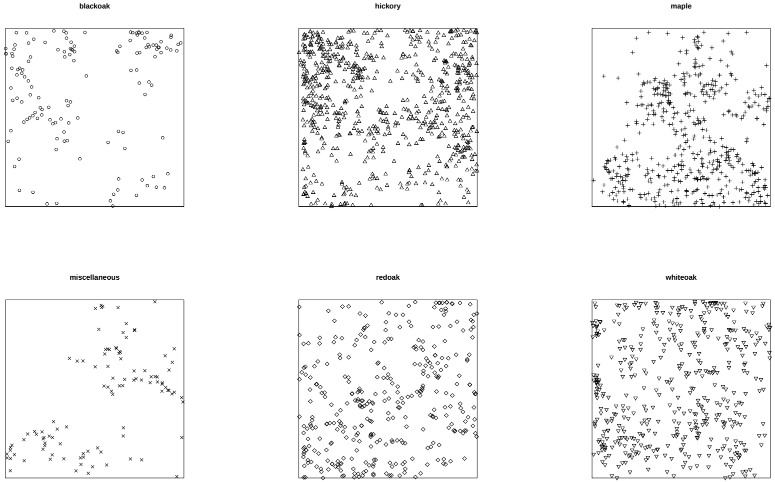
1. bivariate cross summary statistics
2. multivariate log Gaussian Cox process models
3. efficient algorithms and regularization

Example: Lansing Woods data (small)

Locations of 6 types of trees in Lansing Woods, Michigan.



Each type separately:



Objectives of statistical analysis

- Basic: study bivariate dependence for pairs of species
- Advanced: study underlying mechanisms that govern multivariate dependence structure

Both objectives can be addressed using statistics for spatial point processes.

Multivariate point process

Multivariate point process on $\mathbb{R}^2$:

$$\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_p)$$

collection of point processes $\mathbf{X}_i$.

Each $\mathbf{X}_i$ random set of points in $\mathbb{R}^2$ so that $\mathbf{X}_i \cap B$ is finite for any bounded $B \subseteq \mathbb{R}^2$.

Intensity function $\rho_i(\cdot)$:

$$\mathbb{E}\#\mathbf{X}_i \cap B = \int_B \rho_i(u)\mathrm{d}u$$

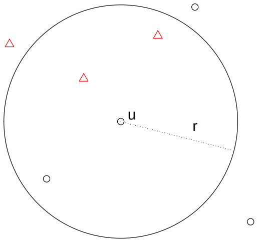
$$\rho_i(u)\mathrm{d}u \approx P(\mathbf{X}_i \text{ has a point at } u)$$

NB: u generic notation for location in $\mathbb{R}^2$.

Cross summary statistics (stationary case)

Stationary case: $\rho_j(u) = \rho_j$ constant.

Consider number of points in $\mathbf{X}_j$ within distance r from $u \in \mathbf{X}_i$.



Cross K_{ij}-function:

$$\rho_j K_{ij}(r) = \mathbb{E}\left[\text{ number of points in } \mathbf{X}_j \text{ within distance } r \text{ from } u \,|u \in \mathbf{X}_i\right]$$

Can be generalized to the case of non-constant intensity $\rho_j(\cdot)$.

Cross pair correlation function

K_{ij} is a cumulative quantity.

Pair correlation function is derivative:

$$g_{ij}(r) = \frac{K'_{ij}(r)}{2\pi r}$$

Infinitesimal interpretation:

$$g_{ij}(\|u - v\|) \approx \frac{P(\mathbf{X}_j \text{ has point at } v \,|\, \mathbf{X}_i \text{ has point at } u)}{P(\mathbf{X}_j \text{ has point at } v)}$$

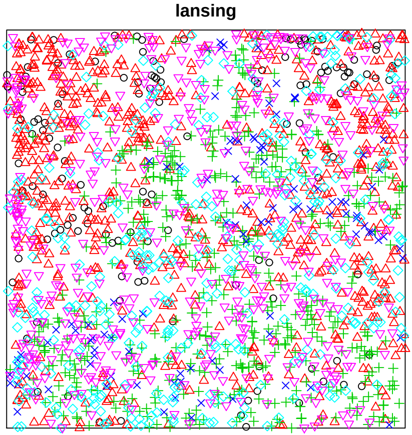
If $\mathbf{X}_i$ and $\mathbf{X}_j$ independent then

$$P(\mathbf{X}_j \text{ has point at } v \,|\, \mathbf{X}_i \text{ has point at } u) = P(\mathbf{X}_j \text{ has point at } v)$$
$$\Rightarrow g_{ij}(\cdot) = 1$$

$g_{ij}(\cdot) = 1 \Rightarrow \mathbf{X}_i$ and $\mathbf{X}_j$ uncorrelated

Example: Lansing woods

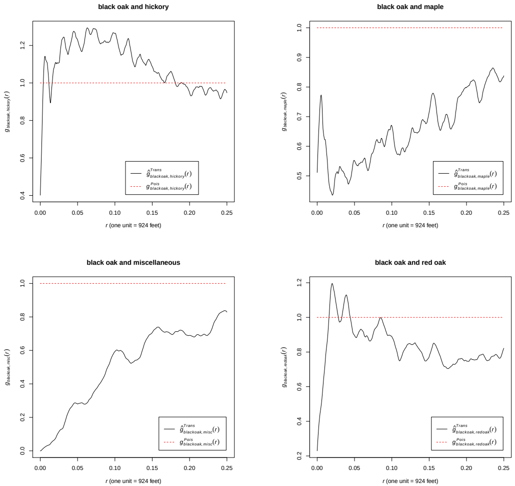
6 species ($\Rightarrow$ 15 pairs of species):



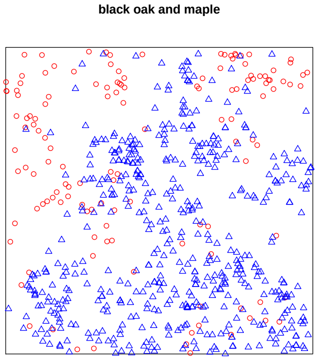
Empirical cross pair correlation functions

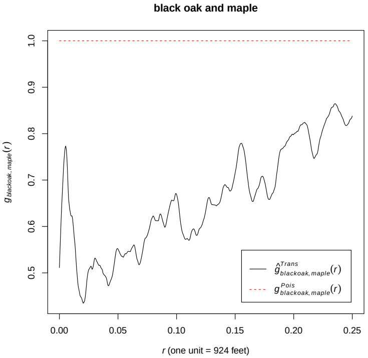
Pair correlation function can be estimated using kernel density estimate.

4 out of 15 cross pair correlation functions:



E.g. black oak and maple:





Seems that these species are segregated.

Perhaps species adapted to different environmental conditions ?

Issues with non-parametric analyses

1. given p species we have many - $O(p^2)$ - cross summary statistics.
   - hard to grasp information in $O(p^2)$ plots.
   - multiple testing.
2. pairwise/bivariate analyses only. Hard to get the big picture.

To learn more we need joint model-based approach.

Waagepetersen, Jalilian, Guan, Mateu (2016): multivariate log Gaussian Cox processes ($p = 9$)

Rajala, Olhede, Murrell (2017): multivariate Gibbs point processes ($p = 83$) - penalized pseudo-likelihood estimation.

I prefer Cox due to easier interpretation - but want higher p ☺

Multivariate Cox processes

Consider a multivariate non-negative random process

$$\Lambda(u) = [\Lambda_1(u), \ldots, \Lambda_p(u)], \quad u \in \mathbb{R}^2$$

A multivariate point process

$$\mathbf{X} = (\mathbf{X}_1, \ldots, \mathbf{X}_p)$$

is a multivariate Cox process if $\mathbf{X}|\Lambda$ is a multivariate Poisson process with intensity function Λ.

Within- and between-species dependence originates from dependencies within and between the Λ_i.

Note Λ is *unobserved* latent process

Multivariate log Gaussian Cox process

$$\log \Lambda_i(u) = z(u)^\mathsf{T}\beta_i + Y_i(u) + U_i(u)$$

where

$$Y_i(u) = \sum_{l=1}^{q} \alpha_{il} E_l(u)$$

and $E_1, \ldots, E_q$, $U_1, \ldots, U_p$ independent Gaussian random fields.

- $z(u)$ observed spatial covariate
- E_l common latent factors (e.g. unobserved environmental covariates).
- U_i species-specific factors (within-species clustering - e.g. seed dispersal)
- known as linear model of coregionalization in geostatistics

Recall:

$$\Lambda_i(u) = \exp[z(u)^\mathsf{T}\beta_i + Y_i(u) + U_i(u)]$$

Intensity function:

$$\rho_i(u) = \mathbb{E}\Lambda_i(u) = \exp[z(u)^\mathsf{T}\beta_i + \sum_{l=1}^{q}\alpha_{il}^2/2 + \sigma_i^2/2] = \exp[\mu + z(u)^\mathsf{T}\beta_i]$$

Cross pair correlation function:

$$g_{ij}(h) = \begin{cases} \exp\left[\sum_{l=1}^{q}\beta_{ijl}c_l(h)\right] & i \neq j \\ \exp\left[\sum_{l=1}^{q}\beta_{ijl}c_l(h) + 1[i=j]\sigma_i^2 c_i(h)\right] & i = j \end{cases} \quad \beta_{ijl} = \alpha_{il}\alpha_{jl}$$

where $c_l(\cdot)$ and $c_i(\cdot)$ correlation functions of the E_l and U_i.

Estimation I

Intensity function can be estimated using composite likelihood approach:

$$\hat{\rho}_i(u) = \exp[\hat{\mu} + z(u)\hat{\beta}_i^\mathsf{T}]$$

Non-parametric kernel density estimates $\hat{g}_{ij}(r)$ of cross pair correlation functions.

Estimation II

Use exponential correlation models for E_l and U_i:
$c(r;\phi) = \exp(-r/\phi)$.

For fixed q minimize weighted least squares criterion to estimate θ (α and covariance parameters)

$$Q(\theta) = \sum_{k,i,j} w_{ijk} [\log \hat{g}_{ij}(t_k) - \log g_{ij}(t_k; \theta, q)]^2$$

Determination of q: K-fold cross-validation based on least squares criterion ($1/K$ of $\log \hat{g}_{ij}(t_k)$ left out)

E.g. $K = 8$ on a multicore machine with 8 CPUs $\rightarrow$ parallel computation

What can be inferred from fitted multivariate LGCP ?

- How many common latent fields $E_1, \ldots, E_q$? q measure of 'complexity'
- Decomposition of covariance into covariance due to common fields $E_1, \ldots, E_q$ and species specific fields U_i.
- Group species according to their pattern of dependence $\alpha_{i1}, \ldots, \alpha_{iq}$ on common fields:

$$Y_i(u) = \alpha_{i1} E_1(u) + \cdots + \alpha_{iq} E_q(u)$$

Decomposition of covariance

$$\log \Lambda_i(u) = z(u)^\mathsf{T}\beta_i + Y_i(u) + U_i(u)$$

Proportions of covariance due to common factors:

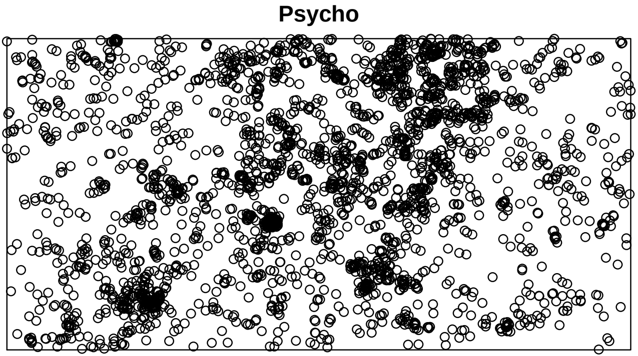
$$PV_i(h) = \frac{\mathbb{C}\mathrm{ov}[Y_i(u), Y_i(u+h)]}{\mathbb{C}\mathrm{ov}[\log \Lambda_i(u), \log \Lambda_i(u+h)]} = \frac{\sum_{l=1}^{q} \alpha_{il}^2 c_l(h)}{\sum_{l=1}^{q} \alpha_{il}^2 c_l(h) + \sigma_i^2 c_i(h)}$$

Application

9 abundant species from Barro Colorado Island plot.

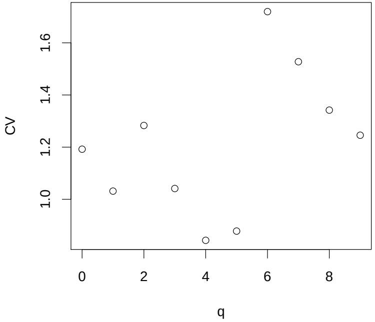
Covariates regarding topography, soil nutrients,...

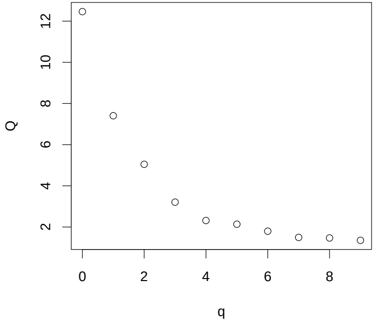
One species *Psychotria* (2640 trees):



Cross-validation

$CV(q)$ $Q(q)$





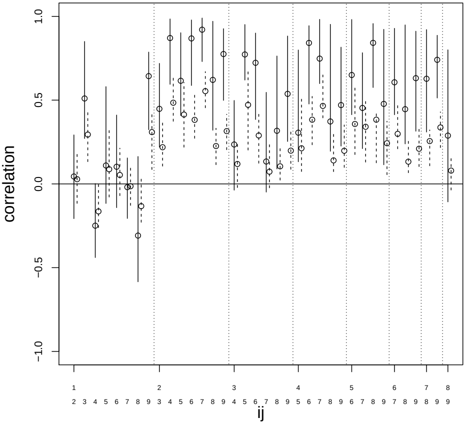
Smallest CV score for $q = 4$.

36 α_{il} and 4 correlation scale parameters for fields E_l. Total 40 parameters for 36 cross g_{ij} functions, $i < j$.

1.1 parameter for each cross pair correlation function.

Estimated correlations at zero lag (with bootstrap confidence intervals)

$$\log \Lambda_i(u) = z(u)^{\mathsf{T}}\beta_i + Y_i(u) + U_i(u)$$

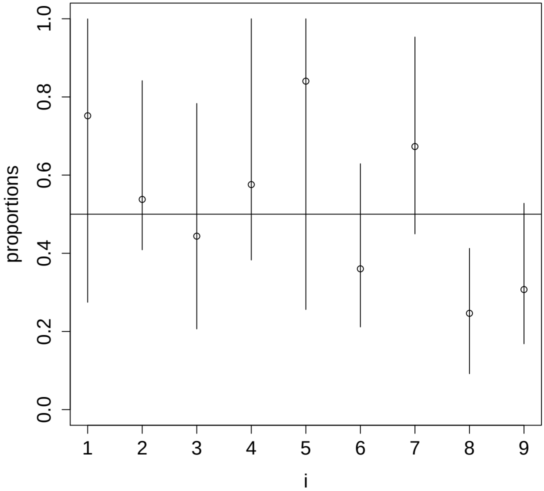


Solid: between $Y_i(u) = \sum_l \alpha_{il} E_l(u)$ and $Y_j(u) = \sum_l \alpha_{jl} E_l(u)$

Dashed: between $\log \Lambda_i(u)$ and $\log \Lambda_j(u)$

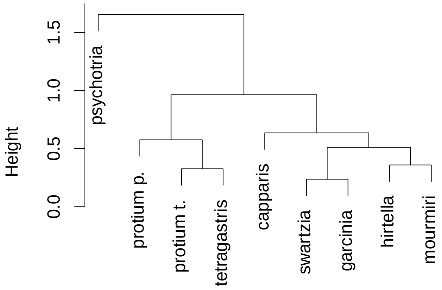
Most species positively correlated. Species 1 (*Psychotria*) is exception.

Proportions of variances at lag zero due to common fields



Clustering of species

Based on similarity of vectors $(\alpha_{i1}, \ldots, \alpha_{iq})$ and $(\alpha_{j1}, \ldots, \alpha_{jq})$.



Psychotria: distinct mode of seed dispersal (bird)

Protium p., Protium t., Tetragastris: the members of the Burseraceae family.

Challenges:

- only considered 9 species
- stability of estimation (numerical minimization)
- interpretability of model

Wishes:

- fast and stable computation.
- encourage sparse results.

Estimation of α_{il}

Focus on parameters α_{il}, $i = 1, \ldots, p$, $l = 1, \ldots, q$.

Fixing all other parameters, object function is of the form

$$\sum_{i,j} \|y_{ij} - x_{ij}\beta_{ij}\|^2$$

where y_{ij} $L \times 1$ 'response vector' and x_{ij} $L \times q$ 'design matrix'.

$$y_{ijk} = \log \hat{g}_{ij}(t_k) \quad (x_{ij})_{kl} = c(t_k; \phi_l) \quad \beta_{ijl} = \alpha_{il}\alpha_{jl}$$

One challenge: non-linear least-squares problem.

Another challenge: high-dimensional α - would be nice to use regularization to promote sparsity and stability of least squares solution.

Regularized least squares

Introduce elastic net penalty

$$\sum_{i,j} \|y_{ij} - x_{ij}\beta_{ij}\|^2 + \lambda p_\xi(\alpha)$$

where

$$p_\xi(\alpha) = \sum_{il} \left[(1-\xi)\alpha_{il}^2 + \xi|\alpha_{il}|\right]$$

Efficient algorithms available for regularized linear models but our problem is non-linear.

Block updates

Consider iterative procedure where α^m is value after m iterations.

Now update ith row $\alpha_{i\cdot} = (\alpha_{i1}, \ldots, \alpha_{iq})$ keeping other rows fixed: minimize

$$Q_i(\alpha_{i\cdot}) = 2 \sum_{\substack{j=1 \\ j \neq i}}^{p} \|y_{ij} - \tilde{x}_{ij}^m \alpha_{i\cdot}\|^2 + \|y_{ii} - x_{ii}\alpha_{i\cdot}^2\|^2 + \lambda p_\xi(\alpha_{i\cdot})$$

Here we rewrote

$$\|y_{ij} - x_{ij}\beta_{ij}^m\|^2 = \|y_{ij} - x_{ij}\mathrm{Diag}(\alpha_{j\cdot}^m)\alpha_{i\cdot}^m\|^2 = \|y_{ij} - \tilde{x}_{ij}^m \alpha_{i\cdot}^m\|^2$$

Note except for 'ii' term $Q_i(\alpha_{i\cdot})$ looks exactly like regularized least squares !

Approximate block update

Consider modified criterion

$$\tilde{Q}_i(\alpha_{i\cdot}) = 2\sum_{\substack{j=1\\ j\neq i}}^{p} \|y_{ij} - \tilde{x}_{ij}^m \alpha_{i\cdot}\|^2 + 2\|y_{ii} - \tilde{x}_{ii}^m \alpha_{i\cdot}\|^2 + \lambda p_\xi(\alpha_{i\cdot})$$

where

$$\tilde{x}_{ii}^m = x_{ii}\mathrm{Diag}(\alpha_{i\cdot}^m)$$

Minimizing $\tilde{Q}_i(\alpha_{i\cdot})$ standard regularized least squares problem (e.g. `glmnet`).

Does it work ?

Gradients of $Q_i(\alpha_{i\cdot})$ and $\tilde{Q}_i(\alpha_{i\cdot})$ coincide.

In simulation studies method works well - although increase in least criterion may be observed in first few iterations.

Wish: more convincing argument that approximate block updates are doing the right thing.

Issue: $\log \hat{g}_{ij}$ is biased estimate of $\log g_{ij}$ (due to kernel smoothing and log transformation)

One more wish: ‘unbiased’ response and design matrix:
$\mathbb{E} Y_{ij} = x_{ij}\beta_{ij}$

Variational approach

Variational point process identity (Jeff) specialized to the isotropic case:

$$\mathbb{E}\left\{\sum_{u\in\mathbf{X}_i,v\in\mathbf{X}_j}^{\neq} e(u,v)h(\|v-u\|)(\log g_{ij})'(\|v-u\|)\right\} =$$
$$-\mathbb{E}\left\{\sum_{u\in\mathbf{X}_i,v\in\mathbf{X}_j}^{\neq} e(u,v)h'(\|v-u\|)\right\},$$

where

$$e(u,v)=\frac{1[u\in W, v\in W]}{\rho_i(u)\rho_j(v)|W\cap W_{v-u}|}$$

and h is continously differentiable with compact support.

In our case,

$$\log g_{ij}(t) = \mathbf{c}(t)\beta_{ij}^{\mathsf{T}} \quad \mathbf{c}(t) = [c(t;\phi_1), \ldots, c(t;\phi_q)] \quad \beta_{ijl} = \alpha_{il}\alpha_{jl}$$

Let

$$h(t) = h_0(t)\mathbf{c}'(t)$$

where h_0 compact support and let

$$\mathbf{A} = \sum_{u,v\in\mathbf{X}\cap W}^{\neq} e(u,v)h_0(\|v-u\|)\mathbf{c}'(\|v-u\|)\{\mathbf{c}'(\|v-u\|)\}^{\top}$$

$$\mathbf{b} = -\sum_{u,v\in\mathbf{X}\cap W}^{\neq} e(u,v)\{h_0'(\|v-u\|)\mathbf{c}'(\|v-u\|) + h_0(\|v-u\|)\mathbf{c}''(\|v-u\|)$$

$\mathbf{A}$ is $q\times q$ and $\mathbf{b}$ is $q\times 1$.

Then from variational equation we obtain unbiased estimating function

$$\mathbf{A}\beta_{ij} - \mathbf{b}.$$

That is,

$$\mathbb{E}[\mathbf{A}\beta_{ij}] = \mathbb{E}\mathbf{b}$$

In terms of α_{il}, procedure can be recast as a least squares problem

$$\|\mathbf{b} - \mathbf{A}\beta_{ij}\|^2 \quad \beta_{ijl} = \alpha_{il}\alpha_{jl}$$

and we can introduce regularization as before.

Further open problems

- validity of using approximate block updates
- choice of λ and ξ (cross validation, BIC,...)
- Inference for proportions of variances, correlations... (bootstrap ?)
- choice of function h_0 in variational equation

References

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