Spatial modeling: a comprehensive framework for Principal Coordinates of Neighbor Matrices (PCNM)

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Introduction

Space in ecological modeling

spatial structure of ecological communities = environment + community-based processes

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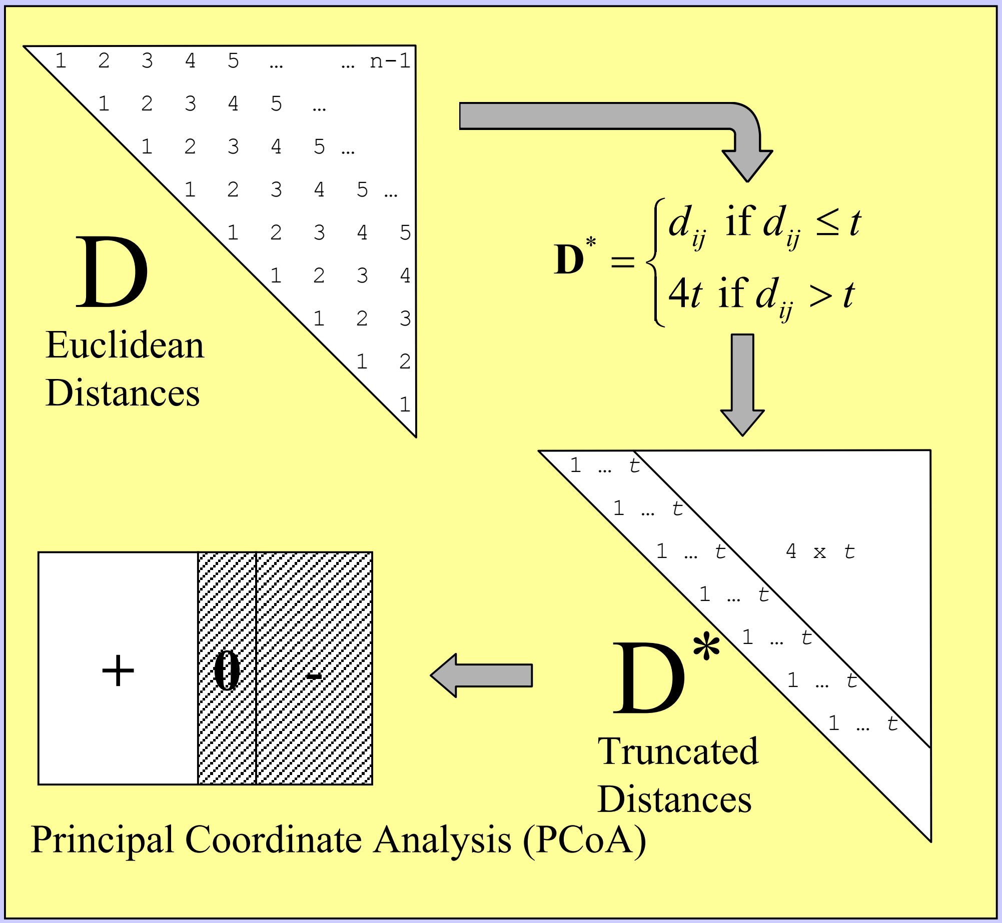
spatial structure of ecological communities	=	environment	+	community-based processes

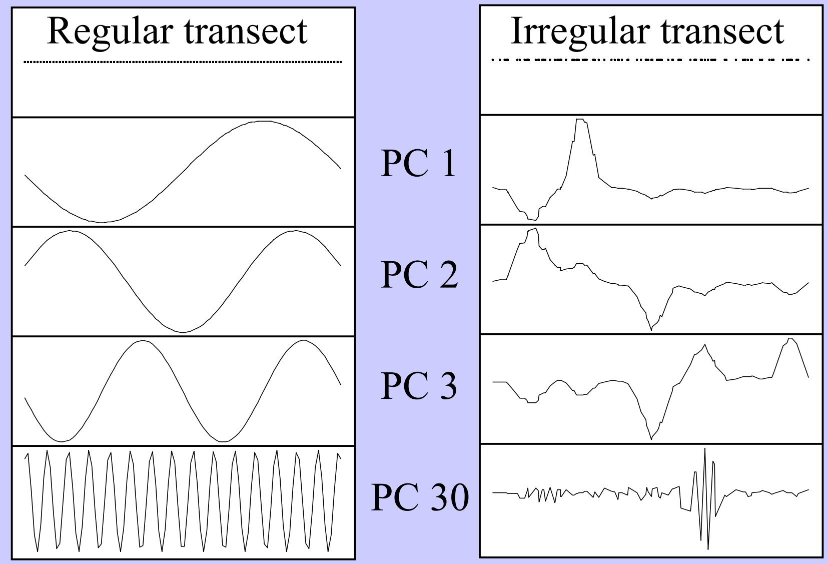
Multiscale spatial descriptors: PCNM

PCNM approach

Principle

BORCARD & LEGENDRE (2002)





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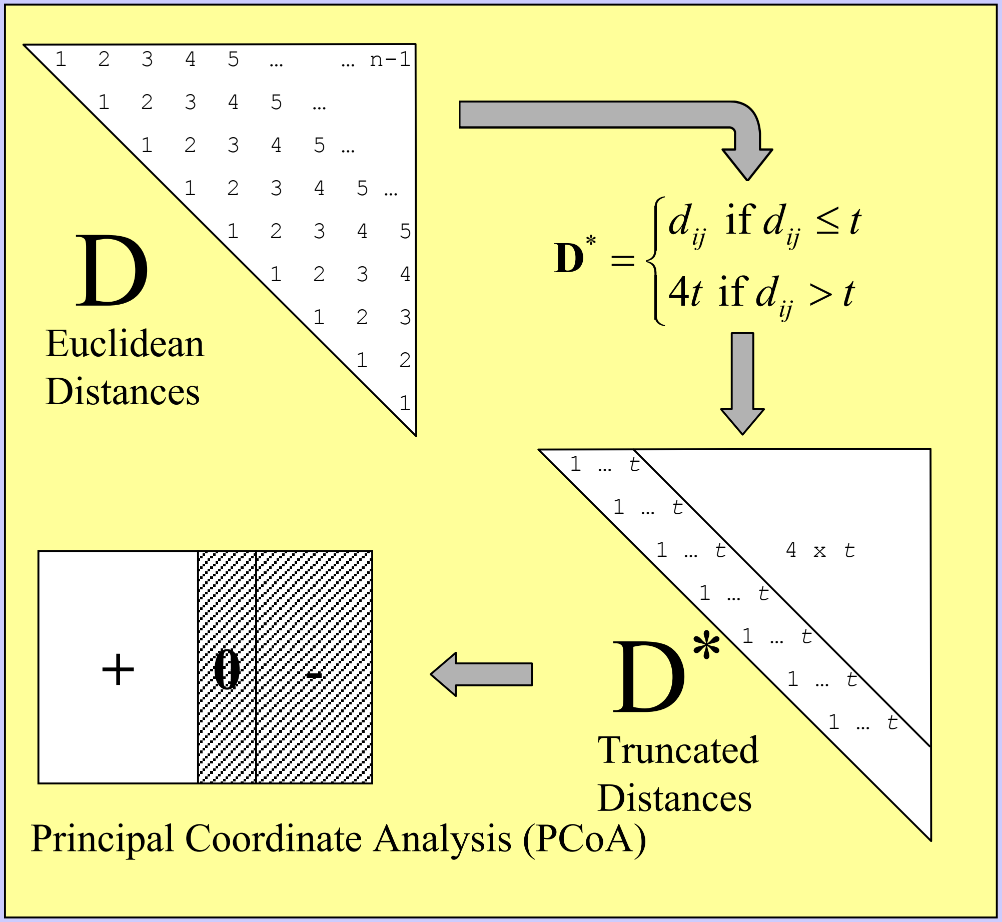

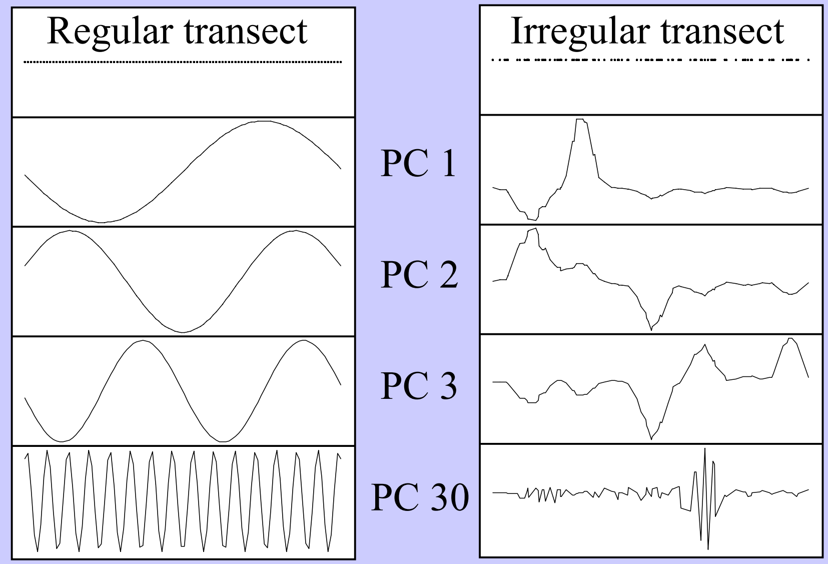

"This paper raises a number of mathematical questions […] We hope that the paper will attract the interest of mathematicians who can help us understand these properties and develop methods of spatial modelling further."

From distances to similarities…

Diagonalization

$$\mathbf{\Delta U} = \mathbf{U\Lambda} \text{ with } \mathbf{U}^t\mathbf{U} = \mathbf{I}$$

$$PC_i = \sqrt{\lambda_i}\,\mathbf{u}_i$$

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- of distances

PCoA of **D**

$$\Delta = -\frac{1}{2}(\mathbf{I} - \frac{\mathbf{11}^t}{n})\mathbf{D_2}(\mathbf{I} - \frac{\mathbf{11}^t}{n})$$

$$= [-\frac{1}{2}(d^2{}_{ij} - d^2{}_{i\bullet} - d^2{}_{\bullet j} + d^2{}_{\bullet\bullet})]$$

PCNM (PCoA of **D***)

$$\Delta^* = -\frac{1}{2}(\mathbf{I} - \frac{\mathbf{11}^t}{n})\mathbf{D}_2^*(\mathbf{I} - \frac{\mathbf{11}^t}{n})$$

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	PCoA of **D**	PCNM (PCoA of $\mathbf{D}^*$)
• of distances	$\Delta = -\frac{1}{2}(\mathbf{I}-\frac{\mathbf{11}^t}{n})\mathbf{D_2}(\mathbf{I}-\frac{\mathbf{11}^t}{n})$ $= [-\frac{1}{2}(d^2{}_{ij} - d^2{}_{i\bullet} - d^2{}_{\bullet j} + d^2{}_{\bullet\bullet})]$	$\Delta^* = -\frac{1}{2}(\mathbf{I}-\frac{\mathbf{11}^t}{n})\mathbf{D}_2^*(\mathbf{I}-\frac{\mathbf{11}^t}{n})$
• of similarities	$\Delta = \frac{1}{2d_{\max}{}^2}(\mathbf{I}-\frac{\mathbf{11}^t}{n})\mathbf{S}(\mathbf{I}-\frac{\mathbf{11}^t}{n})$ where $s_{ij} = 1-\left(\frac{d_{ij}}{d_{\max}}\right)^2$	$\Delta^* = \frac{1}{2d_{\max}{}^2}(\mathbf{I}-\frac{\mathbf{11}^t}{n})\mathbf{S}^*(\mathbf{I}-\frac{\mathbf{11}^t}{n})$ where $s_{ij}^* = 1-\left(\frac{d_{ij}^*}{4t}\right)^2$
	$s_{ij} = 1 \Leftrightarrow d_{ij} = 0$ $s_{ij} = 0 \Leftrightarrow d_{ij} = \max(d_{ij})$	$s_{ij} = 1 \Leftrightarrow d_{ij}^* = d_{ij} = 0$ $s_{ij} = 0 \Leftrightarrow d_{ij}^* = 4t \Leftrightarrow d_{ij} > t$

… to spatial weighting matrix

Spatial weighting matrix

indicates the strength of the potential interaction among the spatial units

$$\mathbf{W} = \underset{\text{connectivity matrix}}{\mathbf{B}} \circ \underset{\text{weighting matrix}}{\mathbf{A}}$$

$$\mathbf{B} = \begin{cases} 1 \text{ if } i \text{ neighbor of } j \\ 0 \text{ otherwise} \end{cases}$$

e.g. geographic similarity

$$1 - \left(d_{ij} / \max(d_{ij}) \right)$$

$$d_{ij}{}^{k},\ d_{ij}{}^{-k},\ \ln d_{ij} \ldots$$

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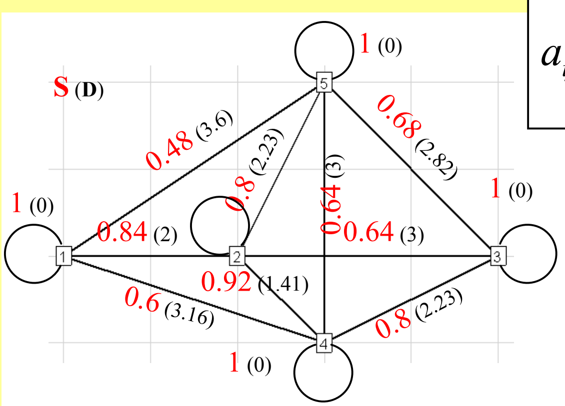
PCoA of **D**

$$\boxed{w_{ij} = s_{ij}}$$

$$b_{ij} = \begin{cases} 1 \Leftrightarrow d_{ij} < \max(d_{ij}) \\ 0 \Leftrightarrow d_{ij} = \max(d_{ij}) \end{cases}$$

$$a_{ij} = 1 - \left(\frac{d_{ij}}{\max(d_{ij})}\right)^2$$



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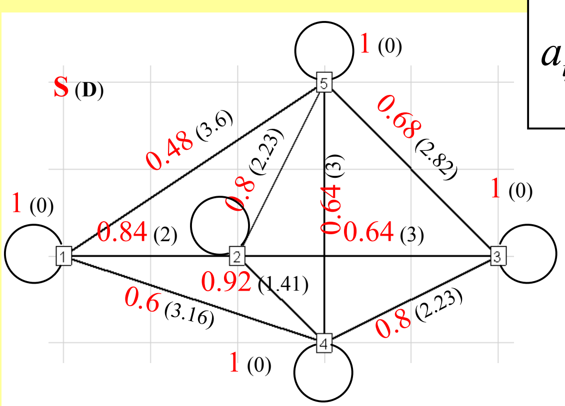

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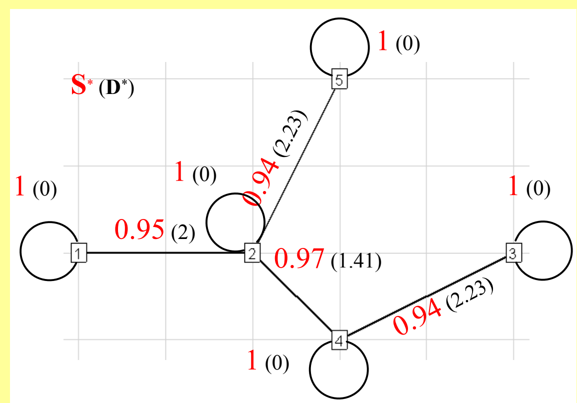

Moran's Eigenvector Maps (MEM)

Spatial autocorrelation

$$I(\mathbf{x}) = \frac{n\sum_{(2)} w_{ij}(x_i - \overline{x})(x_j - \overline{x})}{\sum_{(2)} w_{ij} \sum_{i=1}^{n} (x_i - \overline{x})^2} \qquad I(\mathbf{x}) = \frac{n}{\mathbf{1}^t \mathbf{W} \mathbf{1}} \frac{\mathbf{x}^t (\mathbf{I} - \mathbf{1}\mathbf{1}^t / n) \mathbf{W} (\mathbf{I} - \mathbf{1}\mathbf{1}^t / n) \mathbf{x}}{\mathbf{x}^t (\mathbf{I} - \mathbf{1}\mathbf{1}^t / n) \mathbf{x}}$$

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$$\mathbf{\Omega U} = \mathbf{U\Lambda} \text{ with } \mathbf{U}^t\mathbf{U} = \mathbf{I}$$

A general framework : MEM

- $\mathbf{u}_i$ are vectors with unit norm maximizing Moran's *I* under the constraint of orthogonality

$$\boxed{I(\mathbf{u}_i) = (n/\mathbf{1}^t\mathbf{W1})\lambda_i}$$

- eigenvalues can be either positive or negative

GRIFFITH (1996)

$$\max(I(\mathbf{x})) = (n/\mathbf{1}^t\mathbf{W1})\lambda_{\max}$$
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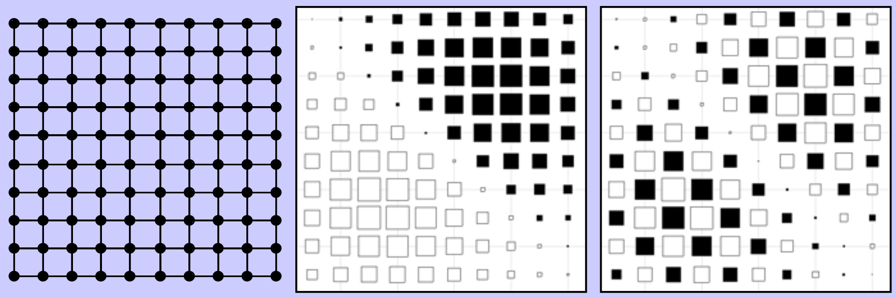

$\lambda_1 = 3.60$ $\lambda_{89} = -3.83$

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DBEM

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$$PCNM \subset DBEM \subset MEM$$

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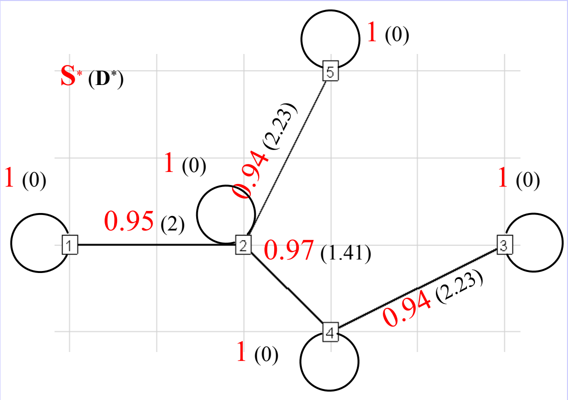

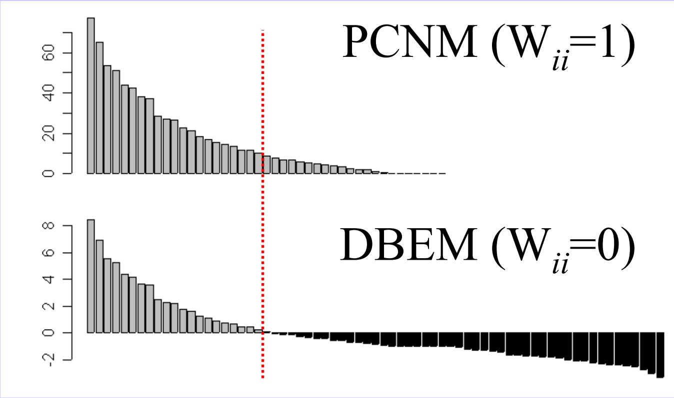

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- 4*t*, why 4?

"beyond a factor of four times the threshold for the 'large' distances, the principal coordinates remain the same to within a multiplicative constant"

BORCARD & LEGENDRE (2002)

$$\boxed{a_{ij} = 1 - \left(\frac{d_{ij}}{4t}\right)^2 \approx 1}$$

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Flexibility

“*the use of a generalised weighting matrix [...] allows the investigator to choose a set of weights which he deems appropriate from prior considerations. This allows great flexibility*”

CLIFF & ORD (1973)

spdep

“*a collection of functions to create* ***spatial weights matrix*** *objects from polygon contiguities, from point patterns by distance and tessellations, for summarising these objects, and for permitting their use in spatial data analysis*”

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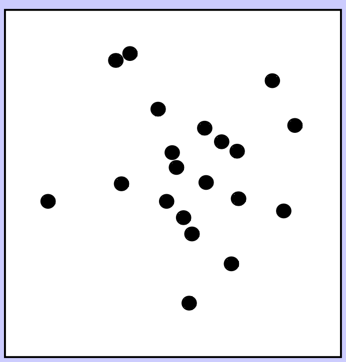

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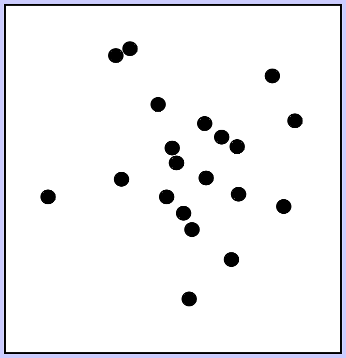

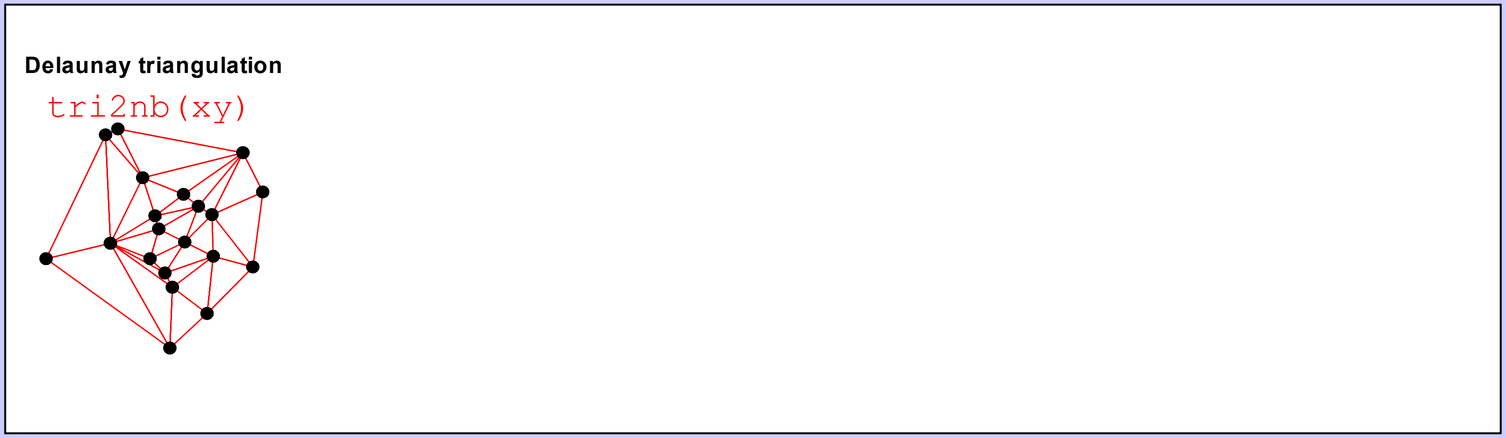

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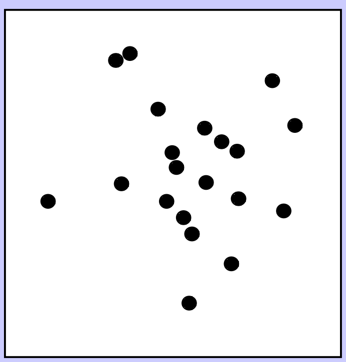

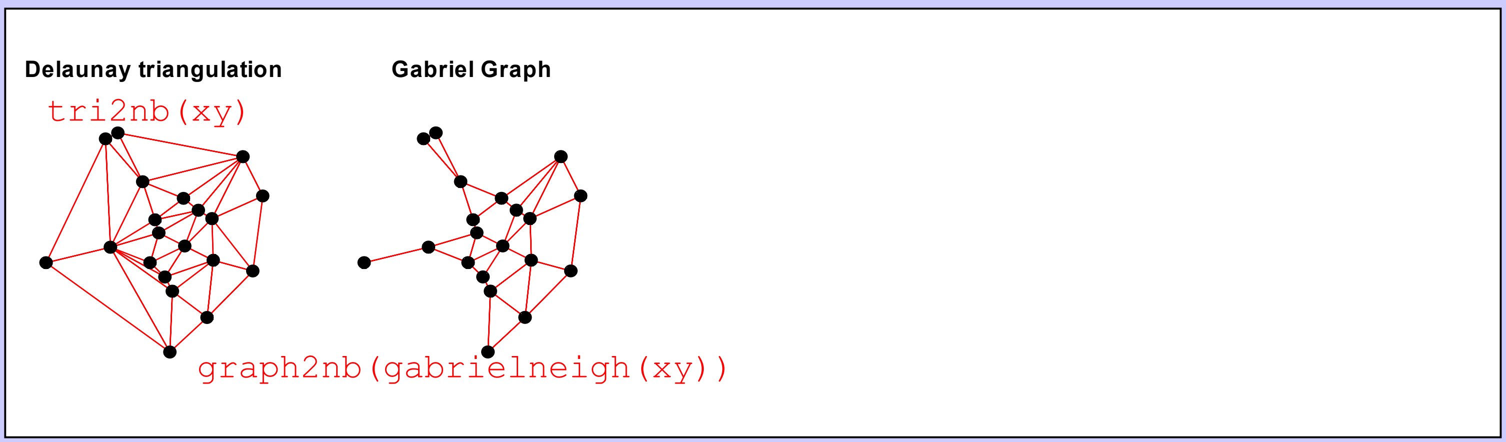

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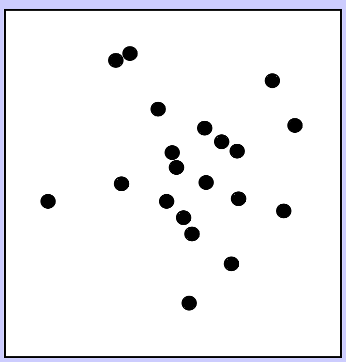

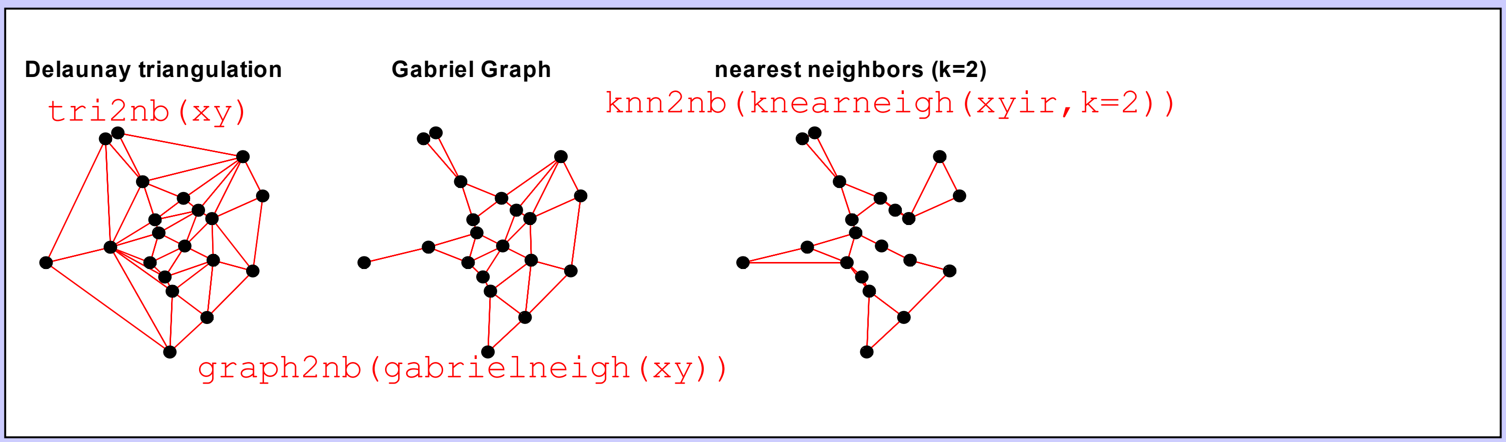

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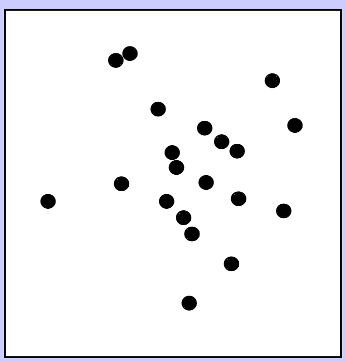

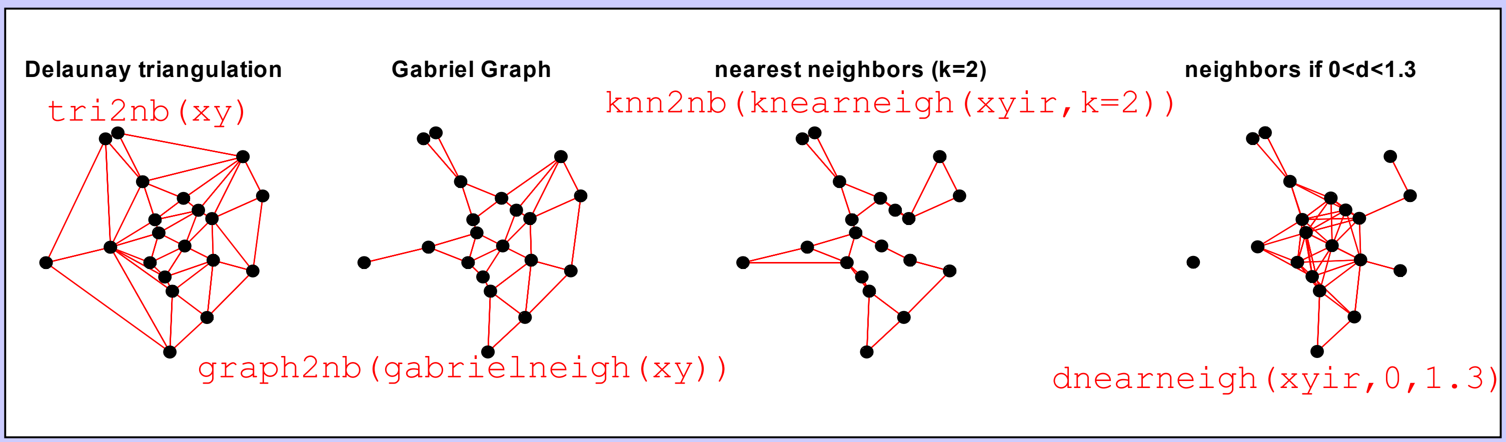

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- Data-driven specification

  For a linear model with n individuals and K variables

  $$\boxed{AIC = -n\log(RSS/n) + 2K}$$

  If n is small

  $$\boxed{AIC_c = AIC + 2K(K+1)/(n-K-1)}$$

  For RDA

  $$\boxed{RSS = trace(\mathbf{Y}^t\mathbf{Y}) - trace(\hat{\mathbf{Y}}^t\hat{\mathbf{Y}})}$$

  GODINEZ-DOMINGUEZ & FREIRE (2003)

Moran's Eigenvector Maps (MEM)

Choice of a spatial weighting matrix

- Theory-driven specification

  matrix constructed upon biological considerations ⇒ difficult for most cases

- Data-driven specification

  For a linear model with n individuals and K variables

  $$AIC = -n\log(RSS/n) + 2K$$

  If n is small

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  For RDA

  $$RSS = trace(\mathbf{Y}^t\mathbf{Y}) - trace(\hat{\mathbf{Y}}^t\hat{\mathbf{Y}})$$

  GODINEZ-DOMINGUEZ & FREIRE (2003)

Define a set of possible spatial weighting matrices

For each candidate

Compute MEM

Sort the eigenvectors by R^2

Enter the K eigenvectors one by one (K models)

Compute AIC_c for each model

Select the spatial weighting matrix corresponding to the model with the lowest AIC_c

Application: Oribatid mite data

W

B

Delaunay triangulation (**tri**)
Gabriel graph (**gab**)
relative neighborhood graph (**rel**)
minimum spanning tree (**mst**)
distance criterion (**dnn**) $d_{ij} < \gamma$

$$1.012 \leq \gamma \leq 4$$

A

$$\mathbf{f}_0 = 1$$

$$\mathbf{f}_1 = 1 - d_{ij} / \max(d_{ij})$$

$$\mathbf{f}_2 = 1 - (d_{ij} / \max(d_{ij}))^{\alpha}$$

$$\mathbf{f}_3 = 1 / d_{ij}^{\ \beta}$$

$$2 \leq \beta \leq 10, 2 \leq \alpha \leq 10$$

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	AIC_c
dnn, $\mathbf{f}_2$ $\gamma = 2.33, \alpha = 2$	**-100.91 (8)**
pcnm	**-92.87 (9)**

Application: Oribatid mite data

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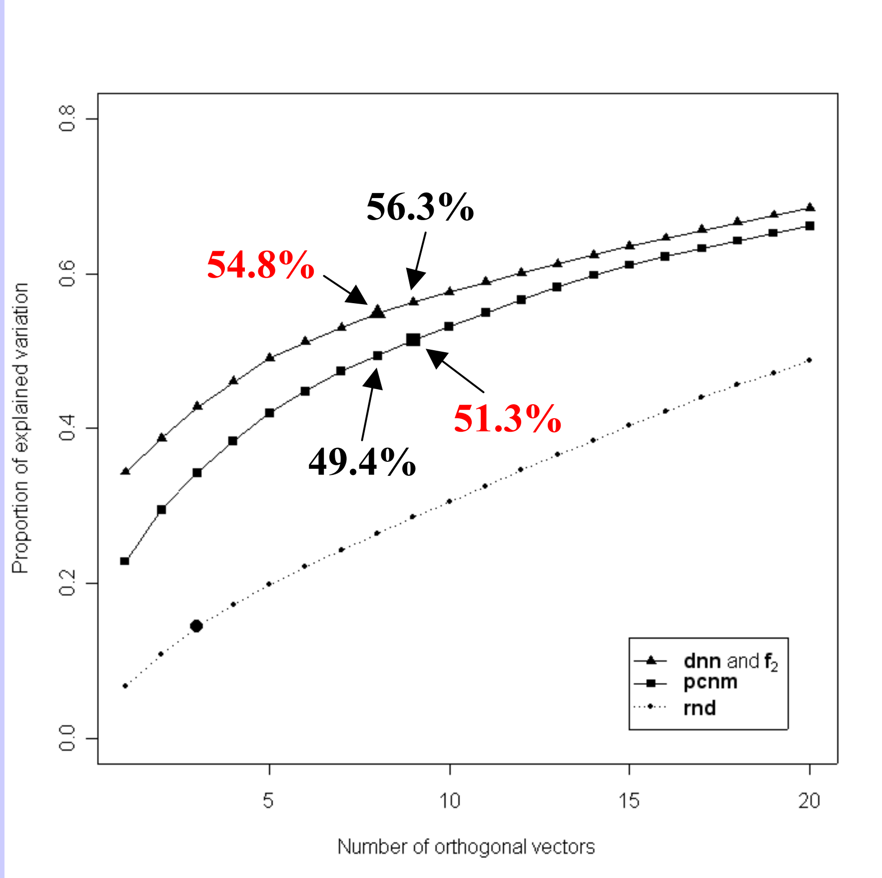

Application: Oribatid mite data

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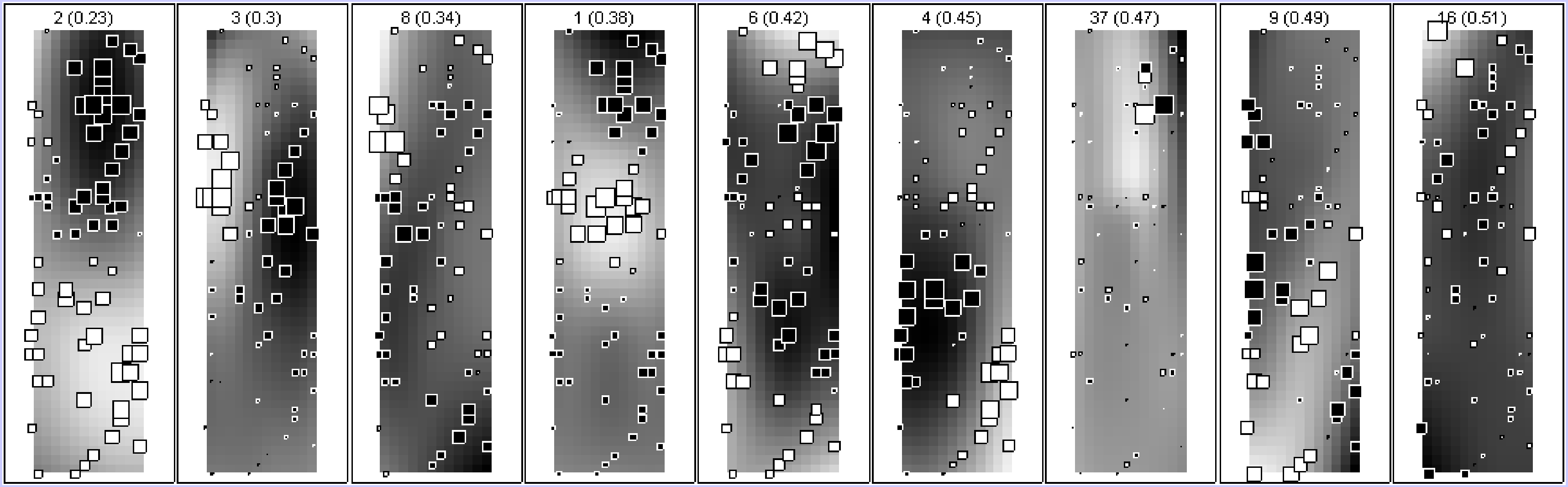
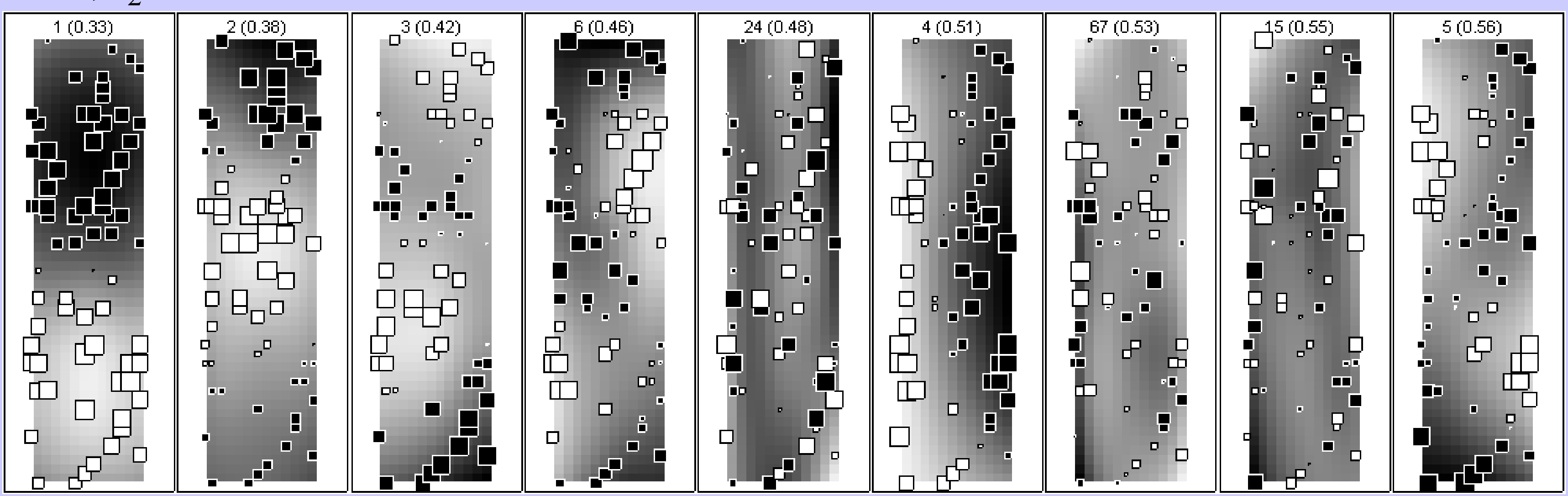


dnn, f_2



Conclusions and perspectives

Mathematical formalism extends the original PCNM approach:

$\Rightarrow$ various definitions of spatial weighting matrices

$\Rightarrow$ negative spatial autocorrelation

$\Rightarrow$ analytical formulation (cos and sin) for regular sampling **(GRIFFITH 2000)**

$\Rightarrow$ very large datasets (*e.g.*, satellite data)

Selection of the eigenvectors to be introduced as spatial predictors

Forward selection is too liberal when K is large

$\Rightarrow$ *AICc*, *RSS* and Moran's I ?

Extension to non-symmetric spatial weighting matrices

e.g., upstream and downstream connectivities in river networks

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