Spatially constrained clustering of ecological networks

Vincent Miele*, Franck Picard and Stéphane Dray

Laboratoire Biométrie et Biologie Evolutive, CNRS, UMR5558, Université de Lyon, Université Lyon 1, Villeurbanne F-69622, France

Summary

1. Spatial ecological networks are widely used to model interactions between georeferenced biological entities (e.g. populations or communities). The analysis of such data often leads to a two-step approach where groups containing similar biological entities are firstly identified and the spatial information is used afterwards to improve the ecological interpretation.

2. We develop an integrative approach to retrieve groups of nodes that are geographically close and ecologically similar. Our model-based spatially constrained method embeds the geographical information within a regularization framework by adding some constraints to the maximum likelihood estimation of parameters.

3. A simulation study and the analysis of two real data sets demonstrate that our approach is able to detect complex spatial patterns that are ecologically meaningful.

4. The model-based framework allows us to consider external information (e.g. geographical proximities, covariates) in the analysis of ecological networks and appears to be an appealing alternative to consider such data.

Key-words: graph Laplacian, model-based clustering, stochastic block model, regularized EM algorithm, spatial partitioning, spatial structure

Introduction

In many ecological studies, researchers must analyse data describing the interactions between biological entities (e.g. individuals, populations, species or communities). These interactions can be directly observed (e.g. trophic relationships in a food web, Krause *et al.* 2003) or they can be inferred from computed distance/similarity measures. Several genetic distances have been developed to summarize allele frequency differences between populations for instance (Kalinowski 2002). In community ecology, species abundance (or presence/absence) data are routinely used to assess turnover (i.e. beta-diversity) between sites based on differences in species composition (Chapter 7 in Legendre & Legendre 2012). Describing and summarizing these sets of pairwise interactions is an important step to better understand the functioning of ecological systems. In a theoretical viewpoint, networks (or graphs) offer a natural and efficient framework to store and analyse interaction data. Whereas food web analysis was a traditional and historical field (Ings *et al.* 2009), network analysis techniques have recently gained popularity in genetics (Albert *et al.* 2013; Keller, Holderegger & van Strien 2013), movement ecology (Jacoby *et al.* 2012), landscape ecology (Bodin & Norberg 2006; Pereira, Segurado & Neves 2011), biogeography (Moalic *et al.* 2012; Thébault 2013) or species distribution modelling (Araujo *et al.* 2011; Foltête *et al.* 2012).

From a statistical perspective, interaction data can be handled using *ecological networks* where biological entities correspond to the nodes while the intensities of interactions are represented by weighted edges (Proulx, Promislow & Phillips 2005). Traditional approaches consist in summarizing the structure of a network using easy-to-compute statistics that relate to ecological properties (connectivity, degree distribution, average path length, Rayfield, Fortin & Fall (2011)). Unsupervised clustering is another common practice to detect groups of biological entities. In ecology, this strategy has been widely applied to find highly intraconnected groups referred to as *modules* : several works have linked the modularity to the stability of the ecological network (Krause *et al.* 2003); searching for modular structure has also helped to identify co-evolution patterns (Dupont & Olesen 2009) and to delineate conservation units (Fortuna *et al.* 2009), habitat patches (Pereira, Segurado & Neves 2011) or biogeographical entities (Moalic *et al.* 2012).

The identification of groups of nodes has received considerable interest in physical sciences (see Newman (2006) or Fortunato (2010) for an extensive review) but also in statistics: in particular, this work relies on well-established model-based clustering procedures (Daudin, Picard & Robin 2008; Picard *et al.* 2009). These methods are fundamentally different from classic approaches by assuming a statistical distribution for interaction data. They are thus very flexible for handling various types of interaction data by specifying adequate statistical distribution to model presence/absence (Bernoulli), abundances (Poisson) or fluxes (Gaussian) or to

integrate external covariates (Mariadassou, Robin & Vacher 2010). These methods among others (Leger, Vacher & Daudin (2013)) can detect hidden connectivity patterns that are not limited to modularity, such as centrality (hubs) or hierarchy (see Picard *et al.* (2009) on a food web of wasps). Lastly, this general statistical framework is adequate for using tools from model selection theory (such as Bayesian information criterion (BIC)) in order to determine the number of groups that structure the data.

In many situations, the nodes correspond to entities that have explicit geographical locations transforming ecological networks into *spatial networks* (Dale & Fortin 2010). When available, this spatial information is often used *posterior* to the identification of groups to improve their ecological interpretation (Araujo *et al.* 2011; Moalic *et al.* 2012; Dáttilo, Guimarães & Izzo 2013). However, if the aim of a study is to identify spatially coherent groups (e.g. habitat patches), this indirect approach may not be optimal as it considers the spatial aspect only after summarizing the network structure. An appropriate technique would integrate spatial information explicitly in the detection of groups. This process is the core of spatially constrained clustering techniques (Gordon 1996; Ambroise & Govaert 1998; Duque, Ramos & Surinach 2007) when ecological observations are stored as raw data tables. When data consist in pairwise interactions stored as a network, no direct technique yet exists to delimit spatial groups except related strategies based on boundary detection (Monmonier 1973).

In this work, we propose an original method to integrate the spatial information in the clustering of ecological interactions. Whereas spatial information is traditionally treated as geographical coordinates, trend surfaces or distance matrix, we used a more efficient strategy that models spatial proximity as a *structural network* where two nodes are connected if they are considered as neighbours (Dray, Legendre & Peres-Neto 2006; Dray *et al.* 2012). This approach offers a great flexibility allowing to include the effect of structural constraints (landscape fragmentation) or physical barriers (rivers, mountains). In our framework, what is usually referred to a spatial network is thus decomposed into a pair of networks: nodes are identical, but edges reflect either biological interactions (ecological network) or spatial connectivity (structural network). Our new model-based approach considers both networks in a single step allowing to identify ecologically homogeneous and spatially coherent groups. The originality of our method is to embed the geographical information within a regularization framework (Ambroise & Govaert 1998; He *et al.* 2011) that has been popularized by the analysis of high-dimensional data sets (Hastie, Tibshirani & Friedman 2001; Buhlmann & van de Geer 2011). We evaluate our new approach by a simulation study and applied it on two real ecological data sets. An R package including methods and data to perform the analysis is also provided at http://lbbe.univ-lyon1.fr/geoclust.

Materials and methods

MODEL-BASED CLUSTERING OF INTERACTION DATA

Our method belongs to the general framework of model-based clustering of network data. This family of models includes the stochastic block model (Airoldi *et al.* 2008) and the MixNet approach (Daudin, Picard & Robin 2008; Mariadassou, Robin & Vacher 2010) among others. We consider data for n interacting entities with Y_{ij} standing for the observed measure of these interactions and $\mathbf{Y} = (Y_{ij})$. Our model is based on group membership of entities, and $\mathbf{Z} = (\mathbf{Z}_1,\ldots,\mathbf{Z}_n)$ denotes the matrix of labels of entities $1,\ldots,n$, *i.e.* $Z_{iq} = 1$ if i belongs to group q and 0 otherwise. In the context of unsupervised clustering, this matrix is unknown and our method aims to recover these labels using the observed information contained in $\mathbf{Y}$. Model-based clustering hypotheses that if labels were known, the distribution of the interaction data would be completely determined. Hence, we start by assuming that there are Q groups with proportions $\boldsymbol{\alpha} = (\alpha_1,\ldots,\alpha_Q)$ such that the distribution of labels $\mathbf{Z}_i = (Z_{i1},\ldots Z_{iQ})$ is multinomial with parameter $\boldsymbol{\alpha}$. The number of groups Q is unknown and will be estimated afterwards. The distribution of the interaction data is specified conditionally to the labels:

$$\mathbf{Z}_i \sim \mathcal{M}(1,\boldsymbol{\alpha}), \ \mathbf{Z}_j \sim \mathcal{M}(1,\boldsymbol{\alpha}), \ Y_{ij}|\{Z_{iq}Z_{i\ell} = 1\} \sim f(\cdot,\theta_{ql}), \qquad \text{eqn 1}$$

where distribution $f(\cdot,\theta_{ql})$ can be Bernoulli to model presence–absence data (Airoldi *et al.* 2008; Daudin, Picard & Robin 2008) and Gaussian or Poisson to model fluxes or abundance data (Mariadassou, Robin & Vacher 2010). The parameters of this model are the proportions for the groups ($\boldsymbol{\alpha}$) and the parameters governing the conditional distribution of the observations ($\boldsymbol{\theta} = (\theta_{q\ell})$). In the following, we note $\boldsymbol{\gamma} = (\boldsymbol{\alpha},\boldsymbol{\theta})$.

The objective is to estimate $\boldsymbol{\gamma}$ and to recover the unobserved labels of the data using the posterior expectation of membership $\mathbb{E}(\mathbf{Z}_i|\mathbf{Y})$. This is achieved using the EM algorithm to maximize the observed-data log likelihood denoted by $\log\mathcal{L}(\mathbf{Y};\boldsymbol{\gamma})$. Unfortunately, the direct maximization of this likelihood is untractable due to the total number of possible partitions ($\mathcal{L}(\mathbf{Y};\boldsymbol{\gamma}) = \sum_{\mathbf{Z}} \mathcal{L}(\mathbf{Y},\mathbf{Z};\boldsymbol{\gamma})$). Hence, we use an iterative algorithm that maximizes the complete-data likelihood:

$$\begin{aligned}\log\mathcal{L}(\mathbf{Y},\mathbf{Z};\boldsymbol{\gamma}) &= \log\mathcal{L}(\mathbf{Z};\boldsymbol{\alpha}) + \log\mathcal{L}(\mathbf{Y}|\mathbf{Z};\boldsymbol{\theta}) \\ &= \sum_{iq} Z_{iq}\log(\alpha_q) + \sum_{ij,q\ell} Z_{iq}Z_{j\ell}\log f(Y_{ij};\theta_{q\ell}) \qquad \text{eqn 2}\end{aligned}$$

The labels being unknown, the algorithm proceeds as follows: the E-step computes the conditional expectation of the complete-data log likelihood defined as:

$$\begin{aligned}\mathcal{Q}(\boldsymbol{\gamma},\boldsymbol{\gamma}^{[h]}) &= \mathbb{E}_{\boldsymbol{\gamma}^{[h]}}\{\log\mathcal{L}(\mathbf{Y},\mathbf{Z};\boldsymbol{\gamma})|\mathbf{Y}\} \\ &= \sum_{iq} \mathbb{E}_{\boldsymbol{\gamma}^{[h]}}(Z_{iq}|\mathbf{Y})\log(\alpha_q) \\ &\quad + \sum_{ij,q\ell} \mathbb{E}_{\boldsymbol{\gamma}^{[h]}}(Z_{iq}Z_{j\ell}|\mathbf{Y})\log f(Y_{ij};\theta_{q\ell}), \qquad \text{eqn 3}\end{aligned}$$

for a current value of the parameters ($\boldsymbol{\gamma}^{[h]}$). Then, the M-step maximizes $\mathcal{Q}$ with respect to $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$. Computational difficulties often arise at the E-step, mainly due to complex dependency structures that can govern the *posterior* distribution of labels given the data. This issue has motivated many methodological developments, in particular in the context of network data, with the use of variational methods (Jordan *et al.* 1999) to approximate this *posterior* distribution (Daudin, Picard & Robin 2008; Mariadassou, Robin & Vacher 2010).

ACCOUNTING FOR SPATIAL CONSTRAINTS IN THE CLUSTERING MODEL

Labels regularization using a structural network

We choose to use a structural network that records the spatial proximity between ecological entities of the ecological network **Y** (see Fig. 1). Structural networks are sometimes directly available such as road networks (Smaltschinski, Seeling & Becker 2012), but they are usually constructed using geographical data with *ad hoc* techniques such as maximum spanning trees (Assunção et al., 2006), k-nearest neighbours (Guo 2008), distance thresholding (Pereira, Segurado & Neves 2011) or edge thinning (Urban & Keitt 2001; Keller, Holderegger & van Strien 2013). In the following, we suppose that the structural network is given and fixed. It is denoted by $\mathbf{X} = (X_{ij})$ such that $(X_{ij} > 0)$ is the geographical proximity between entities i and j and $X_{ij} = 0$ if they are not connected. We assume **X** is symmetric. The entities are the same as in the ecological network **Y**.

We propose to embed the geographical information within a regularization framework by adding some constraints in the maximum likelihood estimation of parameters. In regularization techniques, a constraint defined by a network can be introduced using the graph Laplacian (Jacob, Neuvial & Dudoit 2012). For a network with connection matrix $\mathbf{X} = (X_{ij})$, the Laplacian is defined by $\mathbf{L_x} = \mathbf{D} - \mathbf{X}$ where **D** is the diagonal matrix of degrees with diagonal terms $d_i = \sum_j X_{ij}$. The Laplacian $\mathbf{L_x}$ can then be used as a semi-metric to measure the spatial variability. Indeed, for a given vector $\mathbf{u} = (u_1,\ldots u_n)$, we have:

$$\|\mathbf{u}\|_{\mathbf{L_x}}^2 = \mathbf{u}^T \mathbf{L_x} \mathbf{u} = \sum_{i \sim j} X_{ij}(u_i - u_j)^2,$$
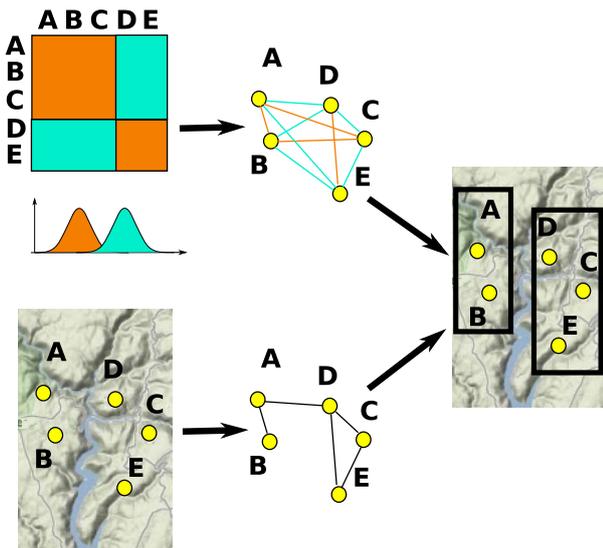

Fig. 1. Framework of our algorithm. The ecological network (top) records the ecological distance between entities. The structural network (bottom) summarizes the proximity between geographical locations. Our method deciphers groups of entities (black squares on the right) using both networks into a model-based strategy associated with a regularization framework. While entities A,B,C and D,E forms two groups in the ecological data, the geographical constraints leads to lastly grouping C with D and E.

which is the squared distance between values of **u** weighted by their spatial proximities contained in **X**. This quantity has been defined as the local variance by Lebart (1969) and is equal to the numerator of the spatial autocorrelation index proposed by Geary (1954).

We develop an original regularization procedure aiming to reduce the variation of labels along the structural network. Whereas the vector of parameters is traditionally regularized, our approach considers that the vector of labels can be regularized using the structural network **X**. Denoting by $\mathbf{Z}^q = (Z_{1q},\ldots,Z_{nq})$ the vector of individuals for label q, we propose the following penalty:

$$\text{pen}(\mathbf{Z}; \mathbf{L_x}) = \sum_{q=1}^{Q} \|\mathbf{Z}^q\|_{\mathbf{L_x}}^2 = \sum_{q=1}^{Q} \sum_{i \sim j} X_{ij}(Z_{iq} - Z_{jq})^2,$$

and the likelihood to maximize by the EM algorithm becomes:

$$\log \mathcal{L}(\mathbf{Y}, \mathbf{Z}; \gamma) - \lambda \times \text{pen}(\mathbf{Z}; \mathbf{L_x}),$$

with λ a constant controlling the amount of penalization that can be estimated adaptively to the data. Let us consider the case where $X_{ij} \in \{0,1\}$ to interpret the penalty. In this case,

$$\text{pen}(\mathbf{Z}; \mathbf{L_x}) = \sum_{q=1}^{Q} \sum_{i \sim j} (Z_{iq} - Z_{jq})^2 = \sum_{q=1}^{Q} \sum_{i \sim j} 1_{\{Z_{iq} \neq Z_{jq}\}}$$

with $i \sim j$ standing for entities i and j connected in the structural network, so that the penalty accounts for the number of edges in the structural network that have discordant labels.

Regularized EM algorithm based on structural network

Considering the new penalized likelihood, the regularized EM algorithm is based on the conditional expectation of the penalized complete-data likelihood

$$\mathcal{Q}(\gamma, \gamma^{[h]}) - \lambda \times \mathbb{E}_{\gamma^{[h]}}\{\text{pen}(\mathbf{Z}; \mathbf{L_x})|\mathbf{Y}\}.$$

As the penalty term does not involve the parameters but only the labels, the maximization step is unchanged (Mariadassou, Robin & Vacher 2010). For instance, if the interaction data are supposed to be Gaussian such that

$$Y_{ij}|\{Z_{iq}Z_{i\ell} = 1\} \sim \mathcal{N}(\mu_{q\ell}, \sigma^2), \qquad \text{eqn 4}$$

we get the following updated estimates (at iteration $[h + 1]$):

$$\hat{\mu}_{ql}^{[h+1]} = \frac{\sum_{ij,q\ell} \hat{Z}_{iq}^{[h]} \hat{Z}_{j\ell}^{[h]} Y_{ij}}{\sum_{ij,q\ell} \hat{Z}_{iq}^{[h]} \hat{Z}_{j\ell}^{[h]}}, \quad \hat{\sigma}^{2[h+1]}$$

$$= \frac{\sum_{ij,q\ell} \hat{Z}_{iq}^{[h]} \hat{Z}_{jl}^{[h]} (Y_{ij} - \hat{\mu}_{ql}^{[h+1]})^2}{\sum_{ij,q\ell} \hat{Z}_{iq}^{[h]} \hat{Z}_{j\ell}^{[h]}},$$

with $(\hat{Z}_{iq}^{[h]})$ the predicted labels provided by the E-step (below).

Network-based regularized E-step. The traditional EM algorithm is not tractable in the case of mixtures for interaction data (Daudin, Picard & Robin 2008). Thus, we use a variational approach which consists in choosing a surrogate *posterior* distribution for the labels that is as close as possible to the true posterior distribution. Moreover, this surrogate *posterior* allows us to suppose that they are conditionally independent (Jordan *et al.* 1999). Denoting by $\tau_{iq} \simeq \mathbb{E}_{\gamma^{[h]}}\{Z_{iq}|\mathbf{Y}\}$ the approximate posterior expectation of labels and by $\tau = (\tau_i) = (\tau_{iq})$, the penalized complete-data likelihood becomes:

$$\mathcal{Q}(\gamma, \gamma^{[h]}) - \lambda \times \mathbb{E}_{\gamma^{[h]}}\{\text{pen}(\mathbf{Z}; \mathbf{L_x})|\mathbf{Y}\} \simeq$$
$$- \sum_{iq} \tau_{iq}\log(\tau_{iq}) + \sum_{iq} \tau_{iq}\log(\alpha_q)$$
$$+ \sum_{ij,q\ell} \tau_{iq}\tau_{j\ell}\log f(Y_{ij}; \theta_{q\ell}) - \lambda \times \sum_{i \sim j} X_{ij}\|\tau_i - \tau_j\|_2^2.$$

The computation of these approximate posterior probabilities is achieved by solving a fixed-point algorithm (Ambroise & Govaert 1998; Mariadassou, Robin & Vacher 2010), and we account for spatial constraints through the penalty term. The derivation of this algorithm is provided in the Appendix S1. Lastly, to retrieve clear and separable groups, we add a classification step corresponding to the classification EM algorithm (Celeux & Govaert 1992). We use the maximum *a posteriori* rule such that $\hat{Z}_{iq} = 1$ if $q = \arg\max_\ell \hat{\tau}_{i\ell}$ and 0 otherwise.

Initialization, λ values and number of groups. It is well known that EM algorithms are very sensitive to the quality of the initialization point. We propose to set up $\tau^{(0)}$ using the clustering partition $\hat{\mathbf{Z}}^0$ obtained with a traditional k-means algorithm as suggested by Daudin, Picard & Robin (2008). Parameter λ increased until $\hat{\lambda}_{\max}$ that corresponds to the maximal spatial homogeneity (i.e. until no further change of labels). Lastly, the number of groups $\hat{Q}(\hat{\lambda}_{\max})$ is chosen using model selection strategy based on the integrated classification likelihood [ICL, Daudin, Picard & Robin (2008)].

Results

SIMULATION STUDY

In this section, we evaluate the relative merits of our method on simulated data that explore different degrees of coherence between the interaction data and the spatial information. For standard clustering methods, the performance only depends on the *group separability*, *i.e.* the ability to delineate groups within the ecological network. However, in the case of spatially constrained clustering, performance is more difficult to explore since it depends on a trade-off between group separability and spatial homogeneity/coherence of the groups. The easiest configuration is when the groups and the spatial information overlap (low *spatial discordance*); the most difficult situation is when groups and spatial information are contradictory (high *spatial discordance*).

We start by simulating a structural network $\mathbf{X}$ that consists of two spatial components of 50 nodes each, related by one single edge only (see Fig. S1). The proximity values stored in the edges in $\mathbf{X}$ are determined using a Gabriel graph (Dale & Fortin 2010). Then, we consider $Q = 2$ groups with equal proportions, the true labels denoted by $\mathbf{Z}^*$. In order to explore different degrees of spatial discordance for the groups, we start by matching labels with the connected components of $\mathbf{X}$ (no spatial discordance), and we randomly sample an increasing number of pairs of nodes from the two spatial components and swap their labels (without modifying $\mathbf{X}$). Then, we use the proportion of edges in $\mathbf{X}$ with discordant labels in the ecological network as a measure of spatial discordance. In the most favourable situation, there is a perfect overlap between labels and the spatial components in $\mathbf{X}$. In the worst situation, labels are spread independently of $\mathbf{X}$. Once the spatial discordance of

labels is determined, we sample a Gaussian interaction network $\mathbf{Y}$ (Eqn 4) with parameters $\sigma = 0.2$ and mean parameters:

$$\boldsymbol{\mu} = \begin{bmatrix} \mu & \nu \\ \nu & \mu \end{bmatrix}.$$

The group separability is governed by $\delta = (\mu - \nu)/\sigma$, which varied from no signal ($\delta = 0$) to high signal levels ($\delta = 1$). Each configuration was repeated 50 times, and we applied our method with spatial penalty or without (*i.e.* $\lambda = 0$). The performance of the method is then assessed by the averaged adjusted Rand Index [aRI, Hubert & Arabie (1985)] that measures the agreement between two partitions. It lies between 0 and 1, 1 being for a perfect match between the simulated and the recovered partition. This index is first used to assess the classification of interactions (between estimated and simulated labels $\mathbf{Z}^*$, referred to as *aRI on $\mathbf{Y}$*) and secondly to assess the spatial homogeneity of groups (between estimated labels and the two spatial components of $\mathbf{X}$, referred to as aRI on $\mathbf{X}$, with the true classification given by the two spatial components).

When groups are highly separable ($\delta \geq 0.5$) and without any spatial discordance, clustering performs perfectly with or without the spatial penalty (aRI $\simeq 1$ on both $\mathbf{X}$ and $\mathbf{Y}$, Fig. 2a–d). The interest in using the spatial penalty is illustrated when the spatial discordance increases until the proportion of spatially discordant labels reaches 50%. In this case, the spatial penalty induces a lower classification performance on the interaction data (decreasing aRI on $\mathbf{Y}$, Fig. 2b), which is compensated by an excellent clustering performance on spatial information (aRI > 0.9 on $\mathbf{X}$, Fig. 2a). Consequently, the effect of the spatial penalty is to maintain the spatial homogeneity of the groups at the price of classification errors on $\mathbf{Y}$. When the separability of the group decreased ($\delta = 0.25$), the performance of clustering also decreased, with a aRI of 0.3 on $\mathbf{Y}$. In this case, the spatial penalty clearly helps to recover the groups when they match the spatial structure (aRI = 0.8 on $\mathbf{X}$ without spatial discordance, $\delta = 0.25$, Fig. 2a,c). In conclusion, when the spatial discordance is low to moderate, the spatial penalty helps in finding the groups, even if the signal in the interaction network is moderate.

Lastly, we evaluate the ability of our method to identify groups when the spatial discordance is high. When looking at the number of groups chosen by the model selection procedure (Fig. 3), it is clear that all nodes are gathered in a single group when the spatial discordance increases. This proves that our method is adaptive to the spatial discordance and searches only for *spatially coherent* groups that are in agreement with ecologically homogeneous subsets.

SPATIAL TURNOVER IN SPECIES COMPOSITION

We re-examine data concerning the presence/absence of 332 genera in 63 hydrothermal fields. This data set was used by Bachraty, Legendre & Desbruyéres (2009) and Moalic *et al.* (2012) to define biogeographical provinces based on the faunal distribution in oceanic hydrothermal vents. We built an ecological network by computing distances in faunal composition
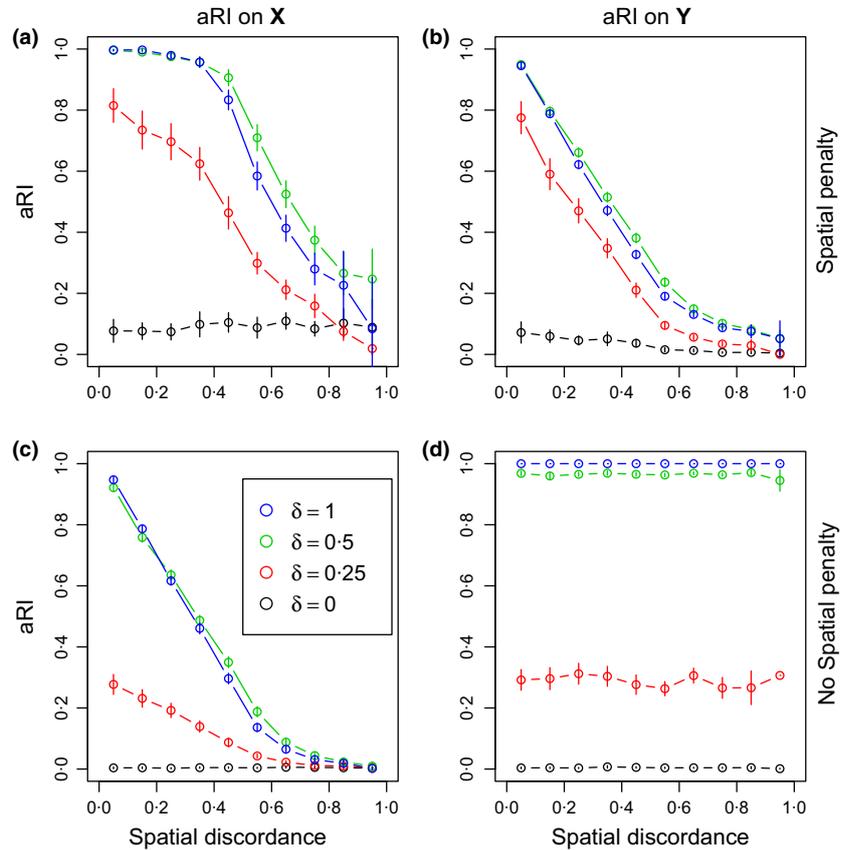
Fig. 2. Performance of our method on simulated data, assessed by the averaged Adjusted Rand Index (aRI), for varying spatial discordance and group separability (δ) values. (a) aRI on **X** with our regularized EM algorithm with spatial penalty. (b) same for aRI on **Y**. (c) aRI on **X** without spatial penalty, i.e λ = 0. (d) same for aRI on **Y**.
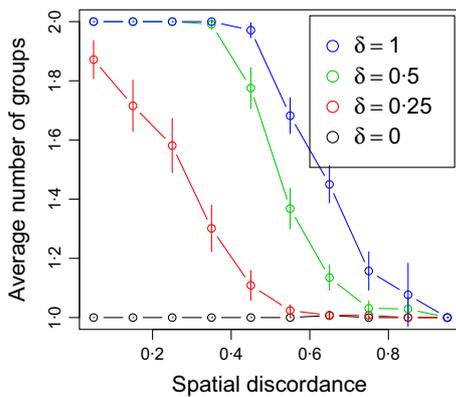

Fig. 3. Average number of groups selected by our model selection approach, on simulated data, for varying spatial discordance and group separability (δ) values.

using Jaccard coefficient (see Chapter 7 in Legendre & Legendre 2012). This fully connected network contains 63 nodes (the fields), and edges are weighted by the ecological distances.

The distribution of Jaccard coefficients was bimodal due to an excess of distance values equal to 1 corresponding to pairs of fields sharing no species; the remaining values, after a logistic transform, follow a Gaussian distribution. Consequently, we modelled data using an inflated Gaussian distribution. We computed spatial proximities among the fields by computing great circle distances. The structural network was then built by removing all the edges corresponding to distances higher than

3600 km (see Fig. 5b). This choice ensures that each node has at least one edge and that only local spatial proximities are considered. Edges were then weighted by spatial distances (max $(d_{ij}) - d_{ij}$).

We first applied our algorithm without spatial penalty (i.e. λ = 0). Fields were partitioned in six groups based on their species composition (Fig. 4). It is clear that fields share more ecological similarities within-groups than between-groups (comparison of diagonal and off-diagonal terms, respectively, in Fig. 4a). This partitioning highlights some geographical patterns: some groups are roughly spatially coherent (groups A, C, D, E), whereas other groups did not show any spatial coherence (Fig. 4b).

If the spatial penalty is applied, the model selection procedure selected also a clustering in six groups (Fig. 5b). In this case, within-group similarities are also higher than the between-group (Fig. 5a). Average within-group Jaccard index (0·944) is slightly higher than for the unconstrained approach (0·928). This loss of ecological homogeneity is counterbalanced by a gain in the spatial aspect (Fig. 5b) as all ecological groups are now spatially coherent. Our results are very similar to those obtained by Bachraty, Legendre & Desbruyéres (2009) and Moalic *et al.* (2012) who used different methods and identified 6 and 5 provinces, respectively. Their partitioning disagreed for the provinces in West Pacific (WP), Indian Ocean (IO) and East Pacific Rise (EPR). We identified a group with only one field (Loihi Seamount, LOS) that shares no species with all others and is poorly spatially connected (only one edge) in the
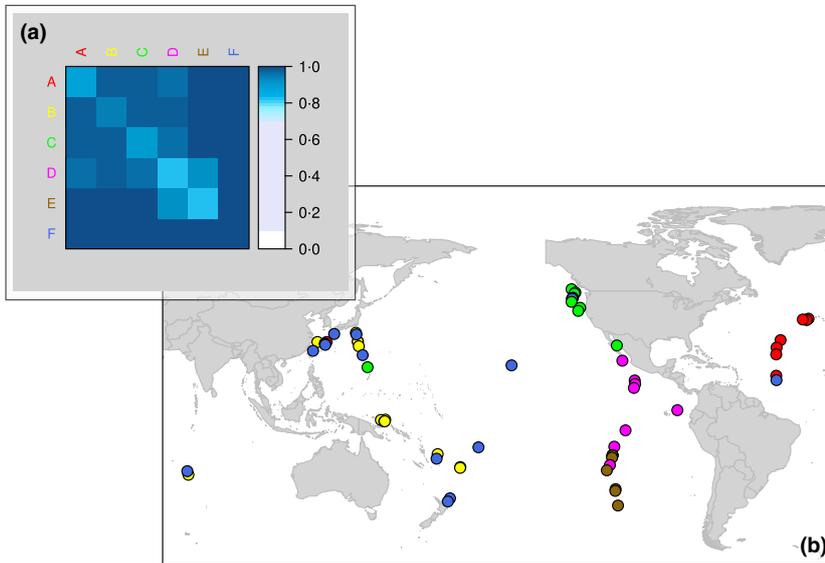
Fig. 4. Clustering of 63 hydrothermal fields in six groups based on similarities in species composition (no spatial penalty). (a) Heatmap showing average ecological distances within and between groups. (b) Map showing the six groups.
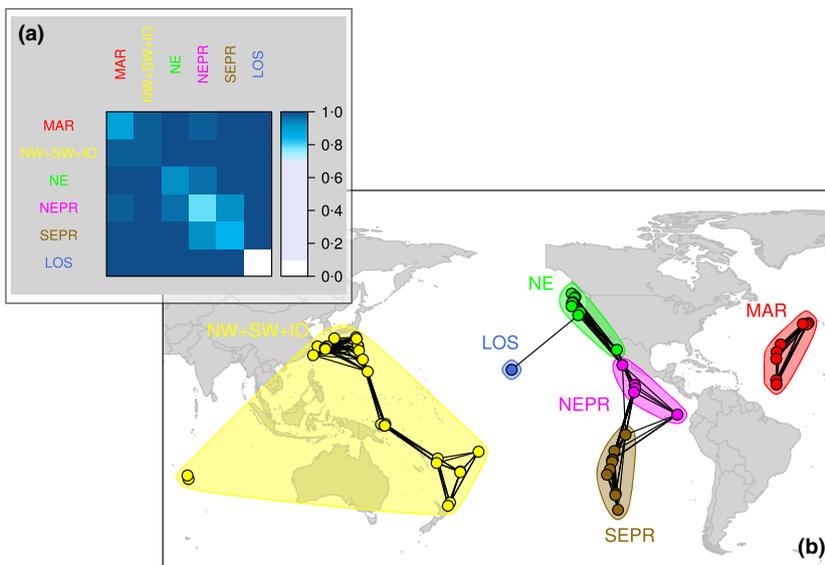

Fig. 5. Spatial clustering of 63 hydrothermal fields in six groups based on similarities in species composition. (a) Heatmap showing average ecological distances within and between groups. (b) Map showing the structural network and the six groups: Loihi Seamount (LOS), Northeast Pacific (NE), Northeast Pacific Rise (NEPR), Northeast Pacific Rise (SEPR), Mid-Atlantic Ridge (MAR) and Northwest Pacific/Southwest Pacific/Indian Ocean (NW + SW + IO).

structural network. As in the mentioned studies, we found the Mid-Atlantic Ridge (MAR) and the Northeast Pacific (NE) provinces, the latter including the Guaymas Basin in our results. We also identified the partitioning between the Northern and Southern Pacific Rise provinces (NEPR and SEPR) that were proposed in Bachraty, Legendre & Desbruyéres (2009) as centres of dispersal for hydrothermal fauna. This shows that our algorithm can separate groups of fields that are spatially connected but very dissimilar according to the ecological network. Our algorithm was not able to partition the global province (NW + SW + IO on Fig. 5b) composed by the Indian Ocean (IO) and Western Pacific zones. Interestingly, both previous studies were discordant for this region: Bachraty, Legendre & Desbruyéres (2009) merged Indian Ocean and Southwest Pacific (SW) and introduced an additional Northwest Pacific province (NW), whereas Moalic *et al.* (2012) proposed a global WP province but kept aside the IO province. Moalic *et al.* (2012) focused on the central role of the

WP province in the biogeography of hydrothermal vents and also mentioned that the existence of the IO province remains unclear due its poor representation in the data. Consequently, the group NW + SW + IO is the most ecologically heterogeneous in our results (Fig. 5a) because our method is more conservative and suggests that any partitioning would be artificial in this region. This merging of IO and Western Pacific zones (SW, NW) demonstrated that our algorithm is able to merge two groups that are ecologically similar but not spatially connected.

SPATIAL TURNOVER OF MUTUALISTIC NETWORKS

This second application illustrates the ability of our approach to study spatial variations of species interaction networks (see e.g. Tylianakis, Tscharntke & Lewis 2007). We analyse the data of Ricciardi, Boyer & Ollerton (2010), which described anemonefish–anemone mutualistic interactions for 16

sampling sites located all over Bunaken Islands and Manado Coast (Indonesia, Fig. 6). For each site, field observations were performed to build interaction matrices between seven anemonefishes and nine anemone species. The ecological dissimilarity between two mutualistic networks can originate from two sources because species compositions and\or species interactions between shared species could vary among sites. Hence, to disentangle these two aspects, we used the additive partitioning framework proposed by Poisot *et al.* (2012) that decomposes network dissimilarity (β_{WN}) into interactions (β_{OS}) and species turnover (β_{ST}) components. We used the betalink package for R (Poisot *et al.* 2012) to build three ecological networks. We chose the Whittaker (1960) index of dissimilarity (index 1 in Koleff, Gaston & Lennon 2003) and computed ecological distances among sites based on β_{WN}, β_{OS} and β_{ST} to study the spatial turnover of the different facets of mutualistic interactions.

The steps to build the structural network are described in Fig. 6a. As this example concerns marine animals and the study area contains land and sea, we used a procedure that considers only sea routes and treats islands as barriers. We firstly divided the study area by computing a Voronoi diagram (step a in Fig. 6a). Then, we removed parts of the Voronoi cells that are not overlapped by the sea (i.e. islands) and built a structural network where two sites are linked by an edge if their Voronoi cells have a common boundary (step b). Lastly, the structural network was pruned by removing all the edges corresponding to sea distances higher than 11·1 km (step c). This choice guarantees that each node has at least one edge and that only local spatial proximities are taken into account. Edges were then weighted by sea distances ($\max(d_{ij}) - d_{ij}$).

The spatial clustering of sites leads to a common partition in two groups for β_{WN} and β_{ST} (Fig. 6b). However, the selection procedure returns only one group for β_{OS}, suggesting that no spatial turnover of interaction networks is observed when considering only shared species. Hence, the partitioning observed for β_{WN} is related to changes in species composition but not in species interactions. For species turnover, we identified a group of two sites (sandy lagoons) characterized by two interacting species (*Stichodactyla haddoni* and *Amphiprion polymnus*) that are not present in other sites. The lack of pattern observed for β_{OS} is coherent with the findings of Ricciardi, Boyer & Ollerton (2010) who suggested that 'competition is not an important factor determining the presence or absence of particular anemonefish/anemone combinations' and that 'a stochastic event on a chronological basis (who arrives first) may determine the presence of an anemonefish in an anemone for long periods, and not a clear niche differentiation or a superiority as competitor against other species'. These stochastic processes increased the spatial homogeneity of mutualistic interactions in the study area so that no pattern can be detected.

Conclusions

The analysis of ecological networks has gained a lot of attention in the past years, and the development of dedicated
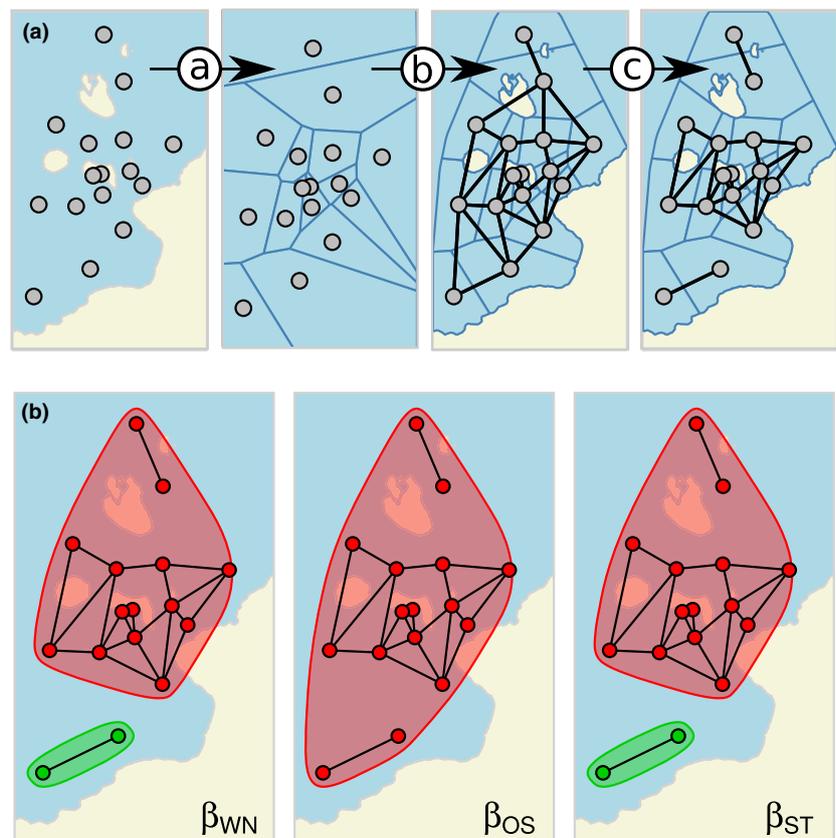

Fig. 6. Analysis of 16 mutualistic networks. (a) The different steps to build the structural network consist in (a) computing a Voronoi diagram, (b) removing lands and building the network and (c) removing the longer edges. (b) Spatial clustering of the 16 sites based on β_{WN}, β_{OS} and β_{ST} similarities.

statistical methods has been challenging. Here, we propose a statistical framework to identify spatial groups of ecological entities based on interaction data. We developed an efficient way to retrieve spatially coherent groups of ecological entities using a regularization framework. The analysis of simulated data and of two real data sets demonstrated the ability of our method to identify groups that match the spatial structure. If no spatial patterns are present in the data, our method did not identify any partitioning, and standard clustering algorithms, which do not consider the spatial aspect, should be preferred in these circumstances.

Whereas classical analysis consists in describing the main structures of ecological networks by summary statistics, our method is based on a model-based framework that assumes and estimates a distribution for interaction data. This approach is already used to analyse genomics data but it has been rarely applied to ecological data (but see Picard *et al.* 2009). We demonstrated that this framework is very promising as it allows to include easily spatial constraints in the estimation procedure. It can be extended to build more complex models by considering covariates measured either on the nodes or the edges of the network (e.g. environmental variables). Lastly, different distributions can be modelled so that the method is applicable to a wide variety of interaction data. For instance, we could assume a multivariate distribution to handle multi-layer ecological networks that record different types of interaction between entities (Kéfi *et al.* 2012).

Acknowledgements

Data accessibility

The hydrothermal fields data set is available online as a supplementary material of Bachraty, Legendre & Desbruyéres (2009) and is integrated in the R package. The anemonefish–anemone data set is available in Ricciardi, Boyer & Ollerton (2010) (geographical positions were provided by Francesco Ricciardi).

References

Airoldi, E., Blei, D., Fienberg, S. & Xing, E. (2008) Mixed-membership stochastic block models. *Journal of Machine Learning Research*, **9**, 1981–2014.

Albert, E.M., Fortuna, M.A., Godoy, J.A. & Bascompte, J. (2013) Assessing the robustness of networks of spatial genetic variation. *Ecology Letters*, **16** (Suppl 1), 86–93.

Ambroise, C. & Govaert, G. (1998) Convergence of an EM-type algorithm for spatial clustering. *Pattern Recognition Letters*, **19**, 919–927.

Araujo, M.B., Rozenfeld, A., Rahbek, C. & Marquet, P.A. (2011) Using species co-occurrence networks to assess the impacts of climate change. *Ecography*, **34**, 897–908.

Assunção, M., Corrêa Neves, M., Câmara, G. & da Costa Freitas, C. (2006) Efficient regionalization techniques for socio-economic geographical units using minimum spanning trees. *International Journal of Geographical Information Science*, **20**, 797–811.

Bachraty, C., Legendre, P. & Desbruyéres, D. (2009) Biogeographic relationships among deep-sea hydrothermal vent faunas at global scale. *Deep Sea Research Part I: Oceano-graphic Research Papers*, **56**, 1371–1378.

Bodin, O. & Norberg, J. (2006) A network approach for analyzing spatially structured populations in fragmented landscape. *Landscape Ecology*, **22**, 31–44.

Buhlmann, P. & van de Geer, S. (2011) *Statistics for High-Dimensional Data: Methods, Theory and Applications.* Springer-Verlag, New York.

Celeux, G. & Govaert, G. (1992) A classification EM algorithm for clustering and two stochastic versions. *Computational Statistics and Data Analysis*, **14**, 315–332.

Dale, M. & Fortin, M.-J. (2010) From graphs to spatial graphs. *Annual Review of Ecology, Evolution, and Systematics*, **41**, 21–38.

Dáttilo, W., Guimarães, P.R. & Izzo, T.J. (2013) Spatial structure of ant-plant mutu-alistic networks. *Oikos*, **122**, 1643–1648.

Daudin, J.J., Picard, F. & Robin, S. (2008) A mixture model for random graphs. *Statistics and Computing*, **18**, 173–183.

Dray, S., Legendre, P. & Peres-Neto, P.R. (2006) Spatial modeling: a comprehensive framework for principal coordinate analysis of neighbor matrices (PCNM). *Ecological Modelling*, **196**, 483–493.

Dray, S., Pélissier, R., Couteron, P., Fortin, M.J., Legendre, P., Peres-Neto, P.R. *et al.* (2012) Community ecology in the age of multivariate multiscale spatial analysis. *Ecological Monographs*, **82**, 257–275.

Dupont, Y.L. & Olesen, J.M. (2009) Ecological modules and roles of species in heathland plant-insect flower visitor networks. *Journal of Animal Ecology*, **78**, 346–353.

Duque, J.C., Ramos, R. & Surinach, J. (2007) Supervised regionalization methods: a survey. *International Regional Science Review*, **30**, 195–220.

Foltête, J.-C., Clauzel, C., Vuidel, G. & Tournant, P. (2012) Integrating graph-based connectivity metrics into species distribution models. *Landscape Ecology*, **27**, 557–569.

Fortuna, M.A., Albaladejo, R.G., Fernańdez, L., Aparicio, A. & Bascompte, J. (2009) Networks of spatial genetic variation across species. *Proceedings of the National Academy of Sciences of the United States of America*, **106**, 19044–19049.

Fortunato, S. (2010) Community detection in graphs. *Physics Reports*, **486**, 75–174.

Geary, R.C. (1954) The contiguity ratio and statistical mapping. *The Incorporated Statistician*, **5**, 115–145.

Gordon, A. (1996) A survey of constrained classification. *Computational Statistics & Data Analysis*, **21**, 17–29.

Guo, D. (2008) Regionalization with dynamically constrained agglomerative clustering and partitioning (redcap). *International Journal of Geographical Information Science*, **22**, 801–823.

Hastie, T., Tibshirani, R. & Friedman, J.H. (2001) *The Elements of Statistical Learning: Data Mining, Inference, and Prediction: with 200 Full-Color Illustrations.* Springer-Verlag, New York.

He, X., Cai, D., Shao, Y., Bao, H. & Han, J. (2011) Laplacian regularized gaussian mixture model for data clustering. *IEEE Knowledge and Data Engineering*, **23**, 1406–1418.

Hubert, L. & Arabie, P. (1985) Comparing partitions. *Journal of Classification*, **2**, 193–218.

Ings, T.C., Montoya, J.M., Bascompte, J., Blüthgen, N., Brown, L., Dormann, C.F. *et al.* (2009) Ecological networks – beyond food webs. *Journal of Animal Ecology*, **78**, 253–269.

Jacob, L., Neuvial, P. & Dudoit, S. (2012) More power via graph-structured tests for differential expression of gene networks. *The Annals of Applied Statistics*, **6**, 561–600.

Jacoby, D.M.P., Brooks, E.J., Croft, D.P. & Sims, D.W. (2012) Developing a deeper understanding of animal movements and spatial dynamics through novel application of network analyses. *Methods in Ecology and Evolution*, **3**, 574–583.

Jordan, M., Ghahramani, Z., Jaakkola, T. & Saul, L. (1999) An introduction to variational methods for graphical models. *Machine Learning*, **37**, 183–233.

Kalinowski, S.T. (2002) Evolutionary and statistical properties of three genetic distances. *Molecular Ecology*, **11**, 1263–1273.

Kéfi, S., Berlow, E.L., Wieters, E.A., Navarrete, S.A., Petchey, O.L., Wood, S.A. *et al.* (2012) More than a meal integrating non feeding interactions into food webs. *Ecology Letters*, **15**, 291–300.

Keller, D., Holderegger, R. & van Strien, M.J. (2013) Spatial scale affects landscape genetic analysis of a wetland grasshopper. *Molecular Ecology*, **22**, 2467–2482.

Koleff, P., Gaston, K.J. & Lennon, J.J. (2003) Measuring beta diversity for presence absence data. *Journal of Animal Ecology*, **72**, 367–382.

Krause, A.E., Frank, K.A., Mason, D.M., Ulanowicz, R.E. & Taylor, W.W. (2003) Compartments revealed in food-web structure. *Nature*, **426**, 282–285.

Lebart, L. (1969) Analyse statistique de la contiguïté. *Publication de l'Institut de Statistiques de l'Université de Paris*, **28**, 81–112.

Legendre, P. & Legendre, L. (2012) *Numerical Ecology*, 3rd edn. Elsevier, Amsterdam.

Leger, J.-B., Vacher, C. & Daudin, J.-J. (2013) Detection of structurally homogeneous subsets in graphs. *Statistics and Computing*, **23**, 1–18.

Mariadassou, M., Robin, S. & Vacher, C. (2010) Uncovering latent structure in valued graphs: a variational approach. *Annals of Applied Statistics*, **4**, 715–742.

Moalic, Y., Desbruyères, D., Duarte, C.M., Rozenfeld, A.F., Bachraty, C. & Arnaud-Haond, S. (2012) Biogeography revisited with network theory: retracing the history of hydrothermal vent communities. *Systematic Biology*, **61**, 127–137.

Monmonier, M. (1973) Maximum-difference barriers: an alternative numerical regionalization method. *Geographical Analysis*, **5**, 245–261.

Newman, M.E.J. (2006) Modularity and community structure in networks. *Proceedings of the National Academy of Sciences of the United States of America*, **103**, 8577–8582.

Pereira, M., Segurado, P. & Neves, N. (2011) Using spatial network structure in land scape management and planning: a case study with pond turtles. *Landscape and Urban Planning*, **100**, 67–76.

Picard, F., Miele, V., Daudin, J.J., Cottret, L. & Robin, S. (2009) Deciphering the connectivity structure of biological networks using MixNet. *BMC Bioinformatics*, **10** (Suppl 6), S17.

Poisot, T., Canard, E., Mouillot, D., Mouquet, N. & Gravel, D. (2012) The dissimilarity of species interaction networks. *Ecology Letters*, **15**, 1353–1361.

Proulx, S.R., Promislow, D.E.L. & Phillips, P.C. (2005) Network thinking in ecology and evolution. *Trends in Ecology and Evolution*, **20**, 345–353.

Rayfield, B., Fortin, M.-J. & Fall, A. (2011) Connectivity for conservation: a framework to classify network measures. *Ecology*, **92**, 847–858.

Ricciardi, F., Boyer, M. & Ollerton, J. (2010) Assemblage and interaction structure of the anemonefish-anemone mutualism across the Manado region of Sulawesi, Indonesia. *Environmental Biology of Fishes*, **87**, 333–347.

Smaltschinski, T., Seeling, U. & Becker, G. (2012) Clustering forest harvest stands on spatial networks for optimised harvest scheduling. *Annals of Forest Science*, **69**, 651–657.

Thébault, E. (2013) Identifying compartments in presence-absence matrices and bipartite networks: insights into modularity measures. *Journal of Biogeography*, **40**, 759–768.

Tylianakis, J.M., Tscharntke, T. & Lewis, O.T. (2007) Habitat modification alters the structure of tropical host-parasitoid food webs. *Nature*, **445**, 202–205.

Urban, D. & Keitt, T. (2001) Landscape connectivity: a graph-theoretic perspective. *Ecology*, **82**, 1205–1218.

Whittaker, R. (1960) Vegetation of the Siskiyou mountains, Oregon and California. *Ecological Monographs*, **30**, 279–338.

Supporting Information

Additional Supporting Information may be found in the online version of this article.

Figure S1. Simulation scheme.

Appendix S1. Fixed point equations.