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Testing Spatial Autocorrelation in Weighted Networks: the Modes Permutation Test

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Abstract. In a weighted spatial network, as specified by an exchange matrix, the variances of the spatial values are inversely proportional to the size of the regions. Spatial values are no more exchangeable under independence, thus weakening the rationale for ordinary permutation and bootstrap tests of spatial autocorrelation. We propose an alternative permutation test for spatial autocorrelation, based upon exchangeable spatial modes, constructed as linear orthogonal combinations of spatial values. The coefficients obtain as eigenvectors of the standardised exchange matrix appearing in spectral clustering, and generalise to the weighted case the concept of spatial filtering for connectivity matrices. Also, two proposals aimed at transforming an acessibility matrix into a exchange matrix with with a priori fixed margins are presented. Two examples (inter-regional migratory flows and binary adjacency networks) illustrate the formalism, rooted in the theory of spectral decomposition for reversible Markov chains.

Keywords: bootstrap, local variance, Markov and semi-Markov processes, Moran's I, permutation test, spatial autocorrelation, spatial filtering, weighted networks

1 Introduction

Permutation tests of spatial autoccorelation are justified under *exchangeability*, that is the premise that the observed scores follow a permutation-invariant joint distribution. Yet, in the frequently encountered case of geographical data collected on regions differing in importance, the variance of a regional score is expected to *decrease* with the size of the region, in the same way that the variance of an average is inversely proportional to the size of the sample in elementary statistics: heteroscedasticity holds in effect, already under spatial independence, thus weakening the rationale of the celebrated spatial autocorrelation permutation test (e.g. Cliff and Ord 1973; Besag and Diggle 1977) in the case of a weighted network.

This paper presents an alternative permutation test for spatial autocorrelation, whose validity extends to the weighted case. The procedure relies upon *spatial modes*, that is linear orthogonal combinations of spatial values, originally based upon the eigenvectors of the standardized connectivity or adjacency matrix (Tiefelsdorf and Boots 1995; Griffth 2000). In contrast to regional scores, the variance of the spatial modes turn out to be constant under spatial independence, thereby justifying the *modes permutation test* for spatial autocorrelation.

Section 2.1 presents the definition of the local variance and Moran's I in the arguably most general setup for spatial autocorrelation, based upon the normalised, symmetrical *exchange matrix*, whose margins define regional weights (Bavaud 2008a). Section 2.2 presents, in the spirit of spatial filtering (Griffth 2000), the spectral decomposition of the exchange matrix, or rather of a standardised version of it, currently used in spectral graph theory (Chung 1997; von Luxburg 2007; Bavaud 2010), supplying the orthogonal components defining in turn the spatial modes. Section 2.3 presents the mode permutation test, and its bootstrap variant, illustrated in section 2.4 on Swiss migratory and linguistic data.

Section 3 addresses the familiar case of binary or weighted adjacency matrices, which have to be first converted into exchange matrices with a priori fixed margins. Two proposals, namely a simple rescaling with diagonal adjustment (Section 3.1) and the construction of time-embeddable exchange matrices (Section 3.2) are presented, and illustrated on the popular "distribution of Blood group A in Eire" dataset (Section 3.3).

2 Spatial autocorrelation in weighted netwoks

2.1 Local covariance and the exchange matrix

Consider a set of n regions with associated weights $f_i > 0$, normalized to $\sum_{i=1}^n f_i = 1$. Weights measure the importance of the regions, and define weighted regional averages and variances as

$$\bar{x} := \sum_{i=1}^n f_i x_i \qquad \mathrm{var}(x) := \sum_{i=1}^n f_i (x_i - \bar{x})^2 = \frac{1}{2} \sum_{ij} f_i f_j (x_i - x_j)^2 \ . \qquad (1)$$

Here $x = (x_i)$ represents a *density variable* or a *spatial field*, that is a numerical quantity attached to region i, transforming under aggregation $i, j \to [i \cup j]$ as $x_{[i \cup j]} = (f_i x_i + f_j x_j)/(f_i + f_j)$, as for instance "cars per inhabitants", "average income" or "proportion of foreigners".

The last identity in (1) is straightforward to check (Lebart 1969), and shows the variance to measure the average squared dissimilarity between pairs (i, j) of regions, selected independently with probability $f_i f_j$. A more general sampling scheme consists in selecting the regional pair (i, j) with probability e_{ij}, such that

$$e_{ij} \geq 0 \qquad e_{ij} = e_{ji} \qquad e_{i\bullet} := \sum_j e_{ij} = f_i \qquad e_{\bullet\bullet} = 1 \qquad (2)$$

where "$\bullet$" denotes the summation over the replaced index. A $n \times n$ matrix $E = (e_{ij})$ obeying (2) is called an *exchange matrix* (Berger and Snell 1957;

Bavaud 2008a), compatible with the regional weights f. The exchange matrix defines an undirected weighted network, with edges weights e_{ij} and regional weights $f_i = e_{i\bullet}$. It contains loops in general ($e_{ii} \geq 0$), denoting regional self-interaction or autarachy (Bavaud 1998).

By construction, the exchange matrix generates a reversible Markov transition matrix $W = (w_{ij})$ (Bavaud 1998) with stationary distribution f:

$$w_{ij} := \frac{e_{ij}}{f_i} \geq 0 \qquad \sum_j w_{ij} = 1 \qquad \sum_i f_i w_{ij} = f_j \qquad f_i w_{ij} = f_j w_{ji} = e_{ij} \quad . \tag{3}$$

W constitutes a row-normalized matrix of spatial weights, entering in the autoregressive models of spatial econometrics (see e.g. Anselin 1988; Cressie 1993; Leenders 2002; Haining 2003; Arbia 2006; LeSage and Pace 2009).

In spatial applications, the components of the exchange matrix are large for nearby regions and small for regions far apart. The quantity

$$\mathrm{var}_{\mathrm{loc}}(x) := \frac{1}{2} \sum_{ij} e_{ij} (x_i - x_j)^2 \tag{4}$$

defines the *local variance*, that is the average squared dissimilarity between neighbours. Comparing the local and the ordinary (weighted) variance defines *Geary's* c and *Moran's* I, measuring spatial autocorrelation (e.g. Geary 1954; Moran 1950 ; Cliff and Ord 1973; Tiefelsdorf and Boots 1995; Anselin 1995). Namely, $c(x) := \mathrm{var}_{\mathrm{loc}}(x)/\mathrm{var}(x)$ (differing from its usual variant by a factor $n/(n-1)$) and

$$I(x) := 1 - c(x) = \frac{\mathrm{var}(x) - \mathrm{var}_{\mathrm{loc}}(x)}{\mathrm{var}(x)} = \frac{\sum_{ij} e_{ij}(x_i - \bar{x})(x_j - \bar{x})}{\sum_i f_i (x_i - \bar{x})^2} \quad .$$

2.2 Spatial filtering and spatial modes

Spatial filtering primarily aims at visualizing and extracting the latent factors involved in spatial autocorrelation (Tiefelsdorf and Boots 1995; Griffith 2000, 2003; Griffith and Peres-Neto 2006; Chun 2008; Dray 2011; and references therein).

Its first step consists in spectrally decomposing a matrix expressing interregional connectivity in some way or another, such as the adjacency matrix or the exchange matrix. Various choices are often equivalent under uniform weighting of the regions, but the general weighted case calls for more precision. Arguably, the most fruitful decomposition considers the so-called *standardized exchange matrix* E^s, with components (Chung 1997, von Luxburg 2007; Bavaud 2010)

$$e^s_{ij} = \frac{e_{ij} - f_i f_j}{\sqrt{f_i f_j}} \quad \text{i.e.} \quad E^s = \Pi^{-\frac{1}{2}}(E - ff')\Pi^{-\frac{1}{2}} \quad \text{with} \quad \Pi = \mathrm{diag}(f) \quad . \tag{5}$$

Its spectral decomposition

$$E^s = U \Lambda U' \qquad \text{with} \quad U = (u_{i\alpha}) \text{ orthogonal and } \Lambda = \mathrm{diag}(\lambda) \text{ diagonal}$$

generates a *trivial* eigenvalue $\lambda_0 = 0$ associated with the trivial eigenvector $u_{i0} = \sqrt{f_i}$. The remaining *non-trivial* decreasingly ordered eigenvalues λ_α (for $\alpha = 1, \ldots, n-1$) lie in the interval $[-1, 1]$, as a consequence of the Perron-Froebenius theorem and the symmetry of E^s.

Also, $\lambda_1 = 1$ iff E is *reducible*, that is consisting of two or more disconnected components (Figure 1), and $\lambda_{n-1} = -1$ iff E is *bipartite*, i.e. partitionable into two sets without within connections (e.g. Kijima 1997; Aldous and Hill 2002).

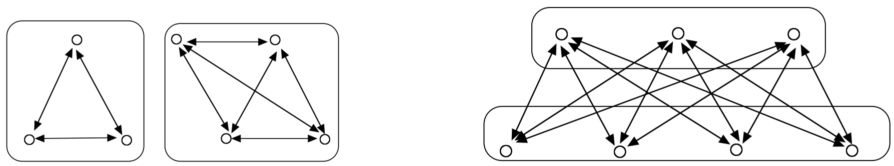

Fig. 1. Reducible network, with $\lambda_1 = 1$ (left) and bipartite network, with $\lambda_{n-1} = -1$ (right)

The exchange matrix itself expresses as

$$e_{ij} = f_i f_j + \sqrt{f_i f_j} \sum_{\alpha=1}^{n-1} \lambda_\alpha u_{i\alpha} u_{j\alpha} = f_i f_j [1 + \sum_{\alpha \geq 1} \lambda_\alpha c_{i\alpha} c_{j\alpha}] \tag{6}$$

where the *raw coordinates*

$$c_{i\alpha} := \frac{u_{i\alpha}}{u_{i0}} = \frac{u_{i\alpha}}{\pm\sqrt{f_i}}$$

can be used at visualizing distinct levels of spatial autocorrelation (Griffith 2003), or at specifying the positions of the n regions in a factor space (Bavaud 2010).

Raw coordinates are orthogonal and standardized, in the sense

$$\sum_i f_i c_{i\alpha} = \delta_{\alpha 0} \qquad\qquad \sum_i f_i c_{i\alpha} c_{i\beta} = \delta_{\alpha\beta} \quad . \tag{7}$$

As a consequence, the n regional values x can be converted into n *modal values* $\hat{x}$, and vice-versa, as

$$\hat{x}_\alpha := \sum_i f_i c_{i\alpha} x_i \qquad\qquad x_i = \sum_{\alpha \geq 0} c_{i\alpha} \hat{x}_\alpha = \bar{x} + \sum_{\alpha \geq 1} c_{i\alpha} \hat{x}_\alpha \quad . \tag{8}$$

Equations (8) express orthogonal, Fourier-like correspondence between regional values and modes. The latter depict global patterns, integrating the contributions from all regions. In particular, the trivial mode yields the field average: $\hat{x}_0 = \bar{x}$.

Borrowing an analogy from solid-state Physics, the spatial field x can describe the individual displacements of each of the n atoms of a crystal. The modes $\hat{x}$

then provide global parameters describing the *collective motion* of atoms, consisting of a superposition of sound waves or *harmonics*, whose specific eigenfrequencies are determined by the nature of the crystal, and whose knowledge permit to reconstruct the individual atomic displacements.

2.3 The modes permutation test

2.3.1 Heterodasticity of the spatial field The hypothesis H_0 of spatial independence requires the covariance matrix of the spatial field $X = (X_1, \ldots, X_n)$ to be diagonal with components *inversely proportional to the spatial weights*, that is of the form (see the Appendix)

$$\sigma_{ij} = \mathrm{Cov}(X_i, X_j) = \delta_{ij}\,\frac{\sigma^2}{f_i} \qquad \text{where} \quad \sigma^2 = \mathrm{Var}(\bar{X}) \ . \tag{9}$$

In its usual form, the *direct* or *regional permutation test* compares the observed value of Moran's $I(x)$ to a set of values $I(\pi(x))$, where $\pi(x)$ denotes a permutation (that is a sampling without replacement) of the n *regional values* x (e.g. Cliff and Ord 1973; Thioulouse et al. 1995; Li and al. 2007; Bivand et al. 2009a). Sampling with replacement, generating *bootstrap resamples* can also be carried out.

Both procedures are justified by the fact that the spatial variables X_i are identically distributed under H_0. Yet, (9) shows the latter assertion to be *wrong whenever the regional weights differ*, thus jeopardizing the rationale of the direct approach, based upon the permutation or the bootstrap of regional values.

The possible heteroscedasticity of regional values has been addressed by quite a few researchers, in particular in epidemiology, and various proposals (transformations of variables or weights, reformulations in terms of residuals, Bayesian approaches) have been investigated (see e.g. Waldhör 1996, Assunção and Reis 1999 or Haining 2003).

2.3.2 Homoscedasticity of the spatial modes As annouced in the introduction, this paper proposes a presumably new *modal test*, identical in spirit to the direct test but based upon *modes permutation*, together with a variant based upon *modes bootstrap*. Its existence results from two fortunate circumstances (see the Appendix), namely i) the homoscedasticity of the modes under H_0

$$\hat{\sigma}_{\alpha\beta} := \mathrm{Cov}(\hat{X}_\alpha, \hat{X}_\beta) = \delta_{\alpha\beta}\,\sigma^2 \qquad \text{with} \qquad \hat{X}_\alpha = \sum_i f_i\, c_{i\alpha}\, X_i \tag{10}$$

and ii) the simplicity of Moran's I expression in terms of spatial modes, which reads

$$I(x) \equiv I(\hat{x}) = \frac{\sum_{\alpha \geq 1} \lambda_\alpha \hat{x}_\alpha^2}{\sum_{\alpha \geq 1} \hat{x}_\alpha^2} \ . \tag{11}$$

As expected, the trivial mode $\hat{x}_0 = \bar{x}$ does not contribute to Moran's I. Under H_0, its expectation and variance under all remaining $(n-1)!$ non-trivial modes permutations read (see the Appendix)

$$E_\pi(I \mid \hat{x}) = \frac{1}{n-1}\sum_{\alpha\geq 1}\lambda_\alpha = \frac{\mathrm{trace}(W)-1}{n-1} \;\geq\; \frac{-1}{n-1} \tag{12}$$

$$\mathrm{Var}_\pi(I \mid \hat{x}) = \frac{s(\hat{x})-1}{(n-1)(n-2)}[\sum_{\alpha\geq 1}\lambda_\alpha^2 - \frac{1}{n-1}(\sum_{\alpha\geq 1}\lambda_\alpha)^2] \tag{13}$$

where

$$s(\hat{x}) := (n-1)\frac{\sum_{\alpha\geq 1}\hat{x}_\alpha^4}{(\sum_{\alpha\geq 1}\hat{x}_\alpha^2)^2} \geq 1$$

is a measure of modes dispersion.

2.3.3 The test The *modes autocorrelation test* consists in refuting H_0, which denies spatial dependence, if the value (11) of $I(\hat{x})$ is extreme w.r.t. the sample $\{I(\pi(\hat{x}))\}$ of B permuted or boostrapped mode values, that is if its quantile is near 1 (evidence of positive autocorrelation) or near 0 (negative autocorrelation).

As expected, the trivial mode $\hat{x}_0 = \bar{x}$ does not contribute to Moran's I. Also, $I(x)$ together with its permuted or boostrapped values lie in an interval comprised in $[\lambda_{n-1}, \lambda_1] \subseteq [-1, 1]$. The interval reduces to a single point $I(\pi(\hat{x})) \equiv I_0$, invariant under permutations or boostraping, with a corresponding variance (13) of zero, thus ruining the autocorrelation test, if (see 11, 13):

a) $s(\hat{x}) = 1$, that is $\hat{x}_\alpha^2 \equiv \hat{x}^2$ or equivalently $\hat{x}_\alpha \equiv \epsilon_\alpha\,\hat{x}$, where $\hat{x} \in \mathbb{R}$ and $\epsilon_\alpha = \pm 1$ for all $\alpha \geq 1$. Following (8), this occurs for "untestable" spatial fields of the form $x_i = \bar{x} + \hat{x}z_i$ where $z_i = \sum_{\alpha\geq 1}\epsilon_\alpha u_{i\alpha}/u_{i0}$ actually defines a set of 2^{n-1} configurations depending on the choice of the ϵ_α, whose sign is arbitrary, as is the sign of the eigenvectors u_α.
   Noticeably, the constant field $x_i \equiv \bar{x}$ is untestable, with a value $I(x) = 0/0$ not even defined. However intriguing, the empirical relevance of those "untestable" spatial fields is debatable, in view of the vanishing probability to encounter *exactly* such a spatial pattern.
b) $\lambda_\alpha \equiv \lambda$ for all $\alpha \geq 1$, as with the :
   i) *frozen networks* $E := E^{(0)}$, where $e_{ij}^{(0)} := f_i\delta_{ij}$ is the disconnected graph[1], associated to the immobile Markov chain with $\lambda_\alpha \equiv 1$ and $I(x) \equiv 1$ (Figure 2 left)
   ii) or as with the *perfectly mobile networks* $E := E^{(\infty)}$, where $e_{ij}^{(\infty)} := f_if_j$ is the complete weighted graph, free of distance-deterrence effects, associated to the memoryless Markov chain with $\lambda_\alpha \equiv 0$ and $I(x) \equiv 0$ (Figure 2 middle)

[1] Here the notations match the *higher-order discrete time extensions* of the exchange matrix, resulting (under weak regularity conditions) from the iteration of the Markov transition matrix as

$$E^{(r)} := \Pi W^r \qquad E^{(0)} = \Pi \qquad E^{(2)} = E\Pi^{-1}E \qquad E^{(\infty)} = ff' \ .$$

as well as with their linear combinations $E := aE^{(0)} + (1-a)E^{(\infty)}$. Also, networks made of $n = 2$ regions are untestable: they automatically satisfy b) and a) above (Figure 2 right).

Under the additional normal assumption $\hat{X}_\alpha \sim N(0, \sigma^2)$ for $\alpha \geq 1$, one can show $E(s(\hat{x})) = 3(n-1)/(n+1)$ by the Pitman-Koopmans theorem (Cliff and Ord 1981 p.43) and hence

$$E(\mathrm{Var}_\pi(I \mid \hat{x})) = \frac{2}{n^2-1}[\sum_{\alpha\geq 1}\lambda_\alpha^2 - \frac{1}{n-1}(\sum_{\alpha\geq 1}\lambda_\alpha)^2]$$
$$= \frac{2}{n^2-1}[\mathrm{tr}(W^2) - 1 - \frac{(\mathrm{tr}(W)-1)^2}{n-1}] \ . \qquad (14)$$

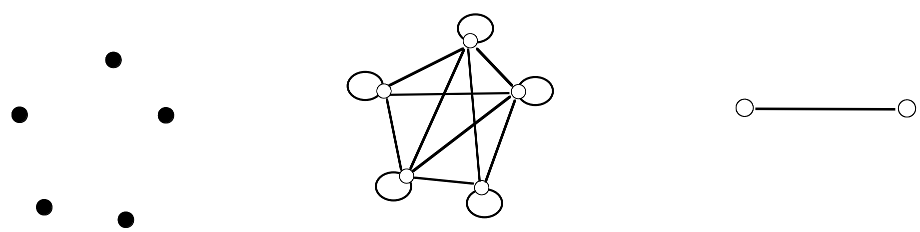

Fig. 2. Moran's $I(x)$ is constant, independent of the value of the field x for the disconnected or frozen network (left), for the fully connected or perfectly mobile network (middle), and their linear combinations. Its minimum $I(x) \equiv -1$ occurs for the loopless network with $n = 2$ (right).

2.4 Illustration: Swiss migratory and linguistic data

Flows constitute a major source of exchange matrices (e.g. Goodchild and Smith 1980; Willekens J. 1983; Fotheringham and O'Kelly, M.E. 1989; Sen and Smith 1995; Bavaud 1998, 2002). Let $n_{ij}(T)$ denote the number of units (people, goods, matter, etc.) initially in region i and located in region j after a time T. *Quasi-symmetric* flows are of the form $n_{ij} = a_i b_j c_{ij}$ with $c_{ij} = c_{ji}$, as predicted by Gravity modelling. They generate *reversible* spatial weights $w_{ij} := n_{ij}/n_{i\bullet}$, with stationary distribution f_i, whose product $f_i w_{ij}$ defines the exchange matrix e_{ij} (Bavaud 2002).

Consider the inter-regional migrations data $n_{ij}(T)$ between the $n = 26$ Swiss cantons for $T = 5$ years (1985-90), together with the spatial fields $x =$ "proportion of germanophones" or $x =$ "proportion of anglophones", for each canton. After determining the quasi-symmetric ML estimates $\hat{n}_{ij}$ (Bavaud 2002), the exchange matrix is computed, and so are the spatial modes $\hat{x}_\alpha$ from (8) and Moran's index $I(\hat{x})$ from (11). Figure 3 depicts the distribution of $10'000$ permutation and boostrap resamples of $I(\pi(\hat{x}))$, from which the bilateral p-values of Table 1 can be computed (see Section 3.2 for the details).

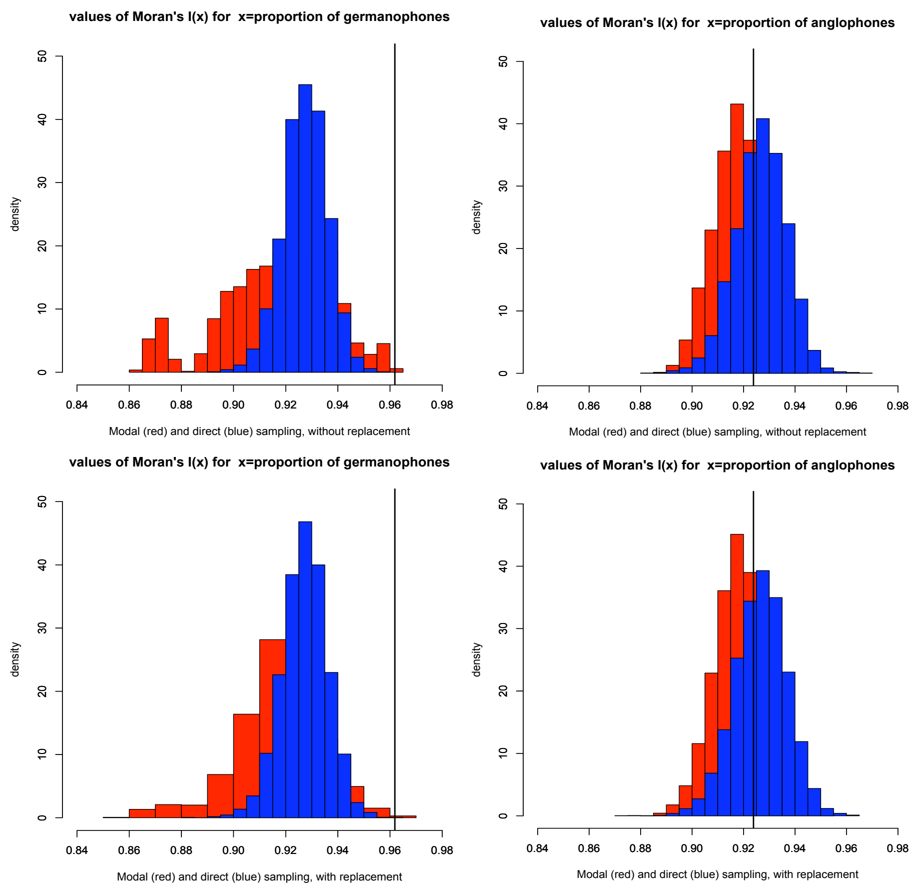

Fig. 3. Permutation (above) and bootstrap (below), modal (red) and regional (blue) testing of the "migation-driven" spatial autocorrelation among germanophones (left) and anglophones (right). $B = 10'000$ samples are generated each time, and compared with the observed I, marked vertically.

Most people do not migrate towards other cantons in five years, thus making the exchange matrix "cold" (that is close to the frozen $E^{(0)}$), with a dominating diagonal, accounting for the high values of I and $E_\pi(I)$ in Table 1.

Swiss native linguistic regions divide into German, French and Italian. Migrants tend to avoid to cross the linguistic barriers, thus accounting for the

	germanophones	anglophones
I	0.962	0.924
$E_\pi(I)$	0.917	0.917
$\mathrm{Var}_\pi(I\|\hat{x})$	0.00044	0.000082
z	2.13	0.74
$s(\hat{x})$	11.29	2.90

	germanophones	anglophones
modal permutation	.0006	.048
regional permutation	.0002	.075
modal bootstrap	.0036	.46
regional bootstrap	.0004	.76

Table 1. Left: observed I, its *modal permutation* expectation (12) and variance (13) together with the z-value $z := (I - E_\pi(I))/\sqrt{\mathrm{Var}_\pi(I|\hat{x})}$ and $s(\hat{x})$ in (13). Right: p-values associated to the modal and direct autocorrelation test, in their permutation and bootstrap variants.

spatial autocorrelation of "germanophones" (Table 1, right). Detecting spatial patterns in the anglophones repartition is, as expected from the above migratory scheme, less evident.

Bootstrap tests (modal or regional) appear here less powerful than permutation tests - a possibly true conjecture in general (Corcoran and Mehta 2002; Janssen and Pauls 2005).

Modal autocorrelation tests of "anglophones" seem more sensitive than their regional conterparts, while the opposite holds for "gemanophones": the usual test of autocorrelation underestimates the dispersion of the resampled values of $I(\pi(\text{germanophones}))$ (Figure 3, left), thus inflating the risk of type I errors for size-unadjusted Moran's I, in accordance with the simulation results of Assunção and Reis (1999).

3 Adjacency graphs and accessibilities

Very commonly, space is defined by a binary, off-diagonal and symmetric *connectivity* or *adjacency* matrix $n \times n$ matrix $A = (a_{ij})$, specifying whether distinct regions i and j are direct neighbours ($a_{ij} = 1$) or not ($a_{ij} = 0$). This scheme can also, as in gravity modelling, be extended to "weighted adjacencies" or *accessibilities* $a_{ij} = f(d_{ij})$ defined by a non-negative *distance deterrence function* $f(d_{ij})$ decreasing with the distance d_{ij} between distinct regions i and j.

In the sequel, we consider accessibility matrices with $a_{ij} \geq 0$, $a_{ij} = a_{ji}$ and $a_{ii} = 0$, with the interpretation that distinct regions i and j are direct neighbours iff $a_{ij} > 0$. By construction, the three quantities

$$\varepsilon_{ij} = \frac{a_{ij}}{a_{\bullet\bullet}} \qquad \kappa_{ij} = \frac{a_{ij}}{a_{i\bullet}} \qquad \sigma_i = \frac{a_{i\bullet}}{a_{\bullet\bullet}} = \varepsilon_{i\bullet} \tag{15}$$

respectively constitute an *exchange matrix*, its associated *transition matrix* and the *stationary distribution*, proportional to the (possibly weighted) number of neighbours or *degree*.

Although the series of steps of Section 2 can be wholly carried out by adopting $\mathcal{E} := (\varepsilon_{ij})$ as the reference exchange matrix, this procedure reveals itself far form satisfactory in general: exchanges between non-adjacent regions are precluded, as are the diagonal exchanges, thus mechanically generating negative eigenvalues in view of $0 = \text{trace}(\mathcal{E}^s) = 1 + \sum_{\alpha \geq 1} \lambda_\alpha$. Even worse, the normalized degree σ in (15), reflecting the regions centrality, strongly differs in general from the regions weights f, reflecting their importance: a densely populated region can be weakly connected to the rest of the territory, and inversely.

Proposals A and B below aim at converting an accessibility matrix A into an exchange matrix E with given margins f, while keeping the neighborhood structure expressed by A as intact as possible.

3.1 Proposal A: simple rescaling with diagonal adjustment

Define the symmetric exchange matrix

$$e_{ij} := \begin{cases} C b_i b_j a_{ij} & \text{if } i \neq j \\ h_i & \text{otherwise.} \end{cases} \tag{16}$$

where C, b and h are non-negative quantities obeying the normalisation condition (recall $a_{ii} = 0$)

$$C b_i \sum_j a_{ij} b_j + h_i = f_i \qquad \text{for all } i. \tag{17}$$

By construction, $e_{i\bullet} = f_i$ and, for $i \neq j$, $e_{ij} = 0$ whenever $a_{ij} = 0$.

An obvious choice, among many possibilities, consists in defining b as the first normalised eigenvector of the accessibility matrix A, that is obeying $Ab = \mu b$, where $\mu > 0$ is the largest eigenvalue of A, and b (normalised to $\sum_i b_i^2 = 1$) is non-negative by the Perron-Froebenius theorem on non-negative matrices. b_i (or b_i^2) is a measure of relative centrality of region i, sometimes referred to as *eigenvector centrality* in the social networks literature.

Condition (17) becomes $C\mu b_i^2 + h_i = f_i$, implying $C = (1-\eta)/\mu$, where the quantity $\eta := \sum_i h_i$ fixes the diagonal parameters to $h_i = f_i - (1-\eta) b_i^2$, and ranges in $\eta \in [H, 1]$ to insure the non-negativity of C and h, where $H := 1 - \min_i (f_i / b_i^2) \geq 0$.

The free parameter η controls the "autarchy of the network": in the limit $\eta \to 1$, one recovers the frozen network of Section 2.3.3, while $\eta \to H$ yields at least one region with $e_{ii} = 0$. Note that $e_{ii} = 0$ cannot hold for all regions, unless $b \equiv \sqrt{f}$ precisely, in which case $H = 0$.

3.2 Proposal B: time-embeddable exchange matrices

The second proposal is based upon the observation that κ_{ij} in (15) constitutes a *jump transition matrix*, defining the probability that j will be the next, *distinct* region to be visited after having been in region i (recall $\kappa_{ii} = 0$). Suppose in addition that, once arrived in j, the state remains in j for a certain random time t_j with cumulative distribution function $F_j(t)$, with average waiting time or *sojurn time* $\tau_j = \int t \, dF_j(t)$. This set-up precisely defines a so-called *semi-Markov process* (e.g. Çinlar 1975, Barbu and Limnios 2008).

Together, the stationary distribution σ_j (15) of the jump transition matrix κ_{ij} and the sojurn times τ_j determine the fraction of time spend in region j, that is the regional weight f_j, as (see e.g. Bavaud 2008b)

$$f_j = \frac{\sigma_j \tau_j}{\tau} \quad \text{where} \quad \tau := \sum_j \sigma_j \tau_j \quad \text{or equivalently} \quad \frac{1}{\tau} = \sum_j \frac{f_j}{\tau_j} \quad . \tag{18}$$

Furthermore, requiring exponentially distributed random times t_j ensures the semi-Markov process to be *continuous* or *time-embeddable*, that is of the form $W(t) = \exp(tR)$ (matrix exponential) where $R = (r_{ij})$ is the $n \times n$ *rate transition matrix*, with components $r_{ij} = (\kappa_{ij} - \delta_{ij})/\tau_i$. In particular,

$$\sum_j r_{ij} = 0 \qquad\qquad \sum_i f_i \, r_{ij} = 0 \quad . \tag{19}$$

The existence of transition matrices $W(t) = (w_{ij}(t))$ defined for *any continuous time* $t \geq 0$, rather than limited to integer values $t = 0, 1, 2, \ldots$, characterises time-embeddable Markov chains. The symmetry of the associated exchange matrices $e_{ij}(t) := f_i \, w_{ij}(t)$ follows from the reversibility of $W(t)$, itself insured by the reversibility of the jump matrix.

In summary, proposal B considers the adjacency matrix A as an *infinitesimal generator* of the exchange matrix E; tuning the freely adjustable sojurn times τ_j in (18) permits to transform any degree distribution σ into any given regional weights f, as required.

To achieve the pratical, numerical construction of the time-embeddable exchange matrix $E(t)$, consider the "standardised rate matrix" $Q = (q_{ij})$ with components

$$q_{ij} := f_i^{\frac{1}{2}} f_j^{-\frac{1}{2}} r_{ij} = \frac{\varepsilon_{ij} - \delta_{ij}\sigma_j}{\tau \sqrt{f_i f_j}} \quad . \tag{20}$$

Q is semi-negative definite (see the Appendix). Its eigenvalues μ_α and associated normalised eigenvectors $u_{i\alpha}$ satisfy $\mu_0 = 0$ with $u_{i0} = \sqrt{f_i}$, together with $\mu_\alpha \leq 0$ for the non-trivial eigenvalues $\alpha = 1, \ldots, n-1$. Now the eigenvectors of the standardized exchange matrix $E^s(t) = (e^s_{ij}(t))$ (5) turn out to be *identical* to those of Q, irrespectively of value of t, (see the Appendix), while the non-trivial eigenvalues of $E^s(t)$ are related to those of Q by $\lambda_\alpha(t) = \exp(\mu_\alpha t)$ for $\alpha = 1, \ldots, n-1$. Substituting back in (6) finally yields the exchange matrix as

$$e_{ij}(t) = f_i f_j [1 + \sum_{\alpha \geq 1} \lambda_\alpha(t) c_{i\alpha} c_{j\alpha}] \quad \text{where}\, c_{i\alpha} = \frac{u_{i\alpha}}{\sqrt{f_i}} \,\text{and}\, \lambda_\alpha(t) = \exp(\mu_\alpha t). \tag{21}$$

The eigenvalues $\lambda_\alpha(t)$ of the standardized exchange matrix $E^s(t)$ (5) are *non-negative*. This characterizes continuous-time Markov chain and *diffusive processes*, by contrast to *oscillatory processes* associated to negative eigenvalues, as in the bipartite network of Figure 1, or as in the direct accessibility-based approach (15).

As a matter of fact, temporal dependence enters through the quantity t/τ only: defining Q^* as (20) with $\tau = 1$ and μ^* as the corresponding non-trivial eigenvalues, one gets $\lambda_\alpha(t) = (\exp(\mu^*_\alpha))^{\frac{t}{\tau}}$, which can be directly susbstituted into (11) to compute Moran's I. Note the modes $\hat{x}_\alpha = \sum_i \sqrt{f_i} u_{i\alpha} x_i$, where the $u_{i\alpha}$ are the eigenvectors of Q^*, to be time-independant.

The free parameter t (or t/τ) represents the (relative) "age of the network". $E(t)$ tends to the frozen network for $t \to 0$, and to the perfectly mobile network for $t \to \infty$ (Section 2.3.3). One expects spatial autocorrelation to be more easily detected for small values of t, that is for networks able to sustain strong contrasts between local and global variances.

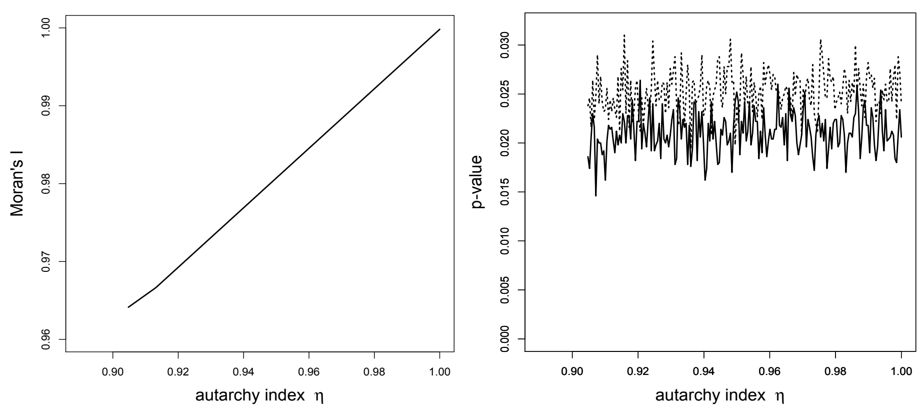

Fig. 4. "Blood group A in Eire" dataset: proposal A. Left: Moran's I as a function of $\eta \in [H, 1]$. Right: two-tailed p-values of the modes autocorrelation test, based upon $B = 10'000$ permutation (bold line) or bootstrap (dashed line) resamples.

3.3 Illustration: the distribution of Blood group A in Eire

Let us revisit the popular "distribution of Blood group A in Eire" dataset (Cliff and Ord 1973; Upton and Fingleton 1985; Griffith 2003; Tiefelsdorf and Griffith 2007), recording the percentage x of the 1958 adult population with of Blood group A in each of the $n = 26$ Eire counties, as well as the relative population size f, and the inter-regional adjacency matrix A (data from the R package `spdep` (Bivand 2009b)).

Following the "proposal A" procedure of Section 3.1 yields $\mu = 5.11$ and $H = 0.904$, echoing the existence of a region whose weight f_i is about ten times smaller than its "eigenvector centrality" b_i^2. Both permutation and boostrap modes autocorrelation tests reveal statistically significant spatial autocorrelation, without obvious dependence upon the autarchy index η.

"Proposal B" procedure of Section 3.2 yields p-values depicted in Figure 5, left. As expected, they reveal statistically significant spatial autocorrelation for small values of t/τ, and increase with t/τ. Starting the procedure with one

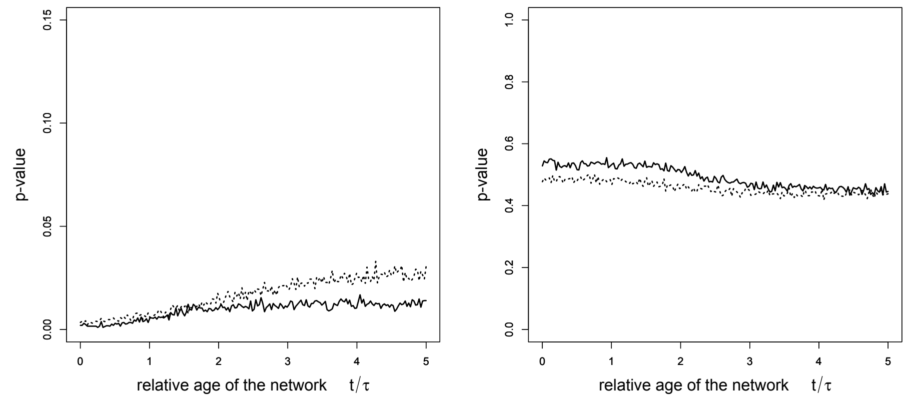

Fig. 5. "Blood group A in Eire" dataset: proposal B. Left: two-tailed p-values of the modes autocorrelation test, based upon $B = 10'000$ permutation (bold line) or bootstrap (dashed line) resamples. Right: the same procedure, applied to an arbitrarily selected permutation $\pi(x)$ of the original spatial field x.

among the many possible permutations of the field produces p-values as in Figure 5 (right) and indicates no spatial autocorrelation, as it must.

4 Conclusion

Real spatial networks are irregular and subject to aggregation. They are bound to exhibit regions differing in sizes or weights. This paper proposes a weighted analysis of Moran's I, in the possibly most general set-up provided by the exchange matrix formalism, rooted in the theory of reversible Markov chains and gravity flows of geographers.

Besides providing a rationale for overcoming the heteroscedasticity problem in the direct application of permutation or boostrap autocorrelation tests, the concept of spatial modes we have elaborated upon arguably generalises the concept of spectrally-based spatial filtering (e.g. Griffith 2003) to a weighted setting, and helps integrating other network-related issues in a unified setting: typically, the first non-trivial raw coordinate c_1 of Section 2.2 has been known for some time to provide the optimal solution to the spectral clustering problem, partitioning a weighted graph into two balanced components (e.g. Chung 1997; von Luxburg 2007; Bavaud 2010).

Finally, local variance (4) can be generalised to local inertias $\frac{1}{2}\sum_{ij} e_{ij} D_{ij}$ (where D represents a squared Euclidean distance between regions) and to local covariances $\frac{1}{2}\sum_{ij} e_{ij}(x_i - x_j)(y_i - y_j)$, whose future study may hopefully enrich formal issues and applications in spatial autocorrelation.

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5 Appendix

Proof of (7): U being orthogonal, $\sum_i f_i c_{i\alpha} c_{i\beta} = \sum_i u_{i\alpha} u_{i\beta} = \delta_{\alpha\beta}$ and $\sum_i f_i c_{i\alpha} = \sum_i \sqrt{f_i} u_{i\alpha} = \sum_i u_{i0} u_{i\alpha} = \delta_{\alpha 0}$.

Proof of (9): independence implies the functional form $\sigma_{ij} = \delta_{ij}\, g(f_i)$ where $g(f)$ expresses a possible size dependence. Consider the aggregation of regions j into super-region J, with aggregated field $X_J = \sum_{j\in J} f_j X_j / f_J$, where $f_J := \sum_{j\in J} f_j$. By construction,

$$g(f_J) = \mathrm{Var}(X_J) = \frac{1}{f_J^2} \sum_{i,j\in J} f_i f_j \sigma_{ij} = \frac{1}{f_J^2} \sum_{j\in J} f_j^2 g(f_j)$$

that is $f_J^2\, g(f_J) = \sum_{j\in J} f_j^2 g(f_j)$, with unique solution $g(f_j) = \sigma^2/f_j$ (and $g(f_J) = \sigma^2/f_J$), where $\sigma^2 = \mathrm{Var}(\bar{X})$.

Proof of (10): $\hat{\sigma}_{\alpha\beta} := \mathrm{Cov}(\hat{X}_\alpha, \hat{X}_\beta) = \sum_{ij} f_i f_j c_{i\alpha} c_{j\beta} \mathrm{Cov}(X_i, X_j) =$
$= \sigma^2 \sum_i f_i c_{i\alpha} c_{i\beta} = \sigma^2 \sum_i u_{i\alpha} u_{i\beta} = \sigma^2 \delta_{\alpha\beta}$.

Proof of (11): $\sum_{\alpha\geq 1} \hat{x}_\alpha^2 = \sum_{ij} \sqrt{f_i f_j} x_i x_j \sum_{\alpha\geq 0} u_{i\alpha} u_{j\alpha} - \hat{x}_0^2 = \sum_i f_i x_i^2 - \bar{x}^2 = \mathrm{var}(x)$. Also, $\mathrm{var}_{\mathrm{loc}}(x) = \frac{1}{2} \sum_{ij} e_{ij} (x_i - x_j)^2 = \sum_i f_i x_i^2 - \sum_{ij} e_{ij} x_i x_j = \sum_i f_i x_i^2 - \bar{x}^2 - \sum_{\alpha\geq 1} \lambda_\alpha \sum_i c_{i\alpha} x_i \sum_j c_{j\alpha} x_j = \mathrm{var}(x) - \sum_{\alpha\geq 1} \lambda_\alpha \hat{x}_\alpha^2$.

Proof of (12) and (13): define

$$a_\alpha := \frac{\hat{x}_\alpha^2}{\sum_{\beta\geq 1} \hat{x}_\beta^2} \qquad \text{with} \qquad \sum_{\alpha\geq 1} a_\alpha = 1 \qquad \text{and} \qquad I(\hat{x}) = \sum_{\alpha\geq 1} \lambda_\alpha a_\alpha \ .$$

Under H_0, the distribution of the non-trivial modes is exchangeable, i.e. $f(a) = f(\pi(a))$. By symmetry, $E_\pi(a_\alpha) = 1/(n-1)$, $E_\pi(a_\alpha^2) = s(x)/(n-1)^2$ where $s(x) = \sum_{\beta\geq 1} a_\beta^2/(n-1)$ and $E_\pi(a_\alpha a_\beta) = (1 - s(x)/(n-1))/[(n-1)(n-2)]$ for $\alpha \neq \beta$. Further substitution proves the result.

Proof of the semi-negative definitness of Q in (20): for any vector h,

$$0 \leq \frac{1}{2} \sum_{ij} \varepsilon_{ij} (h_i - h_j)^2 = \sum_i \sigma_i h_i^2 - \sum_{ij} \epsilon_{ij} h_i h_j = -\sum_{ij} (\epsilon_{ij} - \delta_{ij}\sigma_j) h_i h_j \ .$$

Relation between the eigen-decompositions of $E^s(t)$ and Q in (20): in matrix notation, $Q = \Pi^{\frac{1}{2}} R \Pi^{-\frac{1}{2}}$, and hence $Q\sqrt{f} = 0$ by (19), showing $u_0 = \sqrt{f}$ with $\mu_0 = 0$. Consider another, non-trivial eigenvector u_α of Q, with eigenvalue μ_α, orthogonal to $\sqrt{f}$ by construction. Identity $E(t) = \Pi \exp(tR)$ together with (5) yield

$$E^s(t) = \sum_{k\geq 0} \frac{t^k}{k!} Q^k - \sqrt{f}\sqrt{f}' \qquad\qquad E^s(t) u_\alpha = \sum_{k\geq 0} \frac{t^k \mu_\alpha^k}{k!} u_\alpha = \exp(\mu_\alpha t) u_\alpha \ .$$