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Helene H. Wagner

Stéphane Dray

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Generating spatially-constrained null models for irregularly spaced data using Moran spectral randomization methods

Helene H. Wagner[1] and Stéphane Dray[2]

[1] Department of Ecology and Evolutionary Biology, University of Toronto, 3359 Mississauga Road, Mississauga, ON, Canada L5L 1C6. Phone: +1-905-569-4702, email address: helene.wagner@utoronto.ca

[2] Université de Lyon, F-69000, Lyon ; Université Lyon 1 ; CNRS, UMR5558, Laboratoire de Biométrie et Biologie Evolutive, F-69622, Villeurbanne, France.

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Abstract

1. Spatial autocorrelation jeopardizes the validity of statistical inference, e.g., correlation and regression analysis. Restricted randomization methods can account for the effect of spatial autocorrelation in the observed data by building it into an empirical null model for hypothesis testing. This can be achieved e.g. based on conditional simulation, which fits a highly parameterized geostatistical model to the observed spatial structure, or, for data observed on a regular transect or grid, with Fourier spectral randomization methods that can flexibly model spatial structure at any scale. This paper uses Moran eigenvector maps to extend spectral randomization to irregularly spaced samples.
2. We present different algorithms to perform restricted randomization to suit different types of research questions: individual randomization of each variable, joint randomization of a group of variables while keeping within-group correlations fixed, and randomization with a fixed correlation between original data and randomized replicates (e.g., as input for simulation studies). The performance of the proposed Moran spectral randomization methods for regularly and irregularly spaced samples is assessed with correlation analysis of simulated data.
3. Moran spectral randomization closely matched the spatial structure of original simulated data sets, with identical or nearly identical Moran's *I* values and power spectra, depending on the algorithm. In correlation analysis of two stationary spatially autocorrelated variables, Moran spectral randomization produced correct type I error rates for stationary spatial data, even for very small and highly irregular samples, but was sensitive to linear trend. When one or both

variables lacked spatial structure, Moran spectral randomization tests were more conservative than correlation *t*-tests.

4. The proposed Moran spectral randomization method requires a minimum of parameterization and is able to address multivariate data with spatial structure at multiple scales, with the option of controlling levels of correlation with the original data. It can provide technically unlimited numbers of randomizations even for small samples while closely maintaining the spatial characteristics of uni- or multivariate data at all spatial scales. The method is applicable for correlation analysis of stationary, autocorrelated spatial or temporal series. Further research should assess whether the method can be extended to multiple regression analysis.

Keywords

Spatial autocorrelation, Fourier analysis, Moran eigenvector maps, correlation, time series analysis

Tweetable Abstract (max. 120 characters)

Moran spectral randomization methods for irregularly spaced, spatially autocorrelated, uni- and multivariate data.

Introduction

Ecological data often exhibit spatial autocorrelation, which poses challenges for statistical inference (Legendre 1993). Spatial autocorrelation may affect parameter estimates, type I error rates and statistical power of tests, including significance tests for correlation, partial correlation and regression coefficients that are widely used in ecology (Kühn & Dormann 2012). Methods for dealing with autocorrelation in correlation inference include modified parametric tests with adjustments for effective sample size (Dutilleul *et al*. 1993; Dutilleul, Pelletier & Alpargu 2008) and restricted randomization tests, which preserve the observed spatial autocorrelation and build it into the null model of the statistical hypothesis test (Fortin & Jacquez 2000; Fortin, Jacquez & Shipley 2012). For data sampled on a regular grid, this may be achieved by permuting observed values with toroidal shift methods (Upton & Fingleton 1985), conditional simulation methods that generate new values with similar spatial structure as the observed data (Fortin & Dale 2005), or with spectral randomization methods based on Fourier or wavelet analysis (Deblauwe, Kennel & Couteron 2012).

Conditional autoregressive simulation (Cressie 1991) can be applied to irregularly spaced data, but involves fitting geostatistical models to the observed data and may require substantial computing time (Fortin & Jacquez 2000). Complications may arise (*i*) if the observed spatial pattern (e.g., species abundance) results from multiple processes (e.g., dispersal, competition, predation) acting at different spatial scales, so that the observed data exhibit spatial structure at multiple scales; (*ii*) when analyzing multivariate data, where it may be necessary to randomize one set of variables simultaneously, keeping their correlations constant, while randomizing their correlations with a second set of variables (e.g., to test associations between functional groups of

77 species while keeping associations within groups constant); or (*iii*) when the spatial relationships
78 do not depend on geographic distance per se but on some definition of adjacency formalized in a
79 neighbor matrix (e.g., in a step-wise model of gene flow within a network of discrete populations,
80 or if the data relate to spatial units such as polygons, rather than point locations). The first two
81 situations may require large numbers of geostatistical parameters to be fitted, whereas in the third
82 case, distance-based geostatistical modeling may not be appropriate. Furthermore, conditional
83 simulation methods are not suitable for simulating replicates with a fixed correlation with the
84 original data (e.g., as needed for simulation studies to test performance of estimation methods in
85 regression analysis of spatial data; Beale *et al*. 2010) as they control the parameters of the
86 generating process, not the properties of the observed pattern. This paper provides a new
87 approach, Moran Spectral Randomization (MSR), to generate spatially-structured random
88 variables. Compared to existing approaches, MSR has the main advantages that (*i*) it can deal
89 with irregularly spaced data, (*ii*) it considers a spatial neighbor matrix, rather than geostatistical
90 modeling, and thus requires a minimum of parameterization, (*iii*) it preserves the multiscale
91 properties of spatial structures, (*iv*) and it is able to address multivariate data or (*v*) to control
92 levels of correlation with the original data.

93 Conceptually, MSR is related to Fourier spectral randomization (FSR). FSR is based on
94 Fourier analysis that decomposes an observed, regularly spaced spatial or temporal series into a
95 set of orthogonal sinusoids with different frequencies, i.e., spatial or temporal scales (harmonic
96 regression; Graybill 1976) using discrete Fourier transform (DFT; Cooley & Tukey 1965; Gauss
97 1866). The power spectrum of the series thus describes how the variance of the data is distributed
98 over the frequency components into which it may be decomposed, i.e., the squared correlation of

each sinusoid with the observed data quantifies the intensity of the observed pattern at the scale of the sinusoid.

In MSR, sinusoids are replaced by Moran eigenvector maps (MEM; Borcard & Legendre 2002; Dray, Legendre & Peres-Neto 2006; Griffith & Peres-Neto 2006; Peres-Neto & Legendre 2010) that can also be applied to irregular samples (Borcard & Legendre 2002). MEM are obtained through the eigen analysis of a spatial neighbor matrix which provides orthogonal eigenvectors maximizing the spatial autocorrelation measured by Moran's *I* (Moran 1950). Hence, MEM provides vectors allowing the decomposition of the variance of observed data, similar to the power spectrum in Fourier analysis.

We show that MSR provides technically unlimited numbers of randomizations even for small samples while maintaining the spatial characteristics of uni- or multivariate data at all spatial scales. Specifically, we show how to derive (*i*) replicate autocorrelated patterns under the null hypothesis of an absence of correlation with observed data, (*ii*) replicate autocorrelated multivariate patterns with constant correlation among variables, and (*iii*) replicate autocorrelated patterns that have a predefined correlation with observed data, as used in simulation studies (e.g., Beale *et al*. 2010). The performance of the proposed Moran spectral randomization methods is assessed with correlation analysis of simulated data for different sampling designs.

Methods

Spectral decomposition of variance and correlation using Moran Eigenvector Maps (MEM)

Spatial component regression (SCR; Wagner 2013) uses MEM to decompose the correlation r_{xy} between two variables **x** and **y**, observed at the same *n* sampling locations that may be regularly

or irregularly spaced, by spatial eigenvectors. It defines the correlation r_{xy} as the cross product of the vectors $\mathbf{r}_{xV}$ and $\mathbf{r}_{yV}$ that contain the correlation coefficients between **x** or **y** and each column in a matrix **V** that is defined as a set of orthogonal and uncorrelated (Rodgers, Nicewander & Toothaker 1984) spatial eigenvectors obtained by MEM. In matrix notation:

$$r_{xy} = \mathbf{r}_{xV}^{T} \mathbf{r}_{yV} , \quad (1)$$

where ^{T} indicates the transpose. The columns in **V** are the eigenvectors of a symmetric and doubly centered spatial weight matrix **W** (Dray, Legendre & Peres-Neto 2006). Matrix **W** is constructed by first defining a neighbor matrix of size $n \times n$ that contains values of one for pairs of observations i and j if j is considered a neighbor of i, and zero otherwise. Each neighbor j of observation i is then assigned a spatial weight, which may be binary or e.g. a function of the inverse geographic distance between i and j, and weights may optionally be row-standardized. Note that spatial eigenvectors in **V** are defined as a function of **W** only, without reference to the values of variables **x** or **y** observed at the sampling locations, and **V** is thus the same for **x** and **y**. MEM results in a matrix **V** where the spatial eigenvectors are already sorted from the largest scale to the finest scale.

A set of n observations with a full-rank spatial weights matrix **W** of size $n \times n$ will result in $n - 1$ orthogonal and uncorrelated (Griffith 2000) eigenvectors $\mathbf{V}_k$ associated with eigenvalues λ_k, while a single eigenvector with zero eigenvalue is dropped. Under these conditions, the vector $\mathbf{r}^2_{xV}$ of squared correlations of **x** with eigenvectors in **V** forms a power spectrum (i.e., a spectral decomposition of the variance of the observed data **x** on the orthonormal basis **V**):

$$r^2_{xV} = \mathbf{r}_{xV}^{T} \mathbf{r}_{xV} = 1. \quad (2)$$

Note that if **W** is not of full rank, there will be multiple zero eigenvalues and their associated eigenvectors may not be uncorrelated. To ensure that eq. 2 holds in this situation, a vector of ones is added to the subset of eigenvectors with null eigenvalues, the subspace spanned by these eigenvectors is then re-orthogonalized, the unit eigenvector is removed, and the last eigenvector in the subset is dropped. This procedure is implemented in the R function 'scores.listw' provided in Supporting Material 3.

The variable **x** can be decomposed on an orthonormal basis **V**, so that **x** can be fully recreated from $\mathbf{r}_{\mathbf{xV}}$, **V**, and its mean $\bar{\mathbf{x}}$ and standard deviation $s(\mathbf{x})$:

$$\mathbf{x} = \bar{\mathbf{x}} + s(\mathbf{x})\left(n-1\right)^{0.5}\mathbf{V}\mathbf{r}_{\mathbf{xV}} \quad (3)$$

A key feature of MEM is the additive decomposition of Moran's *I* (Dray, Legendre & Peres-Neto 2006; Dray 2011). Eigenvalues λ_k are conveniently rescaled by multiplication with $h = n / \Sigma_{ij} w_{ij}$, where w_{ij} are the elements of **W**, so that the rescaled eigenvalue $m_k = h\lambda_k$ corresponds to Moran's I_k of eigenvector $\mathbf{v}_k$, with $k = \{1, \ldots, n-1\}$. According to Dray (2011), Moran's $I_{\mathbf{x}}$ of variable **x** can then be found by:

$$I_{\mathbf{x}} = {\mathbf{r}^2_{\mathbf{xV}}}^{\mathrm{T}}\mathbf{m}, \quad (4)$$

which means that global spatial autocorrelation ($I_{\mathbf{x}}$) of the variable **x** is the sum of Moran's *I* of all spatial eigenvectors, weighted by the variance each eigenvector explains in the observed variable **x** (i.e., weighted by the power spectrum).

Basic algorithm for Moran spectral randomization (MSR)

The spatial structure of **x** can be defined by its global level of autocorrelation ($I_{\mathbf{x}} = {\mathbf{r}^2_{\mathbf{xV}}}^{\mathrm{T}}\mathbf{m}$, eq. 4) and its multiscale decomposition defined by its power spectrum ($\mathbf{r}^2_{\mathbf{xV}}$, eq. 2). In this context, MSR

aims to find a vector of coefficients $\mathbf{a} = \left[a_1, \cdots, a_{n-1}\right]^{\mathrm{T}}$ so that the random variable $\mathbf{x}_{\mathrm{rand}} = (n-1)^{0.5}$ **Va** satisfies different conditions. Squared values in **a** should be a power spectrum so that:

$$\sum_{i=1}^{n-1} a_i^{\,2} = 1 \qquad \text{(C1)}$$

To preserve the global level of autocorrelation $I_{\mathbf{x}}$, the vector **a** must satisfy equation 4 and this leads to the second condition:

$$I_{\mathbf{x}} = \sum_{i=1}^{n-1} a_i^{\,2} m_i = \sum_{i=1}^{n-1} r_{\mathbf{xv}_i}^{\,2} m_i \qquad \text{(C2)}$$

Lastly, to preserve the multiscale structure, the vector **a** must satisfy equation 2 and this leads to the third condition:

$$a_i^{\,2} = r_{\mathbf{xv}_i}^{\,2} \qquad \text{(C3)}$$

We provide different algorithms to find adequate values for **a** satisfying strictly or softly the different conditions. Condition C1 is strictly preserved in all algorithms.

The Singleton procedure

Choosing $\left|a_i\right| = r_{\mathbf{xv}_i}$ satisfies both conditions C2 and C3. Hence, the solution consists in randomizing the sign of correlations independently for each single eigenvector (i.e., $a_i = \pm r_{\mathbf{xv}_i}$). This approach allows also generating multivariate replicates with constant correlation among variables (see below).

The Pair procedure

This procedure aims to satisfy strictly condition C2 and softly condition C3. Instead of preserving the contribution of each single eigenvector in the multiscale decomposition, we consider pairs of eigenvectors $\mathbf{v}_i$ and $\mathbf{v}_j$. This subset is stored by column in the matrix $\mathbf{V}_k$. In this case, the condition C3 is partially satisfied by preserving the proportion of variance explained by a pair of eigenvectors. We obtain the new condition C3':

$$R^2_{\mathbf{xV}_k} = a_i^2 + a_j^2 = r_{\mathbf{xv}_i}^2 + r_{\mathbf{xv}_j}^2 \qquad \text{(C3')}$$

The condition C3' corresponds to the equation of a circle of radius $R_{\mathbf{xV}_k} = \sqrt{R^2_{\mathbf{xV}_k}}$. To preserve the level of autocorrelation for the pair of eigenvectors, the condition C2 becomes:

$$I_{\mathbf{xV}_k} = a_i^2 m_i + a_j^2 m_j = r_{\mathbf{xv}_i}^2 m_i + r_{\mathbf{xv}_j}^2 m_j \qquad \text{(C2')}$$

The resolution of the system of equations C2' and C3' leads exactly to the solution provided by the singleton procedure. An alternative is to satisfy only the condition C3' that corresponds to the equation of a circle. The solutions are obtained by drawing a random angle Φ_{rand} from a uniform distribution between [0 – 2π] and then compute the values $\left\{a_i = R_{\mathbf{xV}_k} \cos\left(\Phi_{\text{rand}}\right); a_j = R_{\mathbf{xV}_k} \sin\left(\Phi_{\text{rand}}\right)\right\}$. Note that this method does not completely preserve the global autocorrelation values (condition C2' and C2). However, it will be considered as a valuable alternative as it can be easily extended to generate multivariate replicates with constant correlation among variables or univariate replicates with fixed correlation with observed data (see below).

The Triplet procedure

This procedure aims to satisfy strictly condition C2 and softly condition C3. In this case, the multiscale decomposition is preserved for triplets of eigenvectors $\mathbf{v}_i$, $\mathbf{v}_j$ and $\mathbf{v}_l$ stored by column in matrix $\mathbf{V}_k$. We thus obtain the new condition C3'':

$$R^2_{\mathbf{xV}_k} = a_i^2 + a_j^2 + a_l^2 = r_{\mathbf{xv}_i}^2 + r_{\mathbf{xv}_j}^2 + r_{\mathbf{xv}_l}^2 \qquad \text{(C3'')}$$

The condition C3' corresponds to the equation of a sphere of radius $R_{\mathbf{xV}_k}$. To preserve the level of autocorrelation for the triplet of eigenvectors, the condition C2 becomes:

$$I_{\mathbf{xV}_k} = a_i^2 m_i + a_j^2 m_j + a_l^2 m_l = r_{\mathbf{xv}_i}^2 m_i + r_{\mathbf{xv}_j}^2 m_j + r_{\mathbf{xv}_l}^2 m_l \qquad \text{(C2'')}$$

To satisfy both conditions C2'' and C3'', a first random angle Φ_{rand} is drawn from a uniform distribution between]0 – 2π[(bounds excluded to avoid division by zero). Then, a second angle is computed by $\Theta_{rand} = \text{asin}\left(\sqrt{\frac{I_{\mathbf{xV}_k} / R^2_{\mathbf{xV}_k} - m_l - (m_i - m_l)\sin^2\left(\Phi_{\text{rand}}\right)}{(m_j - m_i)\sin^2\left(\Phi_{\text{rand}}\right)}}\right) = \text{asin}\left(\sqrt{Z}\right)$.

The solutions are then given by

$$\left\{a_i = \pm R_{\mathbf{xV}_k} \cos\left(\Theta_{\text{rand}}\right)\sin\left(\Phi_{\text{rand}}\right); a_j = \pm R_{\mathbf{xV}_k} \sin\left(\Theta_{\text{rand}}\right)\sin\left(\Phi_{\text{rand}}\right); a_l = \pm R_{\mathbf{xV}_k} \cos\left(\Phi_{\text{rand}}\right)\right\}.$$

Practical implementation for Pair and Triplet procedures

MSR consists in randomly redistributing the variance of **x** within blocks of spatial eigenvectors $\mathbf{V}_k$. The following steps are performed:

1. Divide the n-1 eigenvectors in K sets $\mathbf{V}_k$ ($k = \{1,\ldots,K\}$) (see below for details). If the number of eigenvectors is not a multiple of 2 (Pair) or 3 (Triplet), there will be one incomplete block $\mathbf{V}_K$, whose (randomly selected) eigenvectors are treated by the singleton procedure.

2. Repeat for each complete subset $\mathbf{V}_k$.

2.1. Determine the pooled variance in $\mathbf{x}$ explained by the eigenvectors ($R^2_{\mathbf{xV}_k}$), the associated autocorrelation ($I_{\mathbf{xV}_k}$) and (for Pair) the observed angle $\Phi_{\mathbf{x}.k} = \text{atan2}\left(r_{\mathbf{xv}_j}, r_{\mathbf{xv}_i}\right)$.

2.2. Sample the angle Φ_{rand}.

2.3. For the triplet procedure, compute the second angle $\Theta_{\text{rand}} = \text{asin}\left(\sqrt{Z}\right)$. If the value of Φ_{rand} leads to a value of Z not comprised in [0-1], then step 2.2. is repeated. If this existing condition is not satisfied after a number of trials (e.g., 100), the Singleton procedure is used for each eigenvector in the block $\mathbf{V}_k$.

2.4. Determine the coefficients a_i , a_j for the Pair procedure, as $\left\{a_i = R_{\mathbf{xV}_k}\cos\left(\Phi_{\text{rand}}\right); a_j = R_{\mathbf{xV}_k}\sin\left(\Phi_{\text{rand}}\right)\right\}$, or a_i , a_j and a_l for the Triplet procedure, as $\left\{a_i = \pm R_{\mathbf{xV}_k}\cos\left(\Theta_{\text{rand}}\right)\sin\left(\Phi_{\text{rand}}\right); a_j = \pm R_{\mathbf{xV}_k}\sin\left(\Theta_{\text{rand}}\right)\sin\left(\Phi_{\text{rand}}\right); a_l = \pm R_{\mathbf{xV}_k}\cos\left(\Phi_{\text{rand}}\right)\right\}$

3. Optional: Compute the new random variable $\mathbf{x}_{\text{rand}} = \bar{\mathbf{x}} + s(\mathbf{x})\left(n-1\right)^{0.5}\mathbf{V}\mathbf{r}_{\mathbf{xV}}$.

Two or more observed variables may be randomized separately by sampling Φ_{rand} independently for each variable and for each subset $\mathbf{V}_k$. This basic procedure will randomize the correlation between replicates of different variables.

Subsets $\mathbf{V}_k$ (step 1) can be defined randomly or by selecting consecutive eigenvectors. As Triplet preserves values of Moran's $I_{\mathbf{x}}$ (condition C2''), both procedures can be used but empirical experiments showed that the selection of consecutive eigenvectors often produces undetermined results in step 2.3. (i.e., $Z \notin \left[0-1\right]$) and thus leads to the use of the singleton

procedure. Hence, the random assignment of eigenvectors in subsets should be preferred with the Triplet procedure. Here, we restricted random assignment to triplets with all positive or all negative eigenvalues.

Pair procedure does not preserve the global level of autocorrelation (i.e., $I_{\mathbf{x}} \neq I_{\mathbf{x}_{rand}}$). As the spatial eigenvectors in **V** are automatically sorted by decreasing Moran components, i.e., rescaled eigenvalues m_k, pairs of consecutive eigenvectors will have similar autocorrelation. In this case, the use of subsets of consecutive eigenvectors should be preferred as it ensures that the randomized replicate $\mathbf{x}_{\text{rand}}$ will have very similar spatial structure as the original variable **x** (i.e., $I_{\mathbf{x}} \approx I_{\mathbf{x}_{\text{rand}}}$). Supporting Material 1, Fig. S1.1 illustrates the effect of shifting variance between consecutive spatial eigenvectors.

Generating multivariate replicates with constant correlation among variables

To jointly randomize *m* variables, i.e., a data matrix **X** with *n* rows and *m* columns, while maintaining their correlations across all spatial scales, Singleton or Pair procedures may be used. For the Singleton procedure, the sign for correlations with each eigenvector is randomized once for all *m* variables, so that their signs either all change or all remain unchanged. For Pair, a single Φ_{rand} is sampled independently for each subset $\mathbf{V}_k$ and applied to all *m* variables. Then, step 2.4 is performed for each variable **x** using $\Phi_{\text{rand}} + \Phi_{\mathbf{x}.k}$ instead of Φ_{rand}:

$\left\{a_i = R_{x\mathbf{V}_k} \cos\left(\Phi_{\mathbf{x}.k} + \Phi_{\text{rand}}\right); a_j = R_{x\mathbf{V}_k} \sin\left(\Phi_{\mathbf{x}.k} + \Phi_{\text{rand}}\right)\right\}$. See Supporting Material 2 for a mathematical proof.

Generating replicates with fixed correlation with observed data

To obtain a replicate $\mathbf{x}_{rand}$ with similar spatial structure as the observed variable $\mathbf{x}$ and a fixed correlation r_{fix} with $\mathbf{x}$, the Pair method should be used with $\Phi_{rand} = \text{acos}(r_{fix})$, the same for all k, and step 2.4 should be performed using $\Phi_{\mathbf{x}.k} \pm \Phi_{rand}$. The sign needs to be randomized independently for each subset $\mathbf{V}_k$, i.e., each pair of consecutive spatial eigenvectors. The effectiveness of this procedure to obtain multiple non-identical replicates is investigated in the simulation study below.

Illustration with simulated data

All simulations and analyses were performed in R 3.1.1 (R Core Team 2014). The development version of the 'adespatial' package available at https://r-forge.r-project.org/R/?group_id=195 provides general-use functions to implement the proposed Moran spectral randomization procedures. Supporting Material 3 contains a customized version of these functions that can be used with the R code in Supporting Material 4 to reproduce the simulation study.

To illustrate the proposed randomization algorithms, we simulated five standardized variables with different spatial patterns on the same grid with 40 × 40 cells (Supporting Material 1, Fig. S1.1, top row). X0 served as baseline without spatial pattern and was sampled randomly from a standard normal distribution using R function 'rnorm'. X1 and X2 each represent stationary spatial patterns at small (X1) and large scale (X2). The two variables were generated with the function 'RFsimulate' of the R package 'RandomFields' using an isotropic exponential variogram model with variance = 5 and nugget = 0 for both variables, and with scale = 1 for X1 and scale = 3 for X2. Variable X3, which has a more complex spatial structure, was derived as

X3 = X0 + X1 + X2 and is thus correlated with these variables. X4 represents the same spatial pattern as X1 but with an added linear trend along the y-axis, violating the assumption of stationarity.

The full sample (n = 1600) was subsampled in different ways, resulting in ten different samples per simulated data set: a full sample ('Full 1600'); a regular sampling design ('Regular 400'), obtained by discarding every second row and column of the full sample; and a random sample of the same size ('Random 400'). The remaining sampling designs were chosen to illustrate the effect of stronger irregularity in the spacing of observations, as well as a further reduction in sample size. The 70 sampling locations of the well-known oribatid mite data set (Borcard, Legendre & Drapeau 1992; Borcard & Legendre 1994), sampled within an original extent of 2.5 × 10 m, were mapped onto a 40 × 13 grid, resulting in sampling design 'Orib 70', covering one third of the extent of the full sample. The 13 levels of x-coordinates in 'Orib 70' were repeated three times to obtain sample 'Orib 210' with n = 210, covering the extent of the full sample. To further explore the behavior of Moran spectral randomization for small and highly irregularly-spaced samples, we subsampled 'Orib 70' in five different ways to a sample size of 32 – 35: a random subsample ('Random 35'); an artificially spaced out sample, deleting every second level of y coordinates ('Spaced 32'); a clumped sample, retaining only y-coordinates < 23 ('Clumped 35'); a long-stretched sample, retaining only x-coordinates < 8 ('Long 34'); and a bi-modally clustered sample, retaining only y-coordinates that were either < 13 or > 30 ('Bimodal 34').

For the 'Full 1600' and 'Regular 400' sampling designs, we applied queen's case neighbor definition, resulting in an average of 5.06 and 4.44 neighbors per sampling location, respectively.

For all eight irregular sampling designs, we defined neighbors with Gabriel graphs (Supporting Material, Fig. S1.2), resulting in averages of 3.37 – 4.06 neighbors per sampling location. For all sampling designs, **W** was defined using inverse distance weights followed by row-standardization. This means that nearby neighbors receive more weight than more distant ones, and the weights of all neighbors sum to one for each sampling location.

Evaluation of method performance

Statistical properties of replicates

Replicates of spatially autocorrelated variables should mimic the spatial pattern of the original data at all spatial scales but be statistically independent of these. When plotted in space, high and low values should thus show similar spacing but their physical locations should be randomized. In statistical terms, MSR replicates should have the same overall spatial autocorrelation (Moran's *I*) and the same multi-scale spatial structure (power spectrum) as the original variables but, on average, be uncorrelated with the original data, with the same distribution of empirical correlation coefficients as expected from independently simulated data.

To compare these statistical properties between MSR procedures, we simulated a data set with variables X0 – X4, as defined above, and subsampled it for each of the ten sampling designs. For each combination of variable and sampling design, we generated 30 replicates each with the following methods: Singleton, Pair, Triplet, and, for benchmarking, fully independent replicates generated by simulating 30 additional data sets ('Null'). We determined for each combination of simulated variable **x**, sampling design and procedure: (*i*) the correlation of replicates with the original variable (type I error rate of a *t*-test for the correlation of **x** with its

replicates); (*ii*) the preservation of global autocorrelation $I_{\mathbf{x}}$ and of the power spectrum (mean correlation between the power spectrum $\mathbf{r}^2_{\mathbf{xV}}$ of **x** and the power spectra of its replicates); and (*iii*) for the pairs method only, the bias and precision of Moran's *I* of replicates compared to Moran's *I* of **x**. Bias in Moran's *I* was independent of the magnitude of Moran's *I* (controlling for sampling design), hence absolute, not relative deviations were assessed. The entire simulation was repeated 100 times and values averaged across trials.

Spectral randomization tests for correlation

A randomization test for the correlation between two spatial variables sampled from uncorrelated populations should have a correct type I error rate α, i.e., if $\alpha = 0.05$, the null hypothesis of no correlation should be rejected in 5% of independent cases (where the expected correlation is zero), and high power to detect linear dependence (where the expected correlation different from zero). To assess the performance of MSR in significance tests of correlation, we ran 5000 simulations and estimated type I error rates from independent variable pairs, and power from correlated variable pairs. For each simulation run, we generated two data sets, $X0_1 – X4_1$ and $X0_2 – X4_2$, where each pair of corresponding variables (e.g., $X2_1$ and $X2_2$) was simulated independently with the geostatistical parameters defined above and thus had the same expected spatial autocorrelation structure, though empirical values of Moran's *I* may differ. The expected correlation between any two variables from different data sets was zero (linear independence), whereas the expected correlation between X3 and X0, X1, or X2, or between X4 and X1, from the same data set was non-zero (linear dependence). For each sampling design and variable pair, we tested the correlation with four different methods: correlation *t*-test (using R function

347 'cor.test') and three MSR randomization tests with 199 replicates each, using Pair, Triplet
348 (random triplets), and Singleton procedures.

349 *Spectral randomization with additional constraints*
350 To illustrate the implementation of further constraints, we simulated 100 data sets and created 30
351 replicates per data set with the following algorithms: joint MSR of all variables X0 – X4 to
352 maintain their cross-correlations, using Singleton and Pair methods, and MSR with r_{fix}= {0, 0.3, -
353 0.5, 0.7} to obtain replicates that have a fixed correlation with the original variables. We
354 evaluated the distribution of correlation coefficients between the original variables and their
355 replicates, and the distribution of correlation coefficients among replicates.

356 **Results**

357 ***Statistical properties of replicates***
358 For stationary patterns X0 – X3, MSR methods created patterns that were visually comparable to
359 the original data but differed in the locations of low and high values (Supporting Material 1, Fig.
360 S1.3). For X4, a non-stationary pattern with linear trend along the y-axis, replicates included a
361 randomization of the trend angle (Supporting Material 1, Fig. S1.3, bottom). Pairs randomized
362 trend direction more flexibly than Triplet and Singleton methods (Supporting Material 1, Fig.
363 S1.4).
364 MSR replicates of a random normal variable (X0) were uncorrelated on average (mean = 0)
365 with the original variable, but the distribution of correlations had higher variance than expected
366 from true random variables (not shown). This is reflected in higher rates of statistically

significant correlations between each original variable **x** and its replicates, based on a parametric *t*-test for regression coefficients (Fig. 1). On average, correlations with **x** were highest for the Singleton method, lower for Triplet, and lowest for Pair. For variable X2 with stationary, large-scale spatial autocorrelation, replicates of all methods showed increased rates of significant correlations with **x**, with differences between sampling designs that appear to be related to differences in average Moran's *I* (Supporting Material, Fig. S1.5).

Replicate simulations of the data generating process ('Null') showed high variability in their global Moran's *I* (Fig. 2, left: standard deviation rescaled by multiplication with $(n - 1)^{0.5}$ to account for sample size) and power spectra (multi-scale spatial structure), as indicated by a low correlation between the power spectrum of **x** and those of its replicates (Fig. 2, right). In contrast, the Singleton method completely preserved both Moran's *I* and power spectra. The Triplet method preserved Moran's *I* but resulted in some variation in the power spectrum, and the Pair method showed variation both in Moran's *I* and the power spectrum.

The Pair method does not strictly preserve Moran's *I* but its MSR replicates were generally unbiased for the random normal variable X0 (Supporting Material, Fig. S1.6). For the spatially autocorrelated variable X2, bias was negligible for large data sets but Moran's *I* of replicates showed a slight negative bias for the small sampling designs.

Spectral randomization tests for correlation

When correlating two random normal variables $X0_1$ and $X0_2$, or one random normal variable (X0) and one stationary, spatially autocorrelated variable (X1, X2 or X3), the parametric *t*-test produced correct type I error rates. Specifically, the empirical type I error rates fell within the 95% confidence interval for a binomial distribution bin(n, p) with n = 5000 simulated data sets

389 and $p = \alpha = 0.05$ (Fig. 3 A, B). In these situations, all three MSR procedures (especially the
390 Triplet method) showed slightly deflated type I error rates, making tests more conservative.
391 When correlating any two spatially autocorrelated variables (X1, X2, X3 or X4), the *t*-test
392 showed high inflated type I error rates. MSR methods maintained correct or slightly deflated type
393 I error rates for correlations among stationary variables (X1, X2 or X3), but showed considerably
394 deflated error rates for the correlation between X4 and X1, X2 or X3 (Fig. 3 C, D). Error rates
395 were independent of the observed level of Moran's *I* of the randomized variable. When
396 correlating two non-stationary variables $X4_1$ and $X4_2$, where both variables included trend along
397 the y-axis, MSR tests showed generally lower type I error rates than *t*-tests (Fig. 3 E). Especially
398 the Singleton and Triplet procedures were less affected by non-stationarity.
399 When testing the correlation between $X0_1$ and $X3_1$, where the *t*-test was applicable ($X0_1$
400 being a random normal), all three MSR methods had slightly lower statistical power to detect
401 linear dependence than the *t*-test (Fig. 4). Averaged across the five smallest sampling designs,
402 Pair reached approximately 98% of the power of the *t*-test, Triplet 97%, and Singleton 96%. This
403 order remained constant for all other types of variable pairs with linear dependence, where the *t*-
404 test was not applicable (results not shown).

405 ***Spectral randomization with additional constraints***
406 Correlations between variable pairs with linear dependence ($X3_1$ vs. $X0_1$, $X1_1$, or $X2_1$; $X4_1$ vs.
407 $X1_1$) calculated using Equation 1 were identical to Pearson correlation coefficients. When
408 correlated variables were jointly randomized using the Singleton or Pair procedures, their cross-
409 correlations were completely preserved (results not shown).

When each variable was randomized with the additional constraint of a fixed correlation with the original variable, using the Pair method, sampling designs with uneven sample size n ('Random 35', 'Clumped 35') completely preserved the predefined correlation r_{fix} (Supporting Material, Fig. S1.2 A). For even n, the presence of an incomplete block (where the Singleton method was used for one randomly selected spatial eigenvector) introduced some variation in the correlation with the original variable. For large samples ($n \geq 400$), this variation was negligible, but for small samples ($n \leq 100$), there was considerable variation as well as a negative bias, so that on average, correlations with the original variable were slightly weaker than specified by r_{fix}.

For sampling designs with uneven n, the correlation among replicates generated with the constraint of r_{fix} differed systematically from the correlation among replicates generated without such a constraint (Supporting Material, Fig. S1.2 B). The mean correlation among replicates was predictable by r^2_{fix}, whereas the standard deviation varied with r_{fix} and with the level of spatial autocorrelation. The factor by which the standard deviation of the correlation among replicates was inflated, compared to replicates without the constraint of r_{fix}, followed $2^{0.5}(1 - r^2_{fix})$ (Supporting Material, Fig. S1.2 C).

Discussion

Comparisons of Moran spectral randomization procedures

This paper presents algorithms for restricted randomization of irregularly spaced data with Moran spectral randomization that can be applied to a wide range of sampling designs for which restricted randomization methods were limited so far. Moran spectral randomization provides a framework to build spatially constrained null models allowing statistical inference in the presence

of spatial autocorrelation. While Moran spectral randomization has been developed here for two-dimensional spatial data, it is also applicable to one-dimensional transect data or time series analysis. The method produces a technically unlimited number of non-identical replicates even for small samples (except for the Singleton method with $2^{(n-1)}$ unique replicates), without requiring additional parameters beyond the explicit definition of neighbors and spatial weights in matrix **W**.

The MSR replicates mimic the spatial characteristics of the original variables in terms of global autocorrelation and multiscale patterns. These properties allow controlling the type I error rate of statistical tests (e.g., bivariate correlation) in the presence of autocorrelation. Ideally, replicates should also be uncorrelated to the original variable to ensure power. These two objectives (similar spatial structure and independence with the original variables) are antagonist and thus defined a gradient from considering the original variable (spatial properties fully preserved but no independence) to its full randomization (complete independence with the original variable but no spatial constraint). Hence, we provide different procedures that correspond to different trade-offs between these two extremes.

The Singleton procedure imposes the strongest spatial constraints and thus produces replicates with the highest degree of correlation with the original variable. It performs surprisingly well in randomization tests, even for small spatial samples, despite the limitation of $2^{(n-1)}$ unique replicates. The method is simple to implement and can also be used to jointly randomize a group of variables. The Singleton method should be preferred when it is important to strictly preserve the spatial characteristics of the original variables even if this means that its replicates are more correlated with the original variable.

453 The Pair procedure is the least strict concerning the spatial constraints and thus provides
454 MSR replicates with the lowest degree of correlation with the original variables. Spatial
455 characteristics are quite well preserved and thus it appears as good compromise and allows for
456 joint randomization as well as randomization with fixed correlation. The Pair procedure should
457 be used when it is considered important to randomize correlation at each spatial eigenvector and
458 reduce overall correlation with the original variable, or when the slightly lower statistical power
459 or the limited number of 2^{n-1} unique replicates of the Singleton method are of concern.
460 Lastly, the Triplet procedure that is supposed to combine the advantages of singleton and
461 pairs did not perform as well as the other methods and could also be time-consuming (due to the
462 existing conditions is step 2.3). Hence, it is not generally recommended in future work.

463 ***Performance of Moran spectral randomization in correlation analysis***
464 Moran spectral randomization replicates preserved Moran's *I* of the original variable either
465 perfectly (Singleton, Triplet methods) or approximately (Pair). In contrast, replicate simulations
466 of the generating process (i.e., conditional simulation with known geostatistical parameters)
467 resulted in considerable variation of Moran's *I* among replicates (Fig. 2, left). The marked
468 quantitative difference illustrates an important conceptual distinction: spectral randomization
469 methods randomize the observed pattern, whereas conditional simulation simulates independent
470 outcomes of the underlying process, assuming that it has been correctly parameterized, e.g.,
471 through geostatistical analysis of the empirical data. Preserving Moran's *I* may be advantageous
472 when using replicates to control for the effect of spatial autocorrelation in the empirical data on
473 statistical inference, such as correlation or regression analysis. Information on the variability of
474 Moran's *I* given a specified model of the generating process will be most important when the

475 inference concerns the difference between two or more empirically observed patterns (Fortin *et*
476 *al*. 2003; Remmel & Fortin 2013).

477 Moran randomization tests produced correct, or slightly deflated, type I errors for
478 correlation analysis, independent of sample size or sample configuration, unless both variables
479 exhibited non-stationarity, here in the form of linear trend along the y-axis (variable X4).
480 Likewise, Fourier spectral randomization is known to be sensitive to trend. Recently, Deblauwe,
481 Kennel & Couteron (2012) presented a wavelet-based spectral randomization method (dual-tree
482 complex wavelet transform; DT-CWT) that proved more robust than DFT in correlation
483 inference. Wavelet analysis has also been used to control spatial autocorrelation in regression
484 analysis of gridded data (Carl & Kühn 2008), but such wavelet methods are not available for
485 irregularly spaced data. Non-stationarity, which can occur in many different flavors, remains an
486 unsolved problem especially in spatial regression analysis (Beale *et al*. 2010). Further research is
487 needed to assess the performance of Moran spectral randomization in spatial regression analysis
488 when stationarity assumptions are met and its sensitivity to various types of non-stationarity.

489 ***Flexible algorithms for restricted randomization of irregularly spaced spatial data***

490 The proposed algorithms are applicable to a wide range of research questions and hypotheses. We
491 presented MSR in the case of spatial autocorrelation but the method can also be used in the case
492 of temporal of phylogenetic dependence (Peres-Neto 2006). Bivariate correlation analysis can be
493 achieved by randomizing one variable, or randomizing both variables independently (Lennon
494 2000). The possibility to jointly randomize several variables while maintaining their cross-
495 correlations will be especially interesting in ecological community analysis that aims at assessing
496 community interactions. Different groups of species (e.g., functional groups) may thus be

497 randomized separately, maintaining empirical species associations within groups but breaking
498 them between groups. Molecular genetic analysis provides another example where alleles of the
499 same locus may need to be randomized jointly but independently of other loci. While Moran
500 spectral randomization can control correlations among jointly randomized variables even for non-
501 normal data including binary variables, the randomized variables may show a different statistical
502 distribution than the observed variables. Depending on the purpose of randomization, an iterative
503 approach following the steps in iterative amplitude adjusted Fourier transform may be needed
504 (Deblauwe, Kennel & Couteron 2012; Schreiber & Schmitz 1996), where the simulated values
505 are replaced by the observed values according to their rank (though this may alter correlations
506 between variables). Further research should focus on application of MSR to multivariate
507 abundance or presence-absence data.

508 The Pair procedure can be used to generate replicates with similar multi-scale spatial
509 structure (approximate preservation of Moran's I and power spectrum) and a predefined
510 correlation r_{fix} with the original variable. This will be useful in simulation studies aimed e.g. at
511 testing the performance of spatial regression methods in the presence of correlation among
512 predictor variables (multi-collinearity; Beale *et al*. 2010; Dormann *et al*. 2013). In order to
513 completely maintain r_{fix}, an uneven sample size n should be used, though the variation for even n
514 will be negligible for larger samples.

515 ***Conclusion***

516 Moran spectral randomization allows to efficiently use regularly or irregularly spaced spatial data
517 for assessing the correlation between two observed variables. It provides null distributions that
518 explicitly incorporate the observed autocorrelation at all spatial scales without the need for

519 geostatistical parameter estimation as required for conditional simulation. Instead, Moran spectral
520 randomization relies on the definition of spatial relationships in a spatial weights matrix **W**, and
521 the implications of the choice of **W** on correlation and regression analysis with various methods,
522 including those based on MEM, are not well understood (Stakhovych & Bijmolt 2009).
523 In the limited scope of simulations presented here, focusing on correlation analysis under
524 stationary conditions, Moran spectral randomization produced correct or slightly conservative
525 type I error rates and high statistical power (96% - 98% of the power of a parametric *t*-test). MSR
526 thus performed well, even for very small and highly irregularly spaced samples. If the method
527 can be extended to multiple regression analysis, Moran spectral randomization may provide a
528 new avenue for the problem of correctly accounting for spatial autocorrelation in species
529 distribution modeling when the parameters of the underlying spatial ecological process
530 generating the spatial patterns are unknown (e.g.: Beale *et al*. 2010; Kühn & Dormann 2012).

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536 ## Data Accessibility

537 All necessary R code to reproduce the data is provided in Supporting Materials 3 & 4.

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610

Figure captions

Figure 1: Type I error rates for a *t*-test of the correlation between each observed variable and its replicates, for the random normal variable X0 (top row) and variable X2 with stationary, large-scale spatial autocorrelation. 'Null' refers to fully independent replicates of the generating process.

Figure 2: Spatial properties of replicates for fully independent replicates of the generating process ('Null') and for MSR replicates generated with Pair, Triplet or Singleton procedures. Left: bar chart of the mean standard deviation of Moran's *I* of replicates, rescaled by $(n - 1)^{0.5}$ (to account for sample size) and pooled across sampling designs, separately for X0 (dark grey bars) and X2 (light gray bars). Note that Triplet and Singleton methods showed zero variation. Right: bar chart of the mean correlation between the power spectra of the original variable and its replicates, pooled across sampling designs, for X0 (dark gray bars) and X2 (light gray bars).

Figure 3: Boxplots of empirical type I error rates across 5000 simulation runs, for different types of variable pairs and randomization methods, pooled across all 10 sampling designs. Fig. A shows the correlation between two random normal variables, Fig. B the correlation between a random variable X0 and a variable with stationary spatial autocorrelation (X1, X2, or X3), Fig. C the correlation between any two variables with stationary spatial autocorrelation, Fig. D a correlation between a variable with non-stationary spatial autocorrelation (X4: linear trend along y-axis) and any variable with stationary spatial autocorrelation, and Fig. E the correlation between two variables with non-stationary spatial autocorrelation. The number below each boxplot reports the mean, and gray polygons indicate a 95% confidence interval for the expected type I error rate.

633 Fig. 4: Relative power of MSR randomization tests. Each boxplot shows the distribution of
634 ten empirical power estimates to detect the correlation between variables X0 and X3, using Pair,
635 Triplet or Singleton procedures, rescaled by the corresponding empirical power estimate of a
636 parametric correlation *t*-test. The ten values for each method were obtained from 5000 simulated
637 data sets, subsampled with each of the five sampling designs with sample sizes between 32 and
638 35, randomizing either X0 or X3.

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