

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

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

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## **1** Generating spatially-constrained null models for irregularly spaced

## 2 data using Moran spectral randomization methods

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#### 17 Abstract

18 1. Spatial autocorrelation jeopardizes the validity of statistical inference, e.g., correlation and 19 regression analysis. Restricted randomization methods can account for the effect of spatial 20 autocorrelation in the observed data by building it into an empirical null model for hypothesis 21 testing. This can be achieved e.g. based on conditional simulation, which fits a highly 22 parameterized geostatistical model to the observed spatial structure, or, for data observed on a 23 regular transect or grid, with Fourier spectral randomization methods that can flexibly model 24 spatial structure at any scale. This paper uses Moran eigenvector maps to extend spectral 25 randomization to irregularly spaced samples.

26 2. We present different algorithms to perform restricted randomization to suit different types of
27 research questions: individual randomization of each variable, joint randomization of a group
28 of variables while keeping within-group correlations fixed, and randomization with a fixed
29 correlation between original data and randomized replicates (e.g., as input for simulation
30 studies). The performance of the proposed Moran spectral randomization methods for
31 regularly and irregularly spaced samples is assessed with correlation analysis of simulated
32 data.

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

38		variables lacked spatial structure, Moran spectral randomization tests were more conservative
39		than correlation <i>t</i> -tests.
40	4.	The proposed Moran spectral randomization method requires a minimum of parameterization
41		and is able to address multivariate data with spatial structure at multiple scales, with the
42		option of controlling levels of correlation with the original data. It can provide technically
43		unlimited numbers of randomizations even for small samples while closely maintaining the
44		spatial characteristics of uni- or multivariate data at all spatial scales. The method is
45		applicable for correlation analysis of stationary, autocorrelated spatial or temporal series.
46		Further research should assess whether the method can be extended to multiple regression
47		analysis.

### 48 Keywords

49 Spatial autocorrelation, Fourier analysis, Moran eigenvector maps, correlation, time series50 analysis

### 51 **Tweetable Abstract (max. 120 characters)**

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

54

#### 4

#### 55 Introduction

56 Ecological data often exhibit spatial autocorrelation, which poses challenges for statistical 57 inference (Legendre 1993). Spatial autocorrelation may affect parameter estimates, type I error 58 rates and statistical power of tests, including significance tests for correlation, partial correlation 59 and regression coefficients that are widely used in ecology (Kühn & Dormann 2012). Methods 60 for dealing with autocorrelation in correlation inference include modified parametric tests with 61 adjustments for effective sample size (Dutilleul et al. 1993; Dutilleul, Pelletier & Alpargu 2008) 62 and restricted randomization tests, which preserve the observed spatial autocorrelation and build 63 it into the null model of the statistical hypothesis test (Fortin & Jacquez 2000; Fortin, Jacquez & 64 Shipley 2012). For data sampled on a regular grid, this may be achieved by permuting observed 65 values with toroidal shift methods (Upton & Fingleton 1985), conditional simulation methods 66 that generate new values with similar spatial structure as the observed data (Fortin & Dale 2005), 67 or with spectral randomization methods based on Fourier or wavelet analysis (Deblauwe, Kennel 68 & Couteron 2012).

69 Conditional autoregressive simulation (Cressie 1991) can be applied to irregularly spaced 70 data, but involves fitting geostatistical models to the observed data and may require substantial 71 computing time (Fortin & Jacquez 2000). Complications may arise (i) if the observed spatial 72 pattern (e.g., species abundance) results from multiple processes (e.g., dispersal, competition, 73 predation) acting at different spatial scales, so that the observed data exhibit spatial structure at 74 multiple scales; (ii) when analyzing multivariate data, where it may be necessary to randomize 75 one set of variables simultaneously, keeping their correlations constant, while randomizing their 76 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

99 each sinusoid with the observed data quantifies the intensity of the observed pattern at the scale100 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.

108 We show that MSR provides technically unlimited numbers of randomizations even for 109 small samples while maintaining the spatial characteristics of uni- or multivariate data at all 110 spatial scales. Specifically, we show how to derive (i) replicate autocorrelated patterns under the 111 null hypothesis of an absence of correlation with observed data, (ii) replicate autocorrelated 112 multivariate patterns with constant correlation among variables, and (iii) replicate autocorrelated 113 patterns that have a predefined correlation with observed data, as used in simulation studies (e.g., 114 Beale et al. 2010). The performance of the proposed Moran spectral randomization methods is 115 assessed with correlation analysis of simulated data for different sampling designs.

#### 116 Methods

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

118 Spatial component regression (SCR; Wagner 2013) uses MEM to decompose the correlation  $r_{xy}$ 

119 between two variables  $\mathbf{x}$  and  $\mathbf{y}$ , observed at the same *n* sampling locations that may be regularly

120 or irregularly spaced, by spatial eigenvectors. It defines the correlation  $r_{xx}$  as the cross product of 121 the vectors  $\mathbf{r}_{xy}$  and  $\mathbf{r}_{yy}$  that contain the correlation coefficients between x or y and each column in 122 a matrix V that is defined as a set of orthogonal and uncorrelated (Rodgers, Nicewander & 123 Toothaker 1984) spatial eigenvectors obtained by MEM. In matrix notation:  $r_{\mathbf{x}\mathbf{y}} = \mathbf{r}_{\mathbf{x}\mathbf{V}}^{\mathrm{T}}\mathbf{r}_{\mathbf{y}\mathbf{V}},$ 124

(1)

where  $^{T}$  indicates the transpose. The columns in **V** are the eigenvectors of a symmetric and 125 126 doubly centered spatial weight matrix W (Dray, Legendre & Peres-Neto 2006). Matrix W is 127 constructed by first defining a neighbor matrix of size  $n \times n$  that contains values of one for pairs 128 of observations *i* and *j* if *j* is considered a neighbor of *i*, and zero otherwise. Each neighbor *j* of 129 observation *i* is then assigned a spatial weight, which may be binary or e.g. a function of the 130 inverse geographic distance between *i* and *j*, and weights may optionally be row-standardized. 131 Note that spatial eigenvectors in V are defined as a function of W only, without reference to the 132 values of variables x or y observed at the sampling locations, and V is thus the same for x and y. 133 MEM results in a matrix V where the spatial eigenvectors are already sorted from the largest 134 scale to the finest scale.

135 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 136 137  $\lambda_k$ , while a single eigenvector with zero eigenvalue is dropped. Under these conditions, the vector 138  $\mathbf{r}^{2}_{\mathbf{x}\mathbf{V}}$  of squared correlations of **x** with eigenvectors in **V** forms a power spectrum (i.e., a spectral 139 decomposition of the variance of the observed data  $\mathbf{x}$  on the orthonormal basis  $\mathbf{V}$ ):

140 
$$r_{\mathbf{x}\mathbf{V}}^2 = \mathbf{r}_{\mathbf{x}\mathbf{V}}^{T} \mathbf{r}_{\mathbf{x}\mathbf{V}} = 1.$$
(2)

141	Note that if $W$ is not of full rank, there will be multiple zero eigenvalues and their
142	associated eigenvectors may not be uncorrelated. To ensure that eq. 2 holds in this situation, a
143	vector of ones is added to the subset of eigenvectors with null eigenvalues, the subspace spanned
144	by these eigenvectors is then re-orthogonalized, the unit eigenvector is removed, and the last
145	eigenvector in the subset is dropped. This procedure is implemented in the R function
146	'scores.listw' provided in Supporting Material 3.
147	The variable $\mathbf{x}$ can be decomposed on an orthonormal basis $\mathbf{V}$ , so that $\mathbf{x}$ can be fully
148	recreated from $\mathbf{r}_{xV}$ , <b>V</b> , and its mean $\overline{\mathbf{x}}$ and standard deviation $s(\mathbf{x})$ :
149	$\mathbf{x} = \overline{\mathbf{x}} + s(\mathbf{x}) (n-1)^{0.5} \mathbf{V} \mathbf{r}_{\mathbf{x}\mathbf{V}} $ (3)
150	A key feature of MEM is the additive decomposition of Moran's I (Dray, Legendre &
151	Peres-Neto 2006; Dray 2011). Eigenvalues $\lambda_k$ are conveniently rescaled by multiplication with <i>h</i>
152	= $n / \sum_{ij} w_{ij}$ , where $w_{ij}$ are the elements of <b>W</b> , so that the rescaled eigenvalue $m_k = h\lambda_k$ corresponds
153	to Moran's $I_k$ of eigenvector $\mathbf{v}_k$ , with $k = \{1,, n-1\}$ . According to Dray (2011), Moran's $I_x$ of
154	variable $\mathbf{x}$ can then be found by:
155	$I_{\mathbf{x}} = \mathbf{r}_{\mathbf{x}\mathbf{V}}^{2} \mathbf{m}, \tag{4}$

157 *I* of all spatial eigenvectors, weighted by the variance each eigenvector explains in the observed 158 variable  $\mathbf{x}$  (i.e., weighted by the power spectrum).

## 159 Basic algorithm for Moran spectral randomization (MSR)

160 The spatial structure of **x** can be defined by its global level of autocorrelation ( $I_x = \mathbf{r}_{xV}^2 \mathbf{m}$ , eq. 4)

and its multiscale decomposition defined by its power spectrum ( $\mathbf{r}_{xv}^2$ , eq. 2). In this context, MSR

162 aims to find a vector of coefficients  $\mathbf{a} = [a_1, \dots, a_{n-1}]^T$  so that the random variable  $\mathbf{x}_{rand} = (n-1)^{0.5}$ 

163 Va satisfies different conditions. Squared values in a should be a power spectrum so that:

164 
$$\sum_{i=1}^{n-1} a_i^2 = 1$$
 (C1)

165 To preserve the global level of autocorrelation  $I_x$ , the vector **a** must satisfy equation 4 and 166 this leads to the second condition:

167 
$$I_{\mathbf{x}} = \sum_{i=1}^{n-1} a_i^2 m_i = \sum_{i=1}^{n-1} r_{\mathbf{x}\mathbf{v}_i}^2 m_i$$
(C2)

168

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

171 
$$a_i^2 = r_{xv_i}^2$$
 (C3)

172

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.

175

176 The Singleton procedure

177 Choosing  $|a_i| = r_{xv_i}$  satisfies both conditions C2 and C3. Hence, the solution consists in

178 randomizing the sign of correlations independently for each single eigenvector (i.e.,  $a_i = \pm r_{xv_i}$ ).

179 This approach allows also generating multivariate replicates with constant correlation among

180 variables (see below).

182 *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

187 eigenvectors. We obtain the new condition C3':

188 
$$R_{\mathbf{x}_{k}}^{2} = a_{i}^{2} + a_{j}^{2} = r_{\mathbf{x}_{i}}^{2} + r_{\mathbf{x}_{j}}^{2}$$
(C3')

189 The condition C3' corresponds to the equation of a circle of radius  $R_{xv_k} = \sqrt{R_{xv_k}^2}$ . To preserve the 190 level of autocorrelation for the pair of eigenvectors, the condition C2 becomes:

191 
$$I_{\mathbf{x}\mathbf{V}_k} = a_i^2 m_i + a_j^2 m_j = r_{\mathbf{x}\mathbf{v}_i}^2 m_i + r_{\mathbf{x}\mathbf{v}_j}^2 m_j$$
(C2')

192 The resolution of the system of equations C2' and C3' leads exactly to the solution provided by 193 the singleton procedure. An alternative is to satisfy only the condition C3' that corresponds to the 194 equation of a circle. The solutions are obtained by drawing a random angle  $\Phi_{rand}$  from a uniform 195 distribution between  $[0 - 2\pi]$  and then compute the values

196 
$$\left\{a_i = R_{xv_k}\cos(\Phi_{rand}); a_j = R_{xv_k}\sin(\Phi_{rand})\right\}$$
. 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).

201

202 The Triplet procedure

203 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

205 matrix  $\mathbf{V}_k$ . We thus obtain the new condition C3'':

206 
$$R_{\mathbf{x}_{k}}^{2} = a_{i}^{2} + a_{j}^{2} + a_{l}^{2} = r_{\mathbf{x}_{i}}^{2} + r_{\mathbf{x}_{j}}^{2} + r_{\mathbf{x}_{l}}^{2}$$
(C3")

207 The condition C3' corresponds to the equation of a sphere of radius  $R_{xv_k}$ . To preserve the level of 208 autocorrelation for the triplet of eigenvectors, the condition C2 becomes:

209 
$$I_{\mathbf{x}\mathbf{v}_{k}} = a_{i}^{2}m_{i} + a_{j}^{2}m_{j} + a_{l}^{2}m_{l} = r_{\mathbf{x}\mathbf{v}_{i}}^{2}m_{i} + r_{\mathbf{x}\mathbf{v}_{j}}^{2}m_{j} + r_{\mathbf{x}\mathbf{v}_{l}}^{2}m_{l}$$
(C2'')

210 To satisfy both conditions C2'' and C3'', a first random angle 
$$\Phi_{rand}$$
 is drawn from a

uniform distribution between  $]0 - 2\pi[$  (bounds excluded to avoid division by zero). Then, a

212 second angle is computed by 
$$\Theta_{rand} = \operatorname{asin}\left(\sqrt{\frac{I_{\mathbf{x}\mathbf{v}_k} / R_{\mathbf{x}\mathbf{v}_k}^2 - m_l - (m_i - m_l)\sin^2(\Phi_{rand})}{(m_j - m_i)\sin^2(\Phi_{rand})}}\right) = \operatorname{asin}\left(\sqrt{Z}\right).$$
213

The solutions are then given by

214 
$$\left\{a_i = \pm R_{xv_k}\cos(\Theta_{rand})\sin(\Phi_{rand}); a_j = \pm R_{xv_k}\sin(\Theta_{rand})\sin(\Phi_{rand}); a_l = \pm R_{xv_k}\cos(\Phi_{rand})\right\}.$$

215

### 216 Practical implementation for Pair and Triplet procedures

217 MSR consists in randomly redistributing the variance of **x** within blocks of spatial eigenvectors

- 218  $V_k$ . The following steps are performed:
- 219 1. Divide the *n*-1 eigenvectors in *K* sets  $\mathbf{V}_k$  ( $k = \{1, ..., K\}$ ) (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  $V_K$ , whose (randomly selected) eigenvectors are treated by the singleton
- 222 procedure.

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

224 2.1. Determine the pooled variance in **x** explained by the eigenvectors  $(R_{xy}^2)$ , the

- 225 associated autocorrelation  $(I_{\mathbf{x}\mathbf{v}_k})$  and (for Pair) the observed angle  $\Phi_{\mathbf{x},k} = \operatorname{atan2}(r_{\mathbf{x}\mathbf{v}_i}, r_{\mathbf{x}\mathbf{v}_i})$ .
- 226 2.2. Sample the angle  $\Phi_{\text{rand}}$ .
- 227 2.3. For the triplet procedure, compute the second angle  $\Theta_{\text{rand}} = \operatorname{asin}(\sqrt{Z})$ . If the value
- 228 of  $\Phi_{rand}$  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

230 procedure is used for each eigenvector in the block  $\mathbf{V}_k$ .

231 2.4. Determine the coefficients 
$$a_i$$
,  $a_j$  for the Pair procedure, as

232 
$$\left\{a_i = R_{xv_k} \cos(\Phi_{rand}); a_j = R_{xv_k} \sin(\Phi_{rand})\right\}, \text{ or } a_i, a_j \text{ and } a_l \text{ for the Triplet procedure, as}$$

233 
$$\left\{a_i = \pm R_{xv_k} \cos(\Theta_{rand}) \sin(\Phi_{rand}); a_j = \pm R_{xv_k} \sin(\Theta_{rand}) \sin(\Phi_{rand}); a_l = \pm R_{xv_k} \cos(\Phi_{rand})\right\}$$

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

235

236 Two or more observed variables may be randomized separately by sampling  $\Phi_{rand}$ 

independently for each variable and for each subset  $V_k$ . 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  $I_x$  (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.,  $Z \notin [0-1]$ ) 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.,  $I_x \neq I_{x_{rand}}$ ). 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  $\mathbf{x}_{rand}$  will have very similar spatial structure as the original variable  $\mathbf{x}$  (i.e.,  $I_x \approx I_{\mathbf{x}_{rand}}$ ). Supporting Material 1, Fig. S1.1 illustrates the effect of shifting variance between consecutive spatial eigenvectors.

#### 253 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  $\Phi_{rand}$  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  $\Phi_{rand} + \Phi_{\mathbf{x},k}$  instead of  $\Phi_{rand}$ :

260 
$$\left\{a_i = R_{xv_k}\cos\left(\Phi_{x,k} + \Phi_{rand}\right); a_j = R_{xv_k}\sin\left(\Phi_{x,k} + \Phi_{rand}\right)\right\}$$
. See Supporting Material 2 for a  
261 mathematical proof.

#### 262 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  $\Phi_{rand} = a\cos(r_{fix})$ , 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.

#### 269 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 <u>https://r-forge.r-project.org/R/?group\_id=195</u> 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.

275 To illustrate the proposed randomization algorithms, we simulated five standardized 276 variables with different spatial patterns on the same grid with  $40 \times 40$  cells (Supporting Material 277 1, Fig. S1.1, top row). X0 served as baseline without spatial pattern and was sampled randomly 278 from a standard normal distribution using R function 'rnorm'. X1 and X2 each represent 279 stationary spatial patterns at small (X1) and large scale (X2). The two variables were generated 280 with the function 'RFsimulate' of the R package 'RandomFields' using an isotropic exponential 281 variogram model with variance = 5 and nugget = 0 for both variables, and with scale = 1 for X1 282 and scale = 3 for X2. Variable X3, which has a more complex spatial structure, was derived as

 $X_3 = X_0 + X_1 + X_2$  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.

286 The full sample (n = 1600) was subsampled in different ways, resulting in ten different 287 samples per simulated data set: a full sample ('Full 1600'); a regular sampling design ('Regular 288 400'), obtained by discarding every second row and column of the full sample; and a random 289 sample of the same size ('Random 400'). The remaining sampling designs were chosen to 290 illustrate the effect of stronger irregularity in the spacing of observations, as well as a further 291 reduction in sample size. The 70 sampling locations of the well-known oribatid mite data set 292 (Borcard, Legendre & Drapeau 1992; Borcard & Legendre 1994), sampled within an original 293 extent of  $2.5 \times 10$  m, were mapped onto a  $40 \times 13$  grid, resulting in sampling design 'Orib 70', 294 covering one third of the extent of the full sample. The 13 levels of x-coordinates in 'Orib 70' 295 were repeated three times to obtain sample 'Orib 210' with n = 210, covering the extent of the 296 full sample. To further explore the behavior of Moran spectral randomization for small and 297 highly irregularly-spaced samples, we subsampled 'Orib 70' in five different ways to a sample 298 size of 32 – 35: a random subsample ('Random 35'); an artificially spaced out sample, deleting 299 every second level of y coordinates ('Spaced 32'); a clumped sample, retaining only y-300 coordinates < 23 ('Clumped 35'); a long-stretched sample, retaining only x-coordinates < 8 301 ('Long 34'); and a bi-modally clustered sample, retaining only y-coordinates that were either < 302 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.

305 For all eight irregular sampling designs, we defined neighbors with Gabriel graphs (Supporting

306 Material, Fig. S1.2), resulting in averages of 3.37 – 4.06 neighbors per sampling location. For all

307 sampling designs, W was defined using inverse distance weights followed by row-

308 standardization. This means that nearby neighbors receive more weight than more distant ones,

309 and the weights of all neighbors sum to one for each sampling location.

#### 310 Evaluation of method performance

#### 311 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  $I_x$  and of the power spectrum (mean correlation between the power spectrum  $\mathbf{r}^2_{xv}$  of  $\mathbf{x}$  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  $\mathbf{x}$ . 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.

#### 332 Spectral randomization tests for correlation

333 A randomization test for the correlation between two spatial variables sampled from 334 uncorrelated populations should have a correct type I error rate  $\alpha$ , i.e., if  $\alpha = 0.05$ , the null 335 hypothesis of no correlation should be rejected in 5% of independent cases (where the expected 336 correlation is zero), and high power to detect linear dependence (where the expected correlation 337 different from zero). To assess the performance of MSR in significance tests of correlation, we 338 ran 5000 simulations and estimated type I error rates from independent variable pairs, and power 339 from correlated variable pairs. For each simulation run, we generated two data sets,  $X0_1 - X4_1$ 340 and  $XO_2 - XA_2$ , where each pair of corresponding variables (e.g.,  $XZ_1$  and  $XZ_2$ ) was simulated 341 independently with the geostatistical parameters defined above and thus had the same expected 342 spatial autocorrelation structure, though empirical values of Moran's I may differ. The expected 343 correlation between any two variables from different data sets was zero (linear independence), 344 whereas the expected correlation between X3 and X0, X1, or X2, or between X4 and X1, from 345 the same data set was non-zero (linear dependence). For each sampling design and variable pair, 346 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, Triplet348 (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

maintain their cross-correlations, using Singleton and Pair methods, and MSR with  $r_{\text{fix}} = \{0, 0.3, -1\}$ 

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

For stationary patterns X0 – X3, MSR methods created patterns that were visually comparable to
the original data but differed in the locations of low and high values (Supporting Material 1, Fig.
S1.3). For X4, a non-stationary pattern with linear trend along the y-axis, replicates included a
randomization of the trend angle (Supporting Material 1, Fig. S1.3, bottom). Pairs randomized
trend direction more flexibly than Triplet and Singleton methods (Supporting Material 1, Fig.
S1.4).

MSR replicates of a random normal variable (X0) were uncorrelated on average (mean = 0) with the original variable, but the distribution of correlations had higher variance than expected from true random variables (not shown). This is reflected in higher rates of statistically

367	significant correlations between each original variable $\mathbf{x}$ and its replicates, based on a parametric
368	<i>t</i> -test for regression coefficients (Fig. 1). On average, correlations with $\mathbf{x}$ were highest for the
369	Singleton method, lower for Triplet, and lowest for Pair. For variable X2 with stationary, large-
370	scale spatial autocorrelation, replicates of all methods showed increased rates of significant
371	correlations with $\mathbf{x}$ , with differences between sampling designs that appear to be related to
372	differences in average Moran's I (Supporting Material, Fig. S1.5).
373	Replicate simulations of the data generating process ('Null') showed high variability in
374	their global Moran's <i>I</i> (Fig. 2, left: standard deviation rescaled by multiplication with $(n - 1)^{0.5}$ to
375	account for sample size) and power spectra (multi-scale spatial structure), as indicated by a low
376	correlation between the power spectrum of $\mathbf{x}$ and those of its replicates (Fig. 2, right). In contrast,
377	the Singleton method completely preserved both Moran's I and power spectra. The Triplet
378	method preserved Moran's I but resulted in some variation in the power spectrum, and the Pair
379	method showed variation both in Moran's I and the power spectrum.
380	The Pair method does not strictly preserve Moran's I but its MSR replicates were generally
381	unbiased for the random normal variable X0 (Supporting Material, Fig. S1.6). For the spatially
382	autocorrelated variable X2, bias was negligible for large data sets but Moran's I of replicates

383 showed a slight negative bias for the small sampling designs.

Spectral randomization tests for correlation 384

385 When correlating two random normal variables  $X0_1$  and  $X0_2$ , or one random normal variable (X0) 386 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 387 388 95% confidence interval for a binomial distribution bin(n, p) with n = 5000 simulated data sets

autocorrelated variable X2, bias was negligible for large data sets but Moran's I of replicates

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).

Moran spectral randomization

410 When each variable was randomized with the additional constraint of a fixed correlation 411 with the original variable, using the Pair method, sampling designs with uneven sample size n412 ('Random 35', 'Clumped 35') completely preserved the predefined correlation  $r_{fix}$  (Supporting 413 Material, Fig. S1.2 A). For even *n*, the presence of an incomplete block (where the Singleton 414 method was used for one randomly selected spatial eigenvector) introduced some variation in the 415 correlation with the original variable. For large samples  $(n \ge 400)$ , this variation was negligible, 416 but for small samples ( $n \le 100$ ), there was considerable variation as well as a negative bias, so 417 that on average, correlations with the original variable were slightly weaker than specified by  $r_{\text{fix}}$ . 418 For sampling designs with uneven n, the correlation among replicates generated with the 419 constraint of  $r_{\rm fix}$  differed systematically from the correlation among replicates generated without 420 such a constraint (Supporting Material, Fig. S1.2 B). The mean correlation among replicates was 421 predictable by  $r_{\text{fix}}^2$ , whereas the standard deviation varied with  $r_{\text{fix}}$  and with the level of spatial 422 autocorrelation. The factor by which the standard deviation of the correlation among replicates was inflated, compared to replicates without the constraint of  $r_{\text{fix}}$ , followed  $2^{0.5}(1 - r_{\text{fix}}^2)$ 423 424 (Supporting Material, Fig. S1.2 C).

#### 425 **Discussion**

#### 426 Comparisons of Moran spectral randomization procedures

427 This paper presents algorithms for restricted randomization of irregularly spaced data with Moran 428 spectral randomization that can be applied to a wide range of sampling designs for which 429 restricted randomization methods were limited so far. Moran spectral randomization provides a 430 framework to build spatially constrained null models allowing statistical inference in the presence

431 of spatial autocorrelation. While Moran spectral randomization has been developed here for two-432 dimensional spatial data, it is also applicable to one-dimensional transect data or time series 433 analysis. The method produces a technically unlimited number of non-identical replicates even 434 for small samples (except for the Singleton method with  $2^{(n-1)}$  unique replicates), without 435 requiring additional parameters beyond the explicit definition of neighbors and spatial weights in 436 matrix **W**.

437 The MSR replicates mimic the spatial characteristics of the original variables in terms of 438 global autocorrelation and multiscale patterns. These properties allow controlling the type I error 439 rate of statistical tests (e.g., bivariate correlation) in the presence of autocorrelation. Ideally, 440 replicates should also be uncorrelated to the original variable to ensure power. These two 441 objectives (similar spatial structure and independence with the original variables) are antagonist 442 and thus defined a gradient from considering the original variable (spatial properties fully 443 preserved but no independence) to its full randomization (complete independence with the 444 original variable but no spatial constraint). Hence, we provide different procedures that 445 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.

The Pair procedure is the least strict concerning the spatial constraints and thus provides MSR replicates with the lowest degree of correlation with the original variables. Spatial characteristics are quite well preserved and thus it appears as good compromise and allows for joint randomization as well as randomization with fixed correlation. The Pair procedure should be used when it is considered important to randomize correlation at each spatial eigenvector and reduce overall correlation with the original variable, or when the slightly lower statistical power or the limited number of  $2^{n-1}$  unique replicates of the Singleton method are of concern.

Lastly, the Triplet procedure that is supposed to combine the advantages of singleton and pairs did not perform as well as the other methods and could also be time-consuming (due to the 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

The proposed algorithms are applicable to a wide range of research questions and hypotheses. We presented MSR in the case of spatial autocorrelation but the method can also be used in the case of temporal of phylogenetic dependence (Peres-Neto 2006). Bivariate correlation analysis can be achieved by randomizing one variable, or randomizing both variables independently (Lennon 2000). The possibility to jointly randomize several variables while maintaining their crosscorrelations will be especially interesting in ecological community analysis that aims at assessing 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.

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

Moran spectral randomization

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

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

#### 538 **References**

- 539 Beale, C.M., Lennon, J.J., Yearsley, J.M., Brewer, M.J. & Elston, D.A. (2010). Regression
- 540 analysis of spatial data. *Ecology Letters*, **13**, 246-264.
- 541 Borcard, D. & Legendre, P. (1994). Environmental control and spatial structure in ecological
- 542 communities: an example using oribatid mites (Acari, Oribatei). *Environmental and*543 *Ecological Statistics*, 1, 37-61.
- 544 Borcard, D. & Legendre, P. (2002). All-scale spatial analysis of ecological data by means of
- 545 principal coordinates of neighbour matrices. *Ecological Modelling*, **153**, 51-68.
- 546 Borcard, D., Legendre, P. & Drapeau, P. (1992). Partialling out the Spatial Component of
  547 Ecological Variation. *Ecology*, **73**, 1045-1055.
- 548 Carl, G. & Kühn, I. (2008). Analyzing spatial ecological data using linear regression and wavelet
- analysis. Stochastic Environmental Research and Risk Assessment, **22**, 315-324.
- 550 Cooley, J.W. & Tukey, J.W. (1965). An Algorithm for the Machine Calculation of Complex
- 551 Fourier Series. *Mathematics of Computation*, **19**, 297-301.
- 552 Cressie, N. (1991). Statistics for Spatial Data. John Wiley & Sons, New York.
- Deblauwe, V., Kennel, P. & Couteron, P. (2012). Testing Pairwise Association between Spatially
  Autocorrelated Variables: A New Approach Using Surrogate Lattice Data. *PLoS ONE*, 7,
  e48766.
- 556 Dormann, C.F., Elith, J., Bacher, S., Buchmann, C., Carl, G., Carré, G. et al. (2013). Collinearity:
- a review of methods to deal with it and a simulation study evaluating their performance.
- 558 *Ecography*, **36**, 027-046.

559 Dray, S. (2011). A New Perspective about Moran's Coefficient: Spatial Autocorrelation as a 560 Linear Regression Problem. Geographical Analysis, 43, 127-141.

28

- 561 Dray, S., Legendre, P. & Peres-Neto, P.R. (2006). Spatial modelling: a comprehensive
- 562 framework for principal coordinate analysis of neighbour matrices (PCNM). Ecological 563 Modelling, 196, 483-493.
- 564 Dutilleul, P., Clifford, P., Richardson, S. & Hemon, D. (1993). Modifying the t test for assessing 565 the correlation between two spatial processes. *Biometrics*, **49**, 305-314.
- 566 Dutilleul, P., Pelletier, B. & Alpargu, G. (2008). Modified F tests for assessing the multiple
- 567 correlation between one spatial process and several others. Journal of Statistical Planning 568 and Inference, 138, 1402.
- 569 Fortin, M.-., Boots, B., Csillag, F. & Remmel, T.K. (2003). On the role of spatial stochastic 570

models in understanding landscape indices in ecology. *Oikos*, **102**, 203-212.

- 571 Fortin, M. & Dale, M.R.T. (2005). Spatial Analysis: A Guide for Ecologists. Cambridge
- 572 University Press, New York.
- 573 Fortin, M. & Jacquez, G.M. (2000). Randomization tests and spatially auto-correlated data. 574 Bulletin of the Ecological Society of America, 81, 201-205.
- 575 Fortin, M., Jacquez, G.M. & Shipley, B. (2012). Computer-intense methods. Encyclopedia of
- Environmetrics, 2<sup>nd</sup> edition (eds A.H. El-Shaarawi & W.W. Piegorsch), pp. 489-493. Wiley, 576 577 Chichester.
- 578 Gauss, C.F. (1866). Theoria interpolationis methodo nova tractata. Carl Friedrich Gauss Werke.,
- 579 pp. 265-327. Königliche Gesellschaft der Wissenschaften, Göttingen.

- 580 Graybill, F.A. (1976). Theory and Application of the Linear Model. Duxbury Press, Belmont,
  581 CA.
- 582 Griffith, D.A. (2000). Eigenfunction properties and approximations of selected incidence
- 583 matrices employed in spatial analyses. *Linear Algebra and its Applications*, **321**, 95-112.
- Griffith, D.A. & Peres-Neto, P.R. (2006). Spatial Modeling in Ecology: The Flexibility of
  Eigenfunction Spatial Analyses. *Ecology*, 87, 2603-2613.
- 586 Kühn, I. & Dormann, C.F. (2012). Less than eight (and a half) misconceptions of spatial analysis.
   587 *Journal of Biogeography*, **39**, 995-998.
- 588 Legendre, P. (1993). Spatial autocorrelation: trouble or new paradigm? *Ecology*, **74**, 1659-1673.
- Lennon, J.J. (2000). Red shifts and red herrings in geographical ecology. *Ecography*, 23, 101-

590 113.

- 591 Moran, P.A.P. (1950). Notes on continuous stochastic phenomena. *Biometrika*, **37**, 17-23.
- 592 Peres-Neto, P.R. (2006). A unified strategy for estimating and controlling spatial, temporal and
- 593 phylogenetic autocorrelation in ecological models. *Oecologia Brasiliensis*, **10**, 105–119.
- 594 Peres-Neto, P.R. & Legendre, P. (2010). Estimating and controlling for spatial structure in the
- 595 study of ecological communities. *Global Ecology and Biogeography*, **19**, 174-184.
- 596 R Core Team (2014). R: A Language and Environment for Statistical Computing. R Foundation
- 597 for Statistical Computing, Vienna, Austria.
- Remmel, T. & Fortin, M.-J. (2013). Categorical, class-focused map patterns: characterization and
   comparison. *Landscape Ecology*, 28, 1587-1599.
- 600 Rodgers, J.L., Nicewander, W.A. & Toothaker, L. (1984). Linearly Independent, Orthogonal, and
- 601 Uncorrelated Variables. *The American Statistician*, **38**, 133-134.

- Schreiber, T. & Schmitz, A. (1996). Improved Surrogate Data for Nonlinearity Tests. *Physical Review Letters*, 77, 635-638.
- Stakhovych, S. & Bijmolt, T.H.A. (2009). Specification of spatial models: A simulation study on
  weights matrices. *Papers in Regional Science*, **88**, 389-408.
- 606 Upton, G.J.G. & Fingleton, B. (1985). Spatial data analysis by example. Vol. 1: Point pattern and
  607 quantitative data. Wiley, New York.
- 608 Wagner, H.H. (2013). Rethinking the linear regression model for spatial ecological data. *Ecology*,
- **6**09 **94**, 2381-2391.
- 610

# 611 **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, largescale spatial autocorrelation. 'Null' refers to fully independent replicates of the generating process.

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616 Figure 2: Spatial properties of replicates for fully independent replicates of the generating 617 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 618 619 account for sample size) and pooled across sampling designs, separately for X0 (dark grey bars) 620 and X2 (light gray bars). Note that Triplet and Singleton methods showed zero variation. Right: 621 bar chart of the mean correlation between the power spectra of the original variable and its 622 replicates, pooled across sampling designs, for X0 (dark gray bars) and X2 (light gray bars). 623 Figure 3: Boxplots of empirical type I error rates across 5000 simulation runs, for different 624 types of variable pairs and randomization methods, pooled across all 10 sampling designs. Fig. A 625 shows the correlation between two random normal variables, Fig. B the correlation between a 626 random variable X0 and a variable with stationary spatial autocorrelation (X1, X2, or X3), Fig. C 627 the correlation between any two variables with stationary spatial autocorrelation, Fig. D a 628 correlation between a variable with non-stationary spatial autocorrelation (X4: linear trend along 629 y-axis) and any variable with stationary spatial autocorrelation, and Fig. E the correlation 630 between two variables with non-stationary spatial autocorrelation. The number below each 631 boxplot reports the mean, and gray polygons indicate a 95% confidence interval for the expected 632 type I error rate.

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

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