SORT 42 (2) July-December 2018, 125-158 DOI: 10.2436/20.8080.02.72

A contingency table approach based on nearest neighbour relations for testing self and mixed correspondence

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Abstract

Nearest neighbour methods are employed for drawing inferences about spatial patterns of points from two or more classes. We introduce a new pattern called correspondence which is motivated by (spatial) niche/habitat specificity and segregation, and define an associated contingency table called a correspondence contingency table, and examine the relation of correspondence with the motivating patterns (namely, segregation and niche specificity). We propose tests based on the correspondence contingency table for testing self and mixed correspondence and determine the appropriate null hypotheses and the underlying conditions appropriate for these tests. We compare finite sample performance of the tests in terms of empirical size and power by extensive Monte Carlo simulations and illustrate the methods on two artificial data sets and one real-life ecological data set.

MSC: 62M30, 62G10, 62H11, 62P12, 62H30

Keywords: Association, complete spatial randomness, habitat/niche specificity, independence, random labelling, segregation

1. Introduction

The spatial point patterns in natural populations (in $\mathbb{R}^2$ and $\mathbb{R}^3$) have received considerable attention in statistical literature. Among the frequently studied spatial patterns between multiple classes/species are segregation and association (Dixon, 2002a), and niche specificity pattern (Primack, 1998). Pielou (1961) proposed various tests based on nearest neighbour (NN) relations in a two-class setting, namely, tests of segregation, symmetry, and niche specificity, and also a coefficient of segregation. Inspired by niche specificity and segregation, we introduce new multi-class patterns called *self* and *mixed correspondence* in the NN structure. We use the NN relationships for testing these patterns. In this article, we only use the first NN (i.e., 1-NN) of any point so NN always

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Received: July 2015
Accepted: June 2018

refers to the 1-NN. Furthermore, the terms "class" and "species" are used interchangeably and refer to any characteristic of the subjects such as gender, age group, health condition, etc.

We also propose tests for the spatial patterns of *self* and *mixed correspondence* in the NN structure. These tests are based on a contingency table called a *correspondence contingency table* (CCT) which is constructed using the NN relations in the data. A *base-NN pair* (or simply the *NN pair*) is the pair of points (p_1, p_2) in which p_2 is a NN of p_1, and p_1 is called the *base point* and p_2 is called the *NN point*. The NN pair (p_1, p_2) is called a *self pair*, if both p_1 and p_2 are from the same class, while it is called a *mixed pair*, if p_1 and p_2 are from different classes. *Self correspondence* in the NN structure occurs when there is a tendency for points from a class to be NNs to points from the same class. That is, self correspondence occurs when self NN pairs are more abundant than expected. On the other hand, *mixed correspondence* occurs when there is a tendency for points and their NNs to be from different classes, i.e., mixed NN pairs are more abundant than expected.

There are many methods available for testing various types of spatial patterns in literature. These spatial tests include Pielou's test of segregation (Pielou, 1961), Ripley's K-function (Ripley, 2004), or J-function (van Lieshout and Baddeley, 1999), and so on. Some of these methods are based on nearest neighbour (NN) relations between the points in the data set (Dixon, 2002b). For example, Clark and Evans (1954) use the mean distance of points to their NNs in a spatial data set to measure the deviations of plant species from spatial randomness and compare the deviations for multiple species. However, in this article, we base our analysis on the class labels of NN pairs as was done in Pielou (1961) and Dixon (1994). An extensive survey for the tests of spatial point patterns is provided by Kulldorff (2006) who categorized and compared more than 100 such tests. These tests are for testing spatial clustering in a one-class setting or testing segregation of points in a multi-class setting. The null hypothesis is some type of spatial randomness and is usually fully specified, but the alternatives are often not so definite, in the sense that for most tests the alternatives are presented as deviations from the null case are of interest as in pure significance tests of Cox and Hinkley (1974); only a few tests specify an explicit alternative clustering scheme. Most of the tests for multiple classes deal with presence or lack of spatial interaction usually in the form of spatial segregation or association between the classes. However, none of the numerous tests surveyed by Kulldorff (2006) are designed for testing correspondence; and the pattern of correspondence and the associated tests are introduced in this article. The tests for assessing the self and mixed correspondence in the NN structure are based on the CCT which can also be constructed by collapsing the nearest neighbour contingency table (NNCT). See Ceyhan (2010, 2008a) for an extensive treatment of NNCT and tests based on it.

We provide the description of correspondence and related patterns, the list of notations and two motivating (artificial) examples in Section 2. A list of abbreviations used in the article is provided in Table 1. We propose the pattern of correspondence together with the associated tests and the contingency table (i.e., CCT) and the benchmark and the null patterns for correspondence in Section 3 where the asymptotic distributions of the cell counts in the CCT and of the tests based on them are also derived. We prove consistency of the tests in Section 3.3, and provide an extensive empirical size and power analysis by Monte Carlo simulations in Section 4. We also illustrate the methodology on one ecological data set in Section 5 and provide some discussion and guidelines in Section 6.

Table 1: *A list of abbreviations used in the article.*

CSR:	Complete Spatial Randomness
NN:	Nearest Neighbour
NNCT:	Nearest Neighbour Contingency Table
RL:	Random Labelling
CCT:	Correspondence Contingency Table

2. Preliminaries

2.1. Spatial Correspondence and Related Patterns

We first introduce the motivating patterns of niche specificity and segregation and then discuss their connection with correspondence.

Niche/habitat specificity is the collection of biotic and abiotic conditions favouring the development, hence existence and abundance of a species on a spatial scale (Ranker and Haufler, 2008). That is, niche specificity is the dependence of an organism on an environment (i.e., niche or habitat). In literature, niche/habitat specificity is also discussed within the context of species diversity under the title of *habitat association* of two or more species (Primack, 1998). Niche specificity is a broad concept and is determined by partitioning of the niche space. Furthermore, niche space has non-spatial coordinates amenable for niche partitioning; e.g., Fargione and Tilman (2005) uses different phenologies resulting in temporal partitioning of the niche space and Werner and Gilliam (1984) incorporate ontogenetic changes (i.e., changes as an individual develops in size) to partition the niche space. However, in this article, we are mainly concerned with the spatial aspect of multi-class interaction patterns.

In a multi-species setting, *segregation* of a species is the pattern in which members of a species occur near members of the same species (Dixon, 1994). Conversely, *association* of a species to another is the pattern in which members of the former species tend to occur near the members of the latter. That is, under segregation, the members of a class or species enjoy the company of the conspecifics, hence form one class clumps or clusters, while under association they tend to coexist with members of other class(es) and form mixed clumps or clusters (see, e.g., Ceyhan, 2008a for more detail).

Niche specificity can be viewed as a factor that accounts for segregation which can account for self correspondence. In a multi-species setting, if each species were confined to its own support/niche, we would expect one-species clumps (which would tend to exclude other species). So if (spatial) niche specificity is in effect for all species in the study region, self correspondence would occur (i.e., self NN pairs would be more abundant than mixed pairs). On the other hand, if niche specificity is in effect for one species, then that species would exhibit segregation from the rest of the species. Self correspondence is much closer to the concept of segregation compared to niche specificity, as self correspondence and segregation are both based on the spatial proximity of the conspecifics. Self correspondence in the NN structure pertains to the NN pair types as self or mixed for each class among all base-NN pairs and thus to a supra-species characteristic. However segregation is a pattern at the species level, in the sense that one can only talk of segregation of a species from another or others. That is, in a multi-class or multi-species setting, self correspondence refers to the NN preference of species for all species combined and so it is intended to measure whether species prefer their conspecifics in a cumulative fashion, i.e., for all species taken into account together. Thus, segregation is defined at species level, while self correspondence is defined at multi-species level; and the two patterns are related but different in the sense that, e.g., all species together might exhibit self correspondence without significant segregation for any of the species. But segregation of all or most species will usually substantiate the presence of self correspondence, hence segregation can be viewed as a factor that accounts for self correspondence. Lack of segregation might indicate mixed correspondence, which may or may not imply association, since for association one needs to consider each pair of species separately and test the interaction between the two species in the pair. Lack of segregation is guaranteed to imply presence of association in the two-class setting only.

2.2. Notation

For convenience to the reader, following the example of Vichi and Saporta (2009), we provide the notation and terminology used in the article below.

X and Y	class labels (interchangeably 1 and 2, respectively);
$\mathcal{X}_n$ and $\mathcal{Y}_m$	a data set of size n from class X and a data set of size m from class Y;
$\mathcal{W}_n$	represents the combined data set for the CSR setting, and the background points for the RL setting;
$\mathcal{D}_n$	the set of ordered pairs (W_i, L_i), where W_i stands for the location of the point and L_i stands for the corresponding class label;
S_i	the number of self base-NN pairs for class i;
M_i	the number of mixed base-NN pairs with base point being from class i;
S and M	sum of the first column (for self pairs) i.e. $S = \sum_{i=1}^{k} S_i$ and sum of the second column (for mixed pairs) i.e. $M = \sum_{i=1}^{k} M_i$ in the CCT;

N_{ij}	the observed frequency of category (i,j) in the NNCT, i.e., the number of (base,NN) pairs in which base class is i and NN class is j;
C_i	sum of column j in the NNCT;
R and Q	twice the number of reflexive pairs and the number of points with shared NNs, which occurs when two or more points share a NN;
Q_l	the number of points that serve as a NN to other points l times;
Z_{S_i} and Z_S	the test statistics for cell $(i,1)$ in the CCT and for sum of the self column, S;
Z_{ii}	the cell-specific tests for cell (i,i) in the NNCT analysis;
$\mathbf{S}$	the vector of combined S_i values (i.e., the self column in the CCT), i.e., $(S_1, S_2, \ldots, S_k)$;
$\Sigma_{\mathbf{S}}$	the variance-covariance matrix of $\mathbf{S}$;
$\mathscr{X}_C$	the (quadratic form) test statistic for the correspondence;
$\mathscr{X}_D$	the overall segregation test due to Dixon;
$\mathbf{N}$ and $\Sigma_{\mathbf{N}}$	the vector of entries of NNCT concatenated row-wise and its covariance matrix;
A^-	the generalized inverse of a matrix A;
$\chi^2_{\nu,\alpha}$	the $100\alpha^{th}$ percentile of χ^2 distribution with ν degrees of freedom;
N_{mc}	the number of Monte Carlo samples generated for the empirical size and power comparison of the tests;
$\widehat{\alpha}_T$	the empirical size estimate of a test statistic, T, at level $\alpha = 0.05$;
$\widehat{\alpha}_{T_1,T_2}$	the proportion of agreement in rejecting the null hypothesis between test statistics T_1 and T_2;
$\mathscr{U}(A)$	the uniform distribution on region A;
$\text{MatClust}(\kappa, r, \mu)$	Matérn cluster process with Poisson parameters κ and μ and radius r;
$\widehat{\beta}_T$	the empirical power estimate of a test statistic, T, at level $\alpha = 0.05$;
p_{asy}	the p-value based on the asymptotic approximation (i.e., asymptotic critical value);
p_{rand}	the p-value based on Monte Carlo randomization of the labels on the given locations;
p_{mc}	the p-value based on 10000 Monte Carlo replication of the CSR independence pattern in the study region

2.3. Motivating Examples

To motivate the patterns of self/mixed correspondence and how they can be different from segregation/association, we use two artificial data sets, each of which has three classes (representing tree species) say, X, Y and Z in a square study region. We could also choose examples with two classes, but with two classes only one of the newly intro-

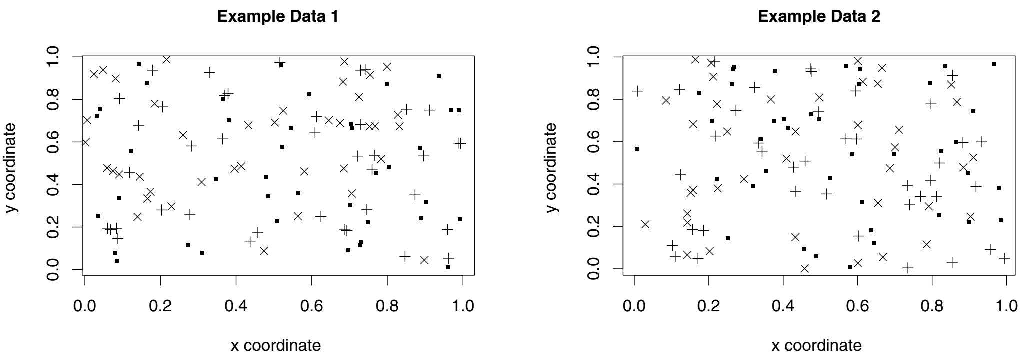

Figure 1: The scatterplots of the locations of three classes (representing three tree species) in our artificial data set 1 (left) and artificial data set 2 (right). There are 40 points in each class/species.

duced tests provide new information compared to the existing segregation tests and there are more possibilities of different types of pairwise interactions between classes with three or more classes. Hence it would be more informative to discuss the differences between the tests and patterns of self/mixed correspondence and segregation/association with three or more classes. We generate 40 points for each class and the locations of the points are plotted in Figure 1. The scatter plot for artificial data set 1 on the left is suggestive of mild self correspondence and segregation with number of self NN pairs being 54 and number of mixed NN pairs being 66. The scatter plot for artificial data set 2 on the right is suggestive of mild mixed correspondence and a lack of segregation with number of self NN pairs being 34 and number of mixed NN pairs being 86. However, these claims are not assessed rigorously yet to attach any significance (or lack of it) to them. We will illustrate the correspondence and segregation patterns and the associated tests using these examples in the following sections.

3. Correspondence in the NN Structure and the Associated Contingency Table

3.1. Benchmark and Null Patterns for Multivariate Spatial Interaction

In this article, we are concerned with the (spatial) interaction between two or more classes of points, particularly with correspondence. For multivariate spatial data analysis, the benchmark pattern is usually complete spatial randomness (CSR) independence or random labelling (RL) (Diggle, 2003) depending on the context. The distinction between CSR independence and RL could be very important in practice. Under CSR independence the (locations of the) points from two classes are *a priori* the result of different processes (for instance, individuals of different species or age cohorts). On the other hand, under RL, some processes affect the individuals of a single population *a posteriori* (for instance, diseased versus non-diseased individuals of a single plant species) (Goreaud and Pélissier, 2003). Under CSR independence, the points from each class are independently uniformly distributed in the region of interest conditioned on the class sizes. That is, the points from each class are independent realizations from a Homogeneous Poisson Process (HPP) with fixed class sizes (i.e., they are independent realizations from a binomial process). On the other hand, under RL, class labels are independently and randomly assigned to a set of given locations which could be a realization from any pattern such as HPP or some clustered or regular pattern.

For simplicity, we describe the benchmark patterns for the two-class case. Extension to multi-class case is straightforward. In a two-class setting, we label the classes as X and Y (or interchangeably 1 and 2, respectively). Let $\mathcal{X}_{n_1}$ be a data set of size n_1 from class X and $\mathcal{Y}_{n_2}$ be a data set of size n_2 from class Y. Then under CSR independence, we have $\mathcal{X}_{n_1} = \{X_1, X_2, \ldots, X_{n_1}\}$ and $\mathcal{Y}_{n_2} = \{Y_1, Y_2, \ldots, Y_{n_2}\}$ which are independent and are both random samples from $\mathcal{U}(S)$, the uniform distribution on the common support $S \subset \mathbb{R}^d$ for classes X and Y where $\mathbb{R}^d$ is the d-dimensional Euclidean space. Unless stated otherwise, for simplicity and practical purposes, we take $d = 2$ (i.e., consider planar data) throughout the article. We combine $\mathcal{X}_{n_1}$ and $\mathcal{Y}_{n_2}$ into one data set $\mathcal{W}_n = \mathcal{X}_{n_1} \cup \mathcal{Y}_{n_2} = \{W_1, W_2, \ldots, W_n\}$ where $n = n_1 + n_2$. In fact, we consider labeled data points as $\mathcal{D}_n = \{(W_i, L_i) \text{ for } i = 1, 2, \ldots, n\}$ where $L_i \in \{0, 1\}$ or $\{X, Y\}$ are the class labels. Notice that under CSR independence, the randomness is in the locations of the points W_i and the class label is a fixed deterministic characteristic of the point. Under the RL pattern, the class labels or marks are assigned randomly to points whose locations are given. The spatial pattern generating these point locations is referred to as the *background pattern* henceforth. Then $\mathcal{W}_n$ is the given set of locations for n points from the background pattern. We have the pair of observations (W_i, L_i) where $L_i \in \{1, 2\}$ or $\{X, Y\}$ is the class label of the point W_i for $i = 1, 2, \ldots, n$. Then n_1 (resp. n_2) of these W_i points are assigned as class X (resp. class Y) randomly; i.e., the labels L_i are 1 or X approximately with probability n_1/n (resp. 2 or Y with probability n_2/n) independently for $i = 1, 2, \ldots, n$. Under RL, the locations of the points are fixed but the randomness is in the label, L_i, associated with these points.

There are two major types of interaction pattern types as deviation from these benchmark patterns in the multivariate spatial pattern analysis. These interaction patterns are segregation and association. Segregation/association, niche specificity and correspondence are related but different concepts (see Section 2.1), and hence the corresponding null hypotheses are different. Niche specificity might account for or explain the self correspondence or segregation patterns. In particular, if niche specificity occurs at significant levels for each species, then there will be significant segregation for each species and significant self correspondence for all species combined. But if niche specificity occurs for some species (but for other species niche specificity is not significant or these other species exist in mixed groups/clumps or scattered around the study region haphazardly), segregation is operating for these species, while self correspondence may or may not be in effect (e.g., segregation of species may not be strong enough to render self pairs significantly larger than expected, or the associated pairs might hinder the occurrence of self correspondence). Hence self correspondence and segregation are different patterns with substantial overlap, but one is not the subset of the other. We provide the explicit forms of the corresponding null hypotheses in the subsequent sections.

3.2. Tests of Correspondence and Their Relation to Segregation

The null case for self or mixed correspondence is that the entries for self (or mixed) pair types in the CCT are as expected under RL or CSR independence.

For a species to exhibit self (resp. mixed) correspondence in the NN structure, self (resp. mixed) NN pairs would be more abundant than expected under RL. To detect such type of pattern, we construct a contingency table where NN pairs are classified as self or mixed for each class. Let S_i be the number of self NN pairs for class i, and M_i be the number of mixed NN pairs with base point being from class i. For simplicity, we assume there are no ties in the NN relations, which occurs with probability one, if $\mathscr{W}_n$ is a random sample from a continuous distribution. Then

$$S_i = \sum_{j \neq i, j=1}^{n} \sum_{i=1}^{n} \mathbf{I}(Z_j \text{ is a NN of } Z_i)\mathbf{I}(L_i = L_j),$$

and

$$M_i = n_i - S_i = \sum_{j \neq i, j=1}^{n} \sum_{i=1}^{n} \mathbf{I}(Z_j \text{ is a NN of } Z_i)\mathbf{I}(L_i \neq L_j).$$

Then the resulting contingency table is a $k \times 2$ contingency table for k classes with first column (called self column) comprising of S_i and the second column (called mixed column) comprising of M_i values. See also Table 3 (left). Notice that row sums are class sizes (i.e., sum of row i is n_i), and sum of the self column is $S = \sum_{i=1}^{k} S_i$ and sum of the mixed column is $M = \sum_{i=1}^{k} M_i$.

Remark 3.1. Ties in the NN Structure. If there are ties in the NN structure, which can happen, e.g., due to truncation of the coordinates of the observations when recording, we can adjust the above formulas for S_i and M_i by inserting a weight term for ties. For instance, we can write $\frac{1}{N_i^{nn}}\mathbf{I}(Z_j \text{ is a NN of } Z_i)$ to account for the ties where N_i^{nn} is the number of NNs of point Z_i. Note that $N_i^{nn} = 1$ with probability 1 when $\mathscr{W}_n$ is a random sample from a continuous distribution. □

The $k \times 2$ CCT is closely related to the $k \times k$ nearest neighbour contingency table (NNCT) based on the same data. Here we provide a brief description of NNCTs (for more detail, see, e.g., Ceyhan, 2008a). NNCTs are constructed using the NN frequencies of classes. Let n_i be the number of points from class i (assumed fixed) for $i \in \{1, 2, \ldots, k\}$ and $n = \sum_{i=1}^{k} n_i$. If we record the class of each point and its NN, the NN relationships fall into the following k^2 categories:

$$(1,1),\,(1,2),\ldots,(1,k);\,(2,1),\,(2,2),\ldots,(2,k);\ldots,(k,k)$$

where in category or cell (i,j), class i is called the *base class*, and class j is called the *NN class*. Denoting N_{ij} as the observed frequency of category (i,j) for $i,j \in \{1,2,\ldots,k\}$, we obtain the NNCT in Table 3 (right). Then,

$$N_{ij} = \sum_{j' \neq i', j'=1}^{n} \sum_{i'=1}^{n} \mathbf{I}(Z_{j'} \text{ is a NN of } Z_{i'})\mathbf{I}(L_{i'} = i)\mathbf{I}(L_{j'} = j).$$

The number of self pairs for class i is same as the number of base-NN pairs with both base and NN classes are from class i. Hence $S_i = N_{ii}$ and $M_i = n_i - N_{ii}$.

Table 3: *The CCT (left) and the NNCT (right) for k classes.*

		pair type		
		self	mixed	total
base class	class 1	S_1	M_1	n_1
	class 2	S_2	M_2	n_2
	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	class k	S_k	M_k	n_k
	total	S	M	n

		NN class			
		class 1	$\ldots$	class k	total
base class	class 1	N_{11}	$\ldots$	N_{1k}	n_1
	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
	class k	N_{k1}	$\ldots$	N_{kk}	n_k
	total	C_1	$\ldots$	C_k	n

Table 4: *The CCT (left) and the NNCT (right) for the three classes in our artificial data set 1.*

		pair type		
		self	mixed	total
base class	class 1	18	22	40
	class 2	18	22	40
	class 3	18	22	40
	total	54	66	120

		NN class			
		class 1	class 2	class 3	total
base class	class 1	18	13	9	40
	class 2	11	18	11	40
	class 3	8	14	18	40
	total	37	45	38	120

Table 5: *The CCT (left) and the NNCT (right) for the three classes in our artificial data set 2.*

		pair type		
		self	mixed	total
base class	class 1	7	33	40
	class 2	19	21	40
	class 3	8	32	40
	total	34	86	120

		NN class			
		class 1	class 2	class 3	total
base class	class 1	7	15	18	40
	class 2	10	19	11	40
	class 3	18	14	8	40
	total	35	48	37	120

We present the CCTs and NNCTs for the artificial data sets 1 and 2 in Tables 4 and 5, respectively. For artificial data set 1, the CCT suggests presence of self correspondence with self column entries being higher than expected. Equivalently, the NNCT diagonal entries are higher than expected suggesting presence of segregation of the classes. For artificial data set 2, based on the CCT, we observe that there seems to be mixed correspondence (with NN pairs in which base points are from classes 1 or 2). Likewise, NNCT suggests that classes 1 and 3 are associated with each other, and there is a lack of segregation for these classes, and class 2 points seem to be segregated from points of other classes.

Under RL, we can determine the exact expected values, variances, and asymptotic distributions of the cell counts in the CCT. In particular,

$$\mathrm{E}[S_i] = \mathrm{E}[N_{ii}] = n_i(n_i-1)/(n-1) \text{ and } \mathrm{E}[M_i] = \mathrm{E}[n_i - N_{ii}] = n_i(n-n_i)/(n-1). \quad (1)$$

Furthermore,

$$\mathrm{Var}[S_i] = \mathrm{Var}[N_{ii}] = (n+R)p_{ii} + (2n-2R+Q)p_{iii} + (n^2-3n-Q+R)p_{iiii} - n^2 p_{ii}^2 \quad (2)$$

and since n_i are fixed

$$\mathrm{Var}[M_i] = \mathrm{Var}[n_i - N_{ii}] = \mathrm{Var}[N_{ii}] = \mathrm{Var}[S_i].$$

In Equation (2), p_{xx}, p_{xxx}, and p_{xxxx} are the probabilities that a randomly picked pair, triplet, or quartet of points, respectively, are the indicated classes and are given by

$$p_{ii} = \frac{n_i(n_i-1)}{n(n-1)}, \; p_{iii} = \frac{n_i(n_i-1)(n_i-2)}{n(n-1)(n-2)}, \; p_{iiii} = \frac{n_i(n_i-1)(n_i-2)(n_i-3)}{n(n-1)(n-2)(n-3)}, \quad (3)$$

and R is twice the number of reflexive pairs and Q is the number of points with shared NNs, which occurs when two or more points share a NN. Then $Q = 2(Q_2 + 3Q_3 + 6Q_4 + 10Q_5 + 15Q_6)$ where Q_l is the number of points that serve as a NN to other points l times. Since n_i are fixed, the covariances of the cell counts can also be obtained as

$$\mathrm{Cov}[S_i, S_j] = \mathrm{Cov}(N_{ii}, N_{jj}) = (n^2-3n-Q+R)p_{iijj} - n^2 p_{ii} p_{jj}$$

and

$$\mathrm{Cov}[M_i, M_j] = \mathrm{Cov}(n_i - N_{ii}, n_j - N_{jj}) = \mathrm{Cov}(N_{ii}, N_{jj})$$

where $p_{iijj} = \frac{n_i(n_i-1)n_j(n_j-1)}{n(n-1)(n-2)(n-3)}$. The covariance of cell counts in different columns is

$$\mathrm{Cov}[S_i, M_j] = \begin{cases} \mathrm{Cov}[N_{ii}, n_i - N_{ii}] = -\mathrm{Var}[N_{ii}] & \text{if } i = j, \\ \mathrm{Cov}[N_{ii}, n_j - N_{jj}] = -\mathrm{Cov}[N_{ii}, N_{jj}] & \text{if } i \neq j. \end{cases} \quad (4)$$

See Dixon (1994, 2002a) for the derivation of the above variance and covariance terms.

In a CCT, deviations of S_i or M_i from their expected values under RL or CSR independence can be assessed. Since $S_i = N_{ii}$, for cell $(i,1)$ of the CCT, we have

$$Z_{S_i} = \frac{S_i - \mathrm{E}[S_i]}{\sqrt{\mathrm{Var}[S_i]}} = \frac{N_{ii} - \mathrm{E}[N_{ii}]}{\sqrt{\mathrm{Var}[N_{ii}]}} \quad (5)$$

for $i = 1,2,\ldots,k$. Notice that $Z_{S_i} = Z_{ii}$ where Z_{ii} is the cell-specific tests for cell (i,i) in the NNCT analysis (see, Dixon, 1994 and Ceyhan, 2008a for more details). Notice also that the mixed column entries carry the same information as the self column entries, and they will yield the test statistic with negative sign. That is, $(M_i - \mathrm{E}[M_i])/\sqrt{\mathrm{Var}[M_i]} = -Z_{S_i}$ for each i, hence the test statistics with mixed column entries are omitted. For large n_i, Z_{S_i} approximately has $N(0,1)$ distribution (Dixon, 2002a).

The test statistics for the self cells of the CCT are as follows: For artificial data set 1, we have $Z_{S_1} = Z_{11} = Z_{S_2} = Z_{22} = Z_{S_3} = Z_{33} = 1.4409$ which is in agreement with our observation in the CCT that all classes exhibit mild segregation. For artificial data set 2, $Z_{S_1} = Z_{11} = -1.8033$, $Z_{S_2} = Z_{22} = 1.7388$, and $Z_{S_3} = Z_{33} = -1.5081$ which is in agreement with our observation in the CCT that classes 1 and 3 exhibit lack of segregation at a moderate level while class 2 exhibits mild level of segregation.

One can combine the S_i values (i.e., the self column in the CCT) into a vector $\mathbf{S} = (S_1,S_2,\ldots,S_k) = (N_{11},N_{22},\ldots,N_{kk})$. So $\mathrm{E}[\mathbf{S}]$ is the vector of expected values of the entries of $\mathbf{S}$. The variance-covariance matrix of $\mathbf{S}$, denoted $\Sigma_{\mathbf{S}}$, is the $k \times k$ matrix with entry (i,i) being $\mathrm{Var}[S_i] = \mathrm{Var}[N_{ii}]$ and entry (i,j) with $i \neq j$ being $\mathrm{Cov}[S_i,S_j] = \mathrm{Cov}[N_{ii},N_{jj}]$. With the self column as the vector $\mathbf{S}$, we have the quadratic form

$$\mathscr{X}_C = (\mathbf{S} - \mathrm{E}[\mathbf{S}])^{\mathsf{T}} \Sigma_{\mathbf{S}}^{-1} (\mathbf{S} - \mathrm{E}[\mathbf{S}]). \tag{6}$$

where $\Sigma_{\mathbf{S}}^{-1}$ is the inverse of $\Sigma_{\mathbf{S}}$. For large n_i, $\mathscr{X}_C$ approximately has a χ^2_k distribution. Observe that the test statistic $\mathscr{X}_C$ is obtained similar to the overall segregation test as described in Ceyhan (2008a). Briefly, the overall segregation test due to Dixon is

$$\mathscr{X}_D = (\mathbf{N} - \mathrm{E}[\mathbf{N}])^{\mathsf{T}} \Sigma_{\mathbf{N}}^{-} (\mathbf{N} - \mathrm{E}[\mathbf{N}]) \tag{7}$$

where $\mathbf{N}$ is the vector of entries of NNCT concatenated row-wise and $\Sigma_{\mathbf{N}}$ is the covariance matrix of $\mathbf{N}$ and A^{-} is the generalized inverse of a matrix A (Searle, 2006).

For the artificial data set 1, we have $\mathscr{X}_C = 5.0761$ $(p = 0.1664)$ and $\mathscr{X}_D = 7.1274$ $(p = 0.3092)$. Notice that neither test is significant, although the correspondence test yields a lower p-value. This suggests lack of significant deviations from the expected cell counts in either contingency table. On the other hand, for the artificial data set 2, we have $\mathscr{X}_C = 9.4670$ $(p = 0.0237)$ and $\mathscr{X}_D = 9.7879$ $(p = 0.1339)$. Notice that the overall segregation test is not significant at the .05 level, which suggests that the cell counts do not deviate significantly from their expected values. On the other hand, $\mathscr{X}_C$ is significant, which is suggesting significant deviation in the first column of CCT (or the diagonal of NNCT). However, to determine the direction of correspondence, we assess the cell counts in the CCT and conclude that there is an abundance of self pairs for class 2, while there is a lower number of self pairs (or there is an abundance of mixed pairs) for the other classes. Together with the column sums in the CCT, we observe that there is evidence for mixed correspondence compared to self correspondence.

Alternatively, we could also concatenate self and mixed columns of CCT to obtain the vector $\mathbf{S}_{II} = (N_{11}, N_{22}, \ldots, N_{kk}, n_1 - N_{11}, n_2 - N_{22}, \ldots, n_k - N_{kk})$ with the test statistic $\mathscr{X}_{II} = (\mathbf{S}_{II} - \mathrm{E}[\mathbf{S}_{II}])' \Sigma_{II}^{-}(\mathbf{S}_{II} - \mathrm{E}[\mathbf{S}_{II}])$, but this version is highly unstable due to severe rank deficiency (see Ceyhan, 2014). Thus we employ the first form of the test statistic, $\mathscr{X}_C$, which is the χ^2 test for the self column and omit $\mathscr{X}_{II}$ in our further discussion.

When $\mathscr{X}_C$ is significant, it implies the presence of significant deviation of some of the cell counts S_i than expected under H_o in Equation (9) or small deviations of cell counts in positive or negative direction might accumulate in the quadratic form in Equation (6) and cause a significant result for $\mathscr{X}_C$. Furthermore, if some significant deviation exists for some cell(s), this deviation could be toward significant segregation or lack of segregation for a class, or significant association of this class with some other class(es). If additionally, the deviations of cells are all toward positive direction (i.e., segregation) or deviations of some cells toward segregation are strong enough, then the self pairs might be more abundant indicating presence of self correspondence. So with $\mathscr{X}_C$ to infer self or mixed correspondence, one needs to check the direction and magnitude of deviation for each class (after a significant $\mathscr{X}_C$), hence should look at the sign and magnitude of the cell-specific Z tests (i.e., the diagonal cell-specific tests) in Equation (5). Thus this process tests self or mixed correspondence by a two-step approach which may be somewhat a subjective assessment of magnitude of the deviations. For example, in our artificial data set 2, the correspondence test statistic is significant, but by itself, does not indicate it is self or mixed correspondence. To determine the type of correspondence, we either look at the CCT or the sign and magnitude of the tests for the cells in the self column of the CCT. In particular, in this data set, we observe that the correspondence is of mixed type due to large negative values for the Z_{S_1} and Z_{S_3}.

As an alternative approach, we propose a test based on the sum of the self column, S, in the CCT. That is,

$$Z_C = \frac{S - \mathrm{E}[S]}{\sqrt{\mathrm{Var}[S]}}. \tag{8}$$

Here

$$\mathrm{E}[S] = \mathrm{E}\left[\sum_{i=1}^{k} N_{ii}\right] = \sum_{i=1}^{k} \mathrm{E}[N_{ii}] = \sum_{i=1}^{k} \frac{n_i(n_i - 1)}{n - 1}$$

and

$$\mathrm{Var}[S] = \mathrm{Var}\left[\sum_{i=1}^{k} N_{ii}\right] = \sum_{i=1}^{k} \mathrm{Var}[N_{ii}] + \sum_{i \neq j}^{k} \mathrm{Cov}[N_{ii}, N_{jj}].$$

Observe that $\mathrm{Var}[S]$ is the sum of entries of Σ_{self}, the covariance matrix of $\mathbf{S}$. As n_i values tend to infinity, Z_C converges in law to $N(0,1)$ distribution. Large (positive) values of Z_C indicate that self pairs are more abundant than expected under RL or CSR independence, hence indicate presence of self correspondence, while smaller (negative) values of Z_C indicate presence of mixed correspondence.

For artificial data set 1, $Z_C = 2.2529$ $(p = 0.0123)$ which indicates that the self column sum is significantly larger than its expected value. Since each cell count deviates in the same direction, this constitutes evidence for self correspondence in the NN structure. Notice that although segregation is mild (and not significant) for each class, their cumulative effect makes the number of self NN pairs significantly higher than expected yielding a significant self correspondence. As for artificial data set 2, $Z_C = -0.8137$ which implies the self column sum in the CCT is not significantly different from its expected value. However, this is not a contradiction with our finding of significant $\mathscr{X}_C$, as the deviations in the first column are in opposite directions, hence cancel each other out in the summation.

Although the test statistics, $\mathscr{X}_C$, Z_{ii}, and Z_C are all related to correspondence and segregation, they test different null hypotheses. The null hypothesis for correspondence is

$$H_o : \text{self (or mixed) NN pairs are as expected under RL and CSR independence.} \tag{9}$$

Hence, by construction, the cell-specific test Z_{ii} tests the hypothesis

$$H_o : \mathrm{E}[Z_{ii}] = \frac{n_i(n_i-1)}{n-1} \tag{10}$$

and $\mathscr{X}_C$ tests the hypothesis

$$H_o : \mathrm{E}[Z_{ii}] = \frac{n_i(n_i-1)}{n-1} \text{ for all } i = 1,2,\ldots,k \tag{11}$$

and Z_C tests the hypothesis

$$H_o : \mathrm{E}[S] = \sum_{i=1}^{k} \frac{n_i(n_i-1)}{n-1}. \tag{12}$$

The right (resp. left) sided alternative for H_o in Equation (12) will imply self (resp. mixed) correspondence, and the right sided alternative for H_o in Equation (10) will imply segregation of species i from others. On the other hand, the left sided alternative for H_o in Equation (10) will imply lack of segregation of species i from others (in a two-class setting, this is equivalent to association of the species with the other, but in a multi-class setting, this may or may not imply association).

For $k = 2$ classes, $\mathscr{X}_C$ is equivalent to the overall test of segregation of Dixon (1994), $\mathscr{X}_D$, since the CCT and NNCT convey the same information and both tests are effectively based on N_{11} and N_{22} only. In particular, N_{11} and N_{22} constitute the first column of the CCT and the diagonal entries of the NNCT and N_{12} and N_{21} constitute the second column of the CCT and the off-diagonal entries of the NNCT. But for $k > 2$, the information conveyed by the NNCT and CCT are different and the $\mathscr{X}_C$ depends only on

$S_i = N_{ii}$ values in CCT, while the overall segregation test depends on all N_{ij} values in NNCT.

Remark 3.2. Relation of Null Hypotheses with CSR Independence and RL. The above null hypotheses in Equation (10)-(12) in terms of the expected values can result from a more general setting. In particular, these null cases follow provided that there is randomness in the NN structure in such a way that the probability of a NN of a point being from a class is proportional to the relative frequency of that class. This assumption holds, e.g., under CSR independence or RL of the points from each class. Both CSR independence and RL patterns imply that there is no correspondence in the NN structure. In fact, it is conceivable that other independence patterns (in which all classes are independently generated from the same process or distribution) can yield the same null hypothesis, but we restrict our attention to RL and CSR independence as they are considered to be the benchmark patterns in spatial data analysis. □

Remark 3.3. Status of Q and R under RL and CSR independence. Note the status of the quantities Q and R under CSR independence and RL models. Under RL, Q and R are fixed, while, under CSR independence, they are random. Hence the tests in Equations (5)-(8) are conditional on the observed values of Q and R under CSR independence while no such conditioning is required under RL. The variance and covariance terms in Section 3.2 and all the corresponding tests also depend on Q and R. Hence these expressions are appropriate for the RL pattern, but for the CSR independence pattern, they are variances and covariances conditioned on Q and R. The unconditional variances and covariances can be obtained by replacing Q and R with their expectations. Under HPP in the infinite plane, Cox (1981) computed $\mathrm{E}[R/n] \to .6215$ and Cuzick and Edwards (1990) computed $\mathrm{E}[Q/n] \to .633$ as $n \to \infty$. However, these results are assuming an infinite plane, and our CSR independence case requires a bounded support (e.g., the unit square) and fixed number of points which renders their computation for exact and asymptotic settings an arduous task (due to, e.g., the edge effects). Alternatively, the expected values of Q and R can be empirically approximated and used in the expressions. For example, for the binomial process on the unit square, $\mathrm{E}[Q/n]$ tends approximately to .6324 and $\mathrm{E}[R/n]$ tends approximately to 0.6219 (estimated empirically based on 1000000 Monte Carlo simulations for increasing values of n). Notice that these estimates are pretty close to the results under HPP. Hence one could also replace Q and R with $0.63n$ and $0.62n$, respectively and obtain the so-called *QR-adjusted* tests but we use the observed values of Q and R in computing our test statistics even when assessing their behavior under CSR independence. As shown in Ceyhan (2008b), QR-adjustment does not improve on the unadjusted NNCT-tests. □

Remark 3.4. Recommended Strategy for $k > 2$ Classes. In the multi-class case with $k > 2$, we recommend the following strategy for the practical implementation of the corresponding tests: Perform $\mathscr{X}_C$ and Z_C to check presence of self or mixed correspondence or any deviation in the self column and then perform the cell-specific tests to determine which species (if any) exhibit segregation or lack of it. □

3.3. Consistency of Tests

A reasonable test should have more power as the sample size increases, so, we prove the consistency of the tests in question under appropriate hypotheses. Let $\chi^2_{\nu,\alpha}$ be the $100\alpha^{\text{th}}$ percentile of χ^2 distribution with ν degrees of freedom.

Theorem 3.5. *Let the CCT be constructed from completely mapped spatial data under RL. Then*

(i) the one-sided (hence the two-sided) cell-specific tests using Z_{ii} given in Equation (5) *rejecting H_o in Equation* (10) *are consistent,*

(ii) the test rejecting H_o in Equation (11) *for $\mathscr{X}_C > \chi^2_{k,1-\alpha}$ with $\mathscr{X}_C$ as in Equation* (6) *is consistent,*

(iii) the one-sided (hence the two-sided) tests using Z_C given in Equation (8) *rejecting H_o in Equation* (12) *are consistent.*

Proof. (i) In the k class case, let $T_{n,i} = \frac{S_i/n - \mathrm{E}[S_i/n]}{\sqrt{\mathrm{Var}[S_i/n]}} = \frac{N_{ii}/n - \mathrm{E}[N_{ii}/n]}{\sqrt{\mathrm{Var}[N_{ii}/n]}}$, then $T_{n,i} = Z_{ii}$ for $i = 1,2,\ldots,k$. Consistency of Z_{ij} was proved in Ceyhan (2010) for all i, j which includes the special case of $i = j$, but we still present it here for the sake of completeness. Under RL, $\mathrm{E}[T_{n,i}] = \mathrm{E}[Z_{ii}] = 0$ and $Z_{ii} = (N_{ii} - \mathrm{E}[N_{ii}])/\sqrt{\mathrm{Var}[N_{ii}]}$ are approximately distributed as $N(0,1)$ for large n_i for $i = 1,2,\ldots,k$. Under the right sided (resp. left sided) alternative H_a, for any $i \in \{1,2,\ldots,k\}$, we have $\mathrm{E}[Z_{ii}|H_a] = \varepsilon_i > 0$ (resp. $\mathrm{E}[Z_{ii}|H_a] = \varepsilon_i < 0$) where ε_i is a parameterization of the alternative for class i for $i = 1,2,\ldots,k$. Let $R(\varepsilon_i)$ and $Q(\varepsilon_i)$ be the numbers of reflexive pairs and shared NNs, respectively, $p_{ii}(\varepsilon_i)$, $p_{iii}(\varepsilon_i)$, and $p_{iiii}(\varepsilon_i)$ be the counterparts of p_{ii}, p_{iii}, and p_{iiii} in Equation (3). Then under H_a, we have $\mathrm{Var}[N_{ii}/n] = (1/n + R(\varepsilon_i)/n^2)p_{ii}(\varepsilon_i) + (2/n - 2R(\varepsilon_i)/n^2 + Q(\varepsilon_i)/n^2)p_{iii}(\varepsilon_i) + (1 - 3/n - Q(\varepsilon_i)/n^2 + R(\varepsilon_i)/n^2)p_{iiii}(\varepsilon_i) - (p_{ii}(\varepsilon_i))^2$. So, under H_a, it follows that $\mathrm{Var}[N_{ii}/n] \to 0$ as $n_i \to \infty$. Hence the test using Z_{ii} is consistent for the right-sided (resp. left sided) alternative. Consistency for the two-sided alternative follows similarly.

(ii) Let $\vec{\varepsilon} = (\varepsilon_1,\ldots,\varepsilon_k)$, then we have $H_a : \vec{\varepsilon} \neq \mathbf{0}$, with $\mathbf{0}$ being the vector of k zeros. Also let $\lambda(\vec{\varepsilon})$ be the non-centrality parameter of χ^2_k distribution for $\mathscr{X}_C$ under H_a. The α-level test based on $\mathscr{X}_C$ is consistent, since $\mathscr{X}_C$ is a quadratic form based on Z_{ii} values, i.e., $\mathscr{X}_C \sim \chi^2_k(\lambda(\vec{\varepsilon}))$ for some $\lambda(\vec{\varepsilon}) > 0$. Furthermore, for large n, the null and alternative hypotheses are equivalent to $H_o : \lambda = 0$ versus $H_a : \lambda = \lambda(\vec{\varepsilon}) > 0$. Then by standard arguments for the consistency of χ^2 tests, consistency follows.

(iii) Let $T_{n,sc} = \frac{S/n - \mathrm{E}[S/n]}{\sqrt{\mathrm{Var}[S/n]}} = \frac{\sum_{i=1}^k N_{ii}/n - \mathrm{E}\left[\sum_{i=1}^k N_{ii}/n\right]}{\sqrt{\mathrm{Var}\left[\sum_{i=1}^k N_{ii}/n\right]}}$, then $T_{n,sc} = Z_C$. Under RL, $\mathrm{E}[T_{n,sc}] = \mathrm{E}[Z_C] = 0$ and $Z_C = (S - \mathrm{E}[S])/\sqrt{\mathrm{Var}[S]}$ is approximately distributed as $N(0,1)$

for large n. Under right-sided (resp. left sided) alternative H_a, we have $\mathrm{E}[S|H_a] = \varepsilon > 0$ (resp. $\mathrm{E}[S|H_a] = \varepsilon < 0$) where ε is a parameterization of the alternative with $\varepsilon > 0$ (resp. $\varepsilon < 0$) characterizing self (resp. mixed) correspondence. Let $R(\varepsilon)$ and $Q(\varepsilon)$ be the numbers of reflexive pairs and shared NNs, respectively, $p_{ii}(\varepsilon)$, $p_{iii}(\varepsilon)$, and $p_{iiii}(\varepsilon)$ be the counterparts of p_{ii}, p_{iii}, and p_{iiii} in Equation (3). Then under H_a, we have $\mathrm{Var}[N_{ii}/n] = (1/n + R(\varepsilon)/n^2)p_{ii}(\varepsilon) + (2/n - 2R(\varepsilon)/n^2 + Q(\varepsilon)/n^2)p_{iii}(\varepsilon) + (1 - 3/n - Q(\varepsilon)/n^2 + R(\varepsilon)/n^2)p_{iiii}(\varepsilon) - (p_{ii}(\varepsilon))^2$ and $\mathrm{Cov}[N_{ii}/n, N_{jj}/n] = (1 - 3/n - Q(\varepsilon)/n^2 + R(\varepsilon)/n^2)p_{iijj} - p_{ii}p_{jj}$. So, under H_a, it follows that $\mathrm{Var}[N_{ii}/n] \to 0$ and $\mathrm{Cov}[N_{ii}/n, N_{jj}/n] \to 0$ as $n_i \to \infty$. Hence $\mathrm{Var}[S] \to 0$ as $n_i \to \infty$. Thus the test using Z_C is consistent for the right-sided (resp. left sided) alternative. Consistency for the two-sided alternative is similar. ■

4. Empirical Size and Power Analysis

In this section we investigate the finite sample performance of the tests under RL or CSR independence and under various alternatives via Monte Carlo simulations.

4.1. Empirical Size Analysis

To determine empirical size performance of the tests, we use CSR independence and RL as our null hypotheses. Under these patterns, correspondence would occur at expected levels. That is, under these patterns we have $\mathrm{E}[S_i] = n_i(n_i - 1)/(n - 1)$ for all $i = 1, 2, \ldots, k$ as in Equation (11) and $\mathrm{E}[S] = \sum_{i=1}^{k} n_i(n_i - 1)/(n - 1)$ as in Equation (12).

We estimate the empirical sizes (i.e., significance levels) based on the asymptotic critical values. For example, let T be a test with a χ^2_{df} distribution asymptotically, and let T_i be the value of test statistic for the sample generated at i^{th} Monte Carlo replication for $i = 1, 2, \ldots, N_{mc}$. Then the empirical size of T at level $\alpha = 0.05$, denoted $\widehat{\alpha}_T$ is computed as $\widehat{\alpha}_T = \frac{1}{N_{mc}} \sum_{i=1}^{N_{mc}} \mathbf{I}\left(T_i \geq \chi^2_{df,0.95}\right)$. Furthermore, let Z be a test with a $N(0,1)$ asymptotic distribution, and let Z_i be the value of test statistic for i^{th} sample generated. Then the empirical size of Z for the left-sided (resp. right-sided) alternative at level $\alpha = 0.05$, denoted $\widehat{\alpha}_Z$ is computed as $\widehat{\alpha}_Z = \frac{1}{N_{mc}} \sum_{i=1}^{N_{mc}} \mathbf{I}(Z_i \leq z_{0.05} = -1.645)$ (resp. $\widehat{\alpha}_Z = \frac{1}{N_{mc}} \sum_{i=1}^{N_{mc}} \mathbf{I}(Z_i \geq z_{0.95} = 1.645)$). The empirical size for the two-sided alternative is computed as $\widehat{\alpha}_Z = \frac{1}{N_{mc}} \sum_{i=1}^{N_{mc}} \mathbf{I}(|Z_i| \geq z_{0.975} = 1.96)$.

4.1.1. Empirical Size Analysis under CSR Independence

We consider the two-class and three-class cases. For the three-class case, we have classes X, Y, and Z (or classes 1, 2, and 3) of sizes n_1, n_2, and n_3 respectively. Under H_o, at each of $N_{mc} = 10000$ replications, we generate n_1 X points $\mathscr{X}_{n_1} = \{X_1, \ldots, X_{n_1}\}$,

n_2 Y points $\mathscr{Y}_{n_2} = \{Y_1,\dots,Y_{n_2}\}$, and n_3 Z points $\mathscr{Z}_{n_3} = \{Z_1,\dots,Z_{n_3}\}$ independently of each other and iid from $\mathscr{U}((0,1)\times(0,1))$ and combine X, Y and Z points as $\mathscr{W}_n = \mathscr{X}_{n_1} \cup \mathscr{Y}_{n_2} \cup \mathscr{Z}_{n_3} = \{W_1,W_2,\dots,W_n\}$. For the two-class case, we only generate points from classes X and Y and combine them as $\mathscr{W}_n = \mathscr{X}_{n_1} \cup \mathscr{Y}_{n_2} = \{W_1,W_2,\dots,W_n\}$. We consider four cases for CSR independence:

$$\begin{aligned}
&\text{CSR Case 1 (with 2 classes)}: n_1 = n_2 = n = 10,20,30,40,50\\
&\text{CSR Case 2 (with 2 classes)}: n_1 = 20 \text{ and } n_2 = 20,30,\dots,60.\\
&\text{CSR Case 3 (with 3 classes)}: n_1 = n_2 = n_3 = n = 10,20,30,40,50\\
&\text{CSR Case 4 (with 3 classes)}: n_1 = 20,\ n_2 = 40, \text{ and } n_3 = 40,40,\dots,80.
\end{aligned}$$

In CSR cases 1 and 3, the sample sizes are equal and increasing, to determine the influence of the increasing balanced sample sizes on the empirical levels of the tests. On the other hand, CSR cases 2 and 4 are designed to determine the influence of differences in the sample sizes (i.e., differences in relative abundances of classes) on the empirical levels of the tests.

The empirical significance levels for the tests under CSR independence are presented in Table 6, where $\widehat{\alpha}_{Z_{11}}$, $\widehat{\alpha}_{Z_{22}}$, and $\widehat{\alpha}_{Z_{33}}$ are for the cell-specific tests for cells $(1,1)$, $(2,2)$, and $(3,3)$ (for segregation); (see, e.g., Dixon, 1994 and Ceyhan, 2008a for details on the cell-specific tests); $\widehat{\alpha}_{\mathscr{X}_C}$ is for the χ^2 test $\mathscr{X}_C$, testing the self column in CCT; $\widehat{\alpha}_{Z_C}$ is for Z_C, testing the sum of the self column; $\widehat{\alpha}_{\mathscr{X}_D}$ is for Dixon's overall segregation test; and $\widehat{\alpha}_{\mathscr{X}_C,Z_C}$ is the proportion of agreement in rejecting the null hypothesis for $\mathscr{X}_C$ and Z_C; $\widehat{\alpha}_{\mathscr{X}_D,\mathscr{X}_C}$ is the proportion of agreement for $\mathscr{X}_D$ and $\mathscr{X}_C$; and $\widehat{\alpha}_{\mathscr{X}_D,Z_C}$ is the proportion of agreement for $\mathscr{X}_D$ and Z_C. For $N_{mc} = 10000$ replications, an empirical size estimate is deemed conservative, if smaller than .0464 while it is deemed liberal, if larger than .0536 at .05 level (based on binomial critical values with $n = 10000$ trials and probability of success 0.05).

In the two-class cases (i.e., CSR cases 1 and 2), we do not present Dixon's overall test of segregation as it is identical to $\mathscr{X}_C$ for two classes. Under CSR case 1, $\mathscr{X}_C$ and Z_C are slightly conservative for smaller sample sizes. Under CSR case 2, $\mathscr{X}_C$ and Z_{11} are conservative (with the latter being more so) when sample sizes are unbalanced (i.e., the relative abundance ratio, n_2/n_1, gets larger than two). Note also that Z_C seems to be robust to differences in relative abundance of the classes. The proportion of agreement in rejecting the null hypothesis by $\mathscr{X}_C$ and Z_C is significantly smaller than .05, which implies these tests have significantly different rejection/acceptance regions (i.e., they are testing substantially different hypotheses).

Under the three-class cases of CSR cases 3 and 4, we also present Dixon's overall test of segregation as it is different from $\mathscr{X}_C$ for more than two classes. Under CSR case 3, all tests are slightly conservative for smaller sample sizes and cell-specific tests are slightly liberal for larger sample sizes. Under CSR case 4, Z_{11} is conservative for all sample size combinations (since it has the smallest sample size in this case where

Table 6: *The empirical significance levels of the tests under CSR independence cases 1-4 with* $N_{mc} = 10000$ *at* $\alpha = .05$. $\widehat{\alpha}_{Z_{11}}$, $\widehat{\alpha}_{Z_{22}}$, *and* $\widehat{\alpha}_{Z_{33}}$ *are the empirical significance levels for the cell-specific tests for cells* $(1,1)$, $(2,2)$, *and* $(3,3)$ *(for segregation);* $\widehat{\alpha}_{\mathscr{X}_D}$ *for Dixon's overall segregation test,* $\mathscr{X}_D$; $\widehat{\alpha}_{\mathscr{X}_C}$ *for the* χ^2 *test* $\mathscr{X}_C$; $\widehat{\alpha}_{Z_C}$ *for* Z_C; *and* $\widehat{\alpha}_{\mathscr{X}_C,Z_C}$ *is the proportion of agreement in rejecting the null hypothesis for* $\mathscr{X}_C$ *and* Z_C; $\widehat{\alpha}_{\mathscr{X}_D,\mathscr{X}_C}$ *is the proportion of agreement for* $\mathscr{X}_D$ *and* $\mathscr{X}_C$; *and* $\widehat{\alpha}_{\mathscr{X}_D,Z_C}$ *is the proportion of agreement for* $\mathscr{X}_D$ *and* Z_C. *Size estimates larger than .0536 (resp. smaller than .0464) are liberal (resp. conservative) and are superscripted with* $^{\ell}$ *(resp.* ^{c}*).*

CSR case 1					
n	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{\mathscr{X}_C,Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$
10	$.0432^c$	$.0439^c$	.0216	$.0454^c$	.0465
20	$.0457^c$	$.0443^c$	.0207	.0517	.0522
30	.0485	$.0462^c$	.0237	.0573	.0493
40	.0501	$.0545^{\ell}$	.0254	.0507	.0525
50	.0472	.0468	.0215	$.0454^c$	.0472

CSR case 2					
n_2	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{\mathscr{X}_C,Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$
20	$.0437^c$	$.0448^c$	.0197	.0482	.0517
30	.0480	.0493	.0253	.0521	.0479
40	.0489	.0521	.0237	$.0313^c$	$.0455^c$
50	$.0427^c$	.0526	.0219	$.0295^c$	.0478
60	$.0452^c$	.0465	.0233	$.0395^c$	.0495

CSR case 3									
n	$\widehat{\alpha}_{\mathscr{X}_D}$	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{\mathscr{X}_D,\mathscr{X}_C}$	$\widehat{\alpha}_{\mathscr{X}_D,Z_C}$	$\widehat{\alpha}_{\mathscr{X}_C,Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$	$\widehat{\alpha}_{Z_{33}}$
10	$.0421^c$	$.0425^c$	.0491	.0179	.0084	.0312	$.0277^c$	$.0283^c$	$.0250^c$
20	$.0408^c$	$.0438^c$	.0481	.0180	.0094	.0293	$.0332^c$	$.0283^c$	$.0318^c$
30	.0465	.0473	.0496	.0204	.0110	.0320	.0530	.0526	$.0549^{\ell}$
40	$.0455^c$	.0495	$.0461^c$	.0205	.0092	$.0320^c$	.0509	$.0558^{\ell}$	$.0595^{\ell}$
50	.0474	.0497	.0504	.0229	.0120	.0329	$.0605^{\ell}$	$.0588^{\ell}$	$.0564^{\ell}$

CSR case 4									
n_3	$\widehat{\alpha}_{\mathscr{X}_D}$	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{\mathscr{X}_D,\mathscr{X}_C}$	$\widehat{\alpha}_{\mathscr{X}_D,Z_C}$	$\widehat{\alpha}_{\mathscr{X}_C,Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$	$\widehat{\alpha}_{Z_{33}}$
40	.0490	.0509	.0492	.0233	.0126	.0342	$.0418^c$	$.0551^{\ell}$	.0510
50	$.0412^c$	$.0443^c$	$.0450^c$	.0187	.0100	.0297	$.0344^c$	$.0460^c$	.0489
60	.0488	.0466	.0528	.0212	.0123	.0354	$.0238^c$	$.0543^{\ell}$	.0492
70	.0528	.0496	.0498	.0261	.0156	.0344	$.0458^c$	.0520	.0517
80	.0509	.0492	.0518	.0228	.0116	.0302	$.0333^c$	$.0431^c$	.0522

there is substantial class imbalance) whereas Z_{33} has the best size performance as it corresponds to the class with the largest samples. The proportions of agreement by the tests in rejecting the null hypothesis are all significantly smaller than .05, which implies these tests have significantly different rejection/acceptance regions (with $\mathscr{X}_C$ and Z_C having the largest overlap (i.e., these statistics are testing more similar hypotheses) and $\mathscr{X}_D$ and Z_C having the smallest overlap in rejection regions (i.e., these statistics are testing more different hypotheses compared to other pairs).

For unbalanced or small sample sizes, the tests are usually conservative (especially for the cell-specific tests for the smaller samples), so we recommend the use of the Monte Carlo randomized versions or the use of Monte Carlo critical values for the cell-specific test for the smaller class. A Monte Carlo critical value is determined as the appropriately ranked value of the test statistic in a certain number of generated data sets from the distribution under the null hypothesis. The class sizes are said to be *balanced*, if the relative abundances of the classes are close to one, and they are called *unbalanced*, if the relative abundances deviate substantially from one.

4.1.2. Empirical Size Analysis under RL

Under the RL pattern, the class labels or marks are assigned randomly to points whose locations are given. Recall that $\mathscr{W}_n = \{w_1, w_2, \ldots, w_n\}$ is the given set of locations for n points from the background pattern. For two classes, at each background realization, n_1 of the points are labeled as class 1 or X and the remaining $n_2 = n - n_1$ points are labeled as class 2 or Y. Similarly, for three classes, at each background realization, n_1 of the points are labeled as class X, n_2 of the points are labeled as class Y, and the remaining $n_3 = n - (n_1 + n_2)$ points are labeled as class Z.

Types of the Background Patterns (Two Classes)

RL Case 1: The background points are a realization of $Z_i \stackrel{iid}{\sim} \mathscr{U}((0,1) \times (0,1))$ for $i = 1, 2, \ldots, n$. That is, the background points, $\mathscr{W}_n$, are generated iid uniform in the unit square $(0,1) \times (0,1)$. We consider $n_1 = n_2 = 10, 20, \ldots, 50$.

RL Case 2: The background points, $\mathscr{W}_n$, are generated as in case 1 above with $n_1 = 20$ and $n_2 = 20, 30, \ldots, 60$.

RL Case 3: The background points, $\mathscr{W}_n$, are generated from a Matérn cluster process, MatClust(κ, r, μ) (Baddeley and Turner, 2005). In this process, first "parent" points are generated from a Poisson process with intensity κ. Then each parent point is replaced by $N \sim$ Poisson(μ) new points which are generated iid inside the circle of radius r centered at the parent point. Each background realization is a realization of $\mathscr{W}_n$ and is generated from MatClust(κ, r, μ). Let n be the number of points in a particular realization. Then $n_1 = \lfloor n/2 \rfloor$ of these points are labeled as class 1 where $\lfloor x \rfloor$ stands for the floor of x, and $n_2 = n - n_1$ as class 2. In our simulations, we use $\kappa = 2, 4, \ldots, 10$, $\mu = \lfloor 100/\kappa \rfloor$, and $r = 0.1$. That is, we take $(\kappa, \mu) \in \{(2,50), (4,25) \ldots, (10,10)\}$ so as to have about 100 background points on the average with about half of them being from class 1 and the other half being from class 2.

To reduce the influence of a particular background realization on the size performance of the tests, we generate 100 different realizations of each background pattern. For each case, the RL scheme described is repeated 1000 times for each (n_1, n_2) combination at each of 100 different background realizations. So we have $N_{mc} = 100000$. In RL cases 1 and 2, the points are from HPP in the unit square with fixed n_1 and n_2 (i.e., from binomial process), where RL case 1 is for assessing the effect of equal but increasing sample sizes on the tests, while RL case 2 is for assessing the effect of increasing differences in sample sizes of the classes (with one class size being fixed, while the other is increasing). On the other hand, in the background realizations of RL case 3, centers and numbers of clusters are random. On the average, with increasing κ, the cluster sizes tend to decrease and the number of clusters tend to increase (so as to have fixed class sizes on the average). Hence in RL case 3, we investigate the influence of increasing number of clusters with randomly determined centers on the size performance of the tests.

The empirical size estimates of the tests for two classes under RL cases 1-3 are presented in Table 7. For $N_{mc} = 100000$ replications, if all the Monte Carlo replications were independent, an empirical size estimate would have been deemed conservative, if smaller than .04887 while it would have been deemed liberal, if larger than .05113 at .05 level (based on binomial critical values with $n = 100000$ trials and probability of success 0.05). This approach is like providing critical values for a two-sided hypothesis test. Equivalently, one might construct a confidence interval (say 95 %) for the proportion of rejections (i.e., empirical size estimate) and check whether it contains the nominal level of .05 or lies completely at one side of .05. However, under our RL scheme, the Monte Carlo replications are not independent as 100 replications are performed at each of 100 background realizations, hence within sample independence is violated rending both the critical value and the confidence interval approaches are not appropriate. But we can account for dependence due to the use of same background realization for 100 of the realizations, at each of which 1000 Monte Carlo replications are performed, by using a linear mixed effects model. In particular, in the "lme4" package in R, we can employ "lmer" command with properly declaring the error structure for dependence in the background realization. For example, let "bg" stand for the background factor (i.e., takes the same value for each Monte Carlo replication at the same background realization). Then we can apply a mixed modeling with "lmer" command by declaring the error structure as "(1|bg)" and construct a 95 % confidence interval for the size estimate value. We mark the empirical sizes not significantly different from .05 with an asterisk.

Under RL case 1, tests are either slightly conservative or liberal (with more conservative for smaller samples), and under RL case 2, cell-specific tests for the smaller sample is moderately conservative, and the other tests are slightly conservative or liberal. The tests have sizes about the nominal level under RL case 3, since in this case, the class sizes are about 50, which seems large enough for the normal approximation to take effect. Moreover, the size performance of the tests does not depend on the number and size of the clusters in the background pattern and the more important factor is the sample sizes.

Types of the Background Patterns (Three Classes)

RL Case (i): Same as in RL Case 1 of the two class setting with $n_1 = n_2 = n_3 = 10, 20, \ldots, 50$.

RL Case (ii): Same as in RL Case 2 of the two class setting with $n_1 = 20$, $n_2 = 40$ and $n_3 = 40, 50, \ldots, 80$.

RL Case (iii): Same as in RL Case 3 of the two class setting with $n_1 = n_2 = \lfloor n/3 \rfloor$ points are labeled as classes 1 and 2 and $n_3 = n - (n_1 + n_2)$ as class 3. In our simulations, we use $\kappa = 2, 4, \ldots, 10$, $\mu = \lfloor 150/\kappa \rfloor$, and $r = 0.1$. That is, we take $(\kappa, \mu) \in \{(2,75), (4,37) \ldots, (10,15)\}$ so as to have about 150 background points on the average with about a third of them being from each of classes 1-3.

Table 7: *The empirical significance levels of the tests for two classes under RL cases 1-3 with $N_{mc} = 100000$ (1000 replications for each of 100 background realizations) at $\alpha = .05$. The empirical size labeling for the tests is as in Table 6. Size estimates not significantly different from .05 are marked with an asterisk.*

RL case 1				
n	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$
10	.04281	.04276	.04513	.04625
20	.04511	.04612	.05349	.05209
30	.04862*	.04616	.05220	.05258
40	.04782	.05398	.05232	.05217
50	.04942*	.04932*	.04740	.04642

RL case 2				
n_2	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$
20	.04602	.04670	.05479	.05414
30	.04735	.04783	.05050*	.04886*
40	.04551	.05357	.03375	.04358
50	.04611	.05649	.03456	.04893*
60	.04395	.04670	.04042	.04749

RL case 3				
κ	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$
2	.04700	.04957*	.04734	.04577
4	.04804	.04959*	.04901*	.04860*
6	.04905*	.05023*	.05103*	.04926*
8	.04859	.04983*	.05096*	.04914*
10	.04869*	.05011*	.05042*	.05097*

The empirical size estimates of the tests for three classes under RL cases (i)-(iii) are presented in Table 8. Under all cases $\mathscr{X}_D$ and $\mathscr{X}_C$ are slightly conservative (with the former being more conservative), and Z_C is closest to the nominal level. Under RL case (i) cell-specific tests are conservative for smaller samples, under RL case (ii), cell-specific tests for the smaller samples are conservative, while larger samples are close to the nominal level. Under RL case (iii) all Z tests are at about the desired level.

Based on the empirical size performance of the tests under CSR independence and RL, we observe that the new tests $\mathscr{X}_C$ and Z_C are more appropriate for both balanced or unbalanced sample sizes (with the latter being more robust to the imbalance in class sizes).

4.2. Empirical Power Analysis

To compare the empirical power performance of the tests, we consider various alternative cases with the two and three classes for deviations from the null case in the NN structure. The empirical power estimates are computed at $\alpha = .05$ as in the size estimation in Section 4.1.

Table 8: *The empirical significance levels of the tests with three classes under RL cases (i)-(iii) with N_{mc} = 10000 at $\alpha = .05$. The notation is as in Table 6. Size estimates not significantly different from .05 are marked with an asterisk.*

RL Case (i)						
n	$\widehat{\alpha}_{\mathscr{X}_D}$	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$	$\widehat{\alpha}_{Z_{33}}$
10	.03879	.03957	.04964*	.02536	.02585	.02528
20	.04479	.04571	.05043*	.03293	.03364	.03175
30	.04558	.04756	.05151	.05292	.05365	.05370
40	.04628	.04773	.04789	.05328	.05231	.05280
50	.04797	.04877*	.05009*	.05855	.05804	.05823

RL Case (ii)						
n_3	$\widehat{\alpha}_{\mathscr{X}_D}$	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$	$\widehat{\alpha}_{Z_{33}}$
40	.04701	.04728	.04674	.04048	.05155*	.04995*
50	.04674	.04736	.05120*	.03374	.04592	.05375
60	.04696	.04578	.05006*	.02355	.05240	.05036*
70	.04870*	.04881*	.04689	.04483	.05102*	.04662
80	.04798	.04970*	.05085*	.03427	.04768	.04747

RL Case (iii)						
κ	$\widehat{\alpha}_{\mathscr{X}_D}$	$\widehat{\alpha}_{\mathscr{X}_C}$	$\widehat{\alpha}_{Z_C}$	$\widehat{\alpha}_{Z_{11}}$	$\widehat{\alpha}_{Z_{22}}$	$\widehat{\alpha}_{Z_{33}}$
2	.04692	.04728	.04940*	.05081*	.05069*	.04764*
4	.04650	.04836	.04878*	.04752	.04813*	.04886*
6	.04860	.04900*	.04927*	.04825*	.04878*	.04959*
8	.04743	.04836	.04736	.04994*	.04923*	.04833*
10	.04693	.04791	.04868*	.04918*	.04881*	.05032*

4.2.1. Empirical Power Analysis for Two Classes

For the two classes, we consider five alternative cases.

Case I: For this class of alternatives, we generate $X_i \overset{iid}{\sim} \mathscr{U}((0,1)\times(0,1))$ for $i = 1,\ldots,n_1$ and $Y_j \overset{iid}{\sim} \mathrm{BVN}(1/2,1/2,\sigma_1,\sigma_2,\rho)$ for $j = 1,\ldots,n_2$, where $\mathrm{BVN}(\mu_1,\mu_2,\sigma_1,\sigma_2,\rho)$ is the bivariate normal distribution with mean (μ_1,μ_2) and covariance $\begin{bmatrix} \sigma_1 & \rho \\ \rho & \sigma_2 \end{bmatrix}$. In our simulations, we set $\sigma_1 = \sigma_2 = \sigma$ and $\rho = 0$. We consider the following three alternatives:

$$H_I^1 : \sigma = 1/5, \quad H_I^2 : \sigma = 2/15, \text{ and } H_I^3 : \sigma = 1/10. \tag{13}$$

The classes 1 and 2 (i.e., X and Y) have different distributions with different local intensities. In particular, X points are a realization of uniform distribution in the unit square, while Y points are clustered around the center of the unit square $(1/2,1/2)$ where the level of clustering increases as σ decreases. This suggests a high level of niche specificity for Y points around the center of the unit square compared to X points, which in turn implies segregation of Y points from X points. Furthermore, self NN pairs would be more likely to occur compared to mixed NN pairs, hence self correspondence is expected to be observed.

The empirical power estimates under the alternatives, $H_I^1 - H_I^3$, with $n_1 = n_2 = 40$ are presented in Table 9, where $\widehat{\beta}_{\mathscr{X}_C}$ is power estimate for the χ^2 test for the self column, $\mathscr{X}_C$; $\widehat{\beta}_{Z_{11}}$ and $\widehat{\beta}_{Z_{22}}$ are for the cell-specific tests for cells $(1,1)$ and $(2,2)$ (for segregation), and $\widehat{\beta}_{Z_C}$ is for the Z test for the sum of self column, Z_C. Under the case I alternatives, the power estimates increase as σ decreases. In particular, the self column test, $\mathscr{X}_C$, and the right-sided cell-specific tests for cells $(1,1)$ and $(2,2)$ have high power estimates, which indicates segregation of Y points from X points and vice versa. Since segregation occurs for both classes, and $\mathscr{X}_C$ has high power implies self correspondence. Also, the right-sided Z test for the sum of the self column has high power, confirming self correspondence in this case. Notice that the Z_C has the highest power estimates.

Case II: For this type of alternatives, first, we generate $X_i \stackrel{iid}{\sim} \mathscr{U}((0,1)\times(0,1))$ for $i = 1,2,\ldots,n_1$ and for each $j = 1,2,\ldots,n_2$, we generate Y_j around a randomly picked X_i with probability p in such a way that $Y_j = X_i + R_j(\cos T_j, \sin T_j)^t$ where v^t stands for transpose of the vector v, $R_j \sim \mathscr{U}(0, \min_{i\neq j} d(X_i, X_j))$ and $T_j \sim \mathscr{U}(0, 2\pi)$ or generate Y_j uniformly in the unit square with probability $1-p$. In the pattern generated, Y_j are more associated with X_i. The three values of p constitute the following alternatives:

$$H_{II}^1 : p = .25, \quad H_{II}^2 : p = .50, \text{ and } H_{II}^3 : p = .75. \tag{14}$$

Table 9: *The power estimates under the case I-III, and V alternatives in Equations* (13)-(15), *and* (17) *with* $N_{mc} = 10000$, $n_1 = n_2 = 40$ *at* $\alpha = .05$. $\widehat{\beta}_{Z_{11}}$ *and* $\widehat{\beta}_{Z_{22}}$ *are is power estimates for the cell-specific tests for cells* $(1,1)$ *and* $(2,2)$ *(for segregation),* $\widehat{\beta}_{\mathscr{X}_C}$ *is for* $\mathscr{X}_C$*, testing deviations in the self column, and* $\widehat{\beta}_{Z_C}$ *is for* Z_C*, testing the sum of self column. The "$>$" (resp. "$<$") sign in the superscript implies the power is estimated for the right-sided (resp. left-sided) alternative.*

Power estimates under case I alternatives				
	$\widehat{\beta}_{\mathscr{X}_C}$	$\widehat{\beta}_{Z_C}^{>}$	$\widehat{\beta}_{Z_{11}}^{>}$	$\widehat{\beta}_{Z_{22}}^{>}$
H_I^1	.2226	.4167	.2648	.3320
H_I^2	.8523	.9599	.8403	.9164
H_I^3	.9929	.9994	.9887	.9972

Power estimates under case II alternatives				
	$\widehat{\beta}_{\mathscr{X}_C}$	$\widehat{\beta}_{Z_C}^{<}$	$\widehat{\beta}_{Z_{11}}^{<}$	$\widehat{\beta}_{Z_{22}}^{<}$
H_{II}^1	.1469	.3998	.2658	.2330
H_{II}^2	.4051	.7788	.5625	.4054
H_{II}^3	.5393	.9003	.7373	.3366

case III alternatives				
	$\widehat{\beta}_{\mathscr{X}_C}$	$\widehat{\beta}_{Z_C}^{>}$	$\widehat{\beta}_{Z_{11}}^{>}$	$\widehat{\beta}_{Z_{22}}^{>}$
H_{III}^1	.4196	.6812	.5141	.5134
H_{III}^2	.9247	.9876	.9437	.9439
H_{III}^3	.9999	1.000	.9999	.9997

case V alternatives				
	$\widehat{\beta}_{\mathscr{X}_C}$	$\widehat{\beta}_{Z_C}^{<}$	$\widehat{\beta}_{Z_{11}}^{<}$	$\widehat{\beta}_{Z_{22}}^{<}$
H_V^1	.1795	.3499	.2160	.3867
H_V^2	.4384	.7081	.5562	.6280
H_V^3	.6808	.8937	.7937	.7795

In this case, X points constitute a realization of the uniform distribution in the unit square, while Y points are clustered around the X points, and the level of clustering increases as p increases. The empirical power estimates under the alternatives, $H^1_{II} - H^3_{II}$, with $n_1 = n_2 = 40$ are presented in Table 9. Notice that $\mathscr{X}_C$ implies significant deviations in the self column, but Z_{11} and Z_{22} have high power estimates for the left-sided alternative, which implies significant association between the classes. Z_{11} having higher power for the left-sided alternative is due to severe lack of segregation of class X points from class Y points (or class Y points being significantly associated with class X points), and Z_{22} has smaller power since Y points are clustered around X points, which also causes slight clustering of Y points. Furthermore, Z_C has high power for the left-sided alternative, which implies mixed NN pairs are more abundant, hence there is significant mixed correspondence in the NN structure.

Case III: For this class of alternatives, we consider $X_i \overset{iid}{\sim} \mathscr{U}((0,1-s)\times(0,1-s))$ for $i=1,\ldots,n_1$, and $Y_j \overset{iid}{\sim} \mathscr{U}((s,1)\times(s,1))$ for $j=1,\ldots,n_2$. The three values of s constitute the following alternatives;

$$H^1_{III}: s = 1/6, \quad H^2_{III}: s = 1/4, \text{ and } H^3_{III}: s = 1/3. \tag{15}$$

Notice that these alternatives are the segregation alternatives considered for Monte Carlo simulations in Ceyhan (2010). The empirical power estimates under the segregation alternatives $H^1_{III} - H^3_{III}$ are presented in Table 9. The tests have high power which increases as s increases. There is significant segregation (at the same level for both classes by construction), and the cell-specific tests are also significant for the right-sided alternatives. Furthermore, $\mathscr{X}_C$ indicates significant deviations in the self column, and Z_C has high power for the right-sided alternative, indicating self correspondence in the NN structure.

Case IV: We also consider alternatives in which, by construction, self-reflexive pairs are more frequent than expected under CSR independence. We generate $X_i \overset{iid}{\sim} S_1$ for $i=1,\ldots,\lfloor n_1/2 \rfloor$ and $Y_j \overset{iid}{\sim} S_2$ for $j=1,\ldots,\lfloor n_2/2 \rfloor$. Then for $k=\lfloor n_1/2 \rfloor+1,\ldots,n_1$, we generate $X_k = X_{k-\lfloor n_1/2 \rfloor} + r(\cos T_j, \sin T_j)^t$ and for $l = \lfloor n_2/2 \rfloor + 1,\ldots,n_2$, we generate $Y_l = Y_{l-\lfloor n_1/2 \rfloor} + r(\cos T_j, \sin T_j)^t$ where $r \in (0,1)$ and $T_j \sim \mathscr{U}(0,2\pi)$. Appropriate small choices of r will yield an abundance of self-reflexive pairs. The three values of r we consider constitute the self-reflexivity alternatives at each support pair (S_1,S_2). Then the nine alternative combinations we consider are given by

$$\begin{aligned}
&(i)\ H^1_{IV}: S_1 = S_2 = (0,1)\times(0,1), \text{ (a) } r=1/7, \text{ (b) } r=1/8, \text{ (c) } r=1/9,\\
&(ii)\ H^2_{IV}: S_1 = (0,5/6)\times(0,5/6) \text{ and } S_2 = (1/6,1)\times(1/6,1), \text{ (a) } r=1/7, \text{ (b) } r=1/8, \text{ (c) } r=1/9,\\
&(iii)\ H^3_{IV}: S_1 = (0,3/4)\times(0,3/4) \text{ and } S_2 = (1/4,1)\times(1/4,1) \text{ (a) } r=1/7, \text{ (b) } r=1/8, \text{ (c) } r=1/9.
\end{aligned} \tag{16}$$

Table 10: *The power estimates under the case IV alternatives with $N_{mc} = 10000$, $n_1 = n_2 = 40$ at $\alpha = .05$. The empirical power labeling and superscripting for "<" and ">" are as in Table 9.*

Power estimates under the case IV alternatives					
	r	$\widehat{\beta}_{\mathscr{X}_C}$	$\widehat{\beta}^{>}_{Z_C}$	$\widehat{\beta}^{>}_{Z_{11}}$	$\widehat{\beta}^{>}_{Z_{22}}$
H^1_{IV}	1/7	.8671	.9572	.8866	.8848
	1/8	.9377	.9834	.9455	.9436
	1/9	.9735	.9949	.9746	.9743
H^2_{IV}	1/7	.9440	.9885	.9522	.9523
	1/8	.9740	.9949	.9769	.9779
	1/9	.9890	.9982	.9895	.9908
H^3_{IV}	1/7	.9930	.9990	.9925	.9932
	1/8	.9973	.9996	.9967	.9973
	1/9	.9991	.9999	.9984	.9989

In this case, under H^2_{IV} and H^3_{IV}, by construction, there is segregation of the classes due to the choices of the supports. The empirical power estimates under the alternatives $H^1_{IV} - H^3_{IV}$ are presented in Table 10. Notice that the tests all have very high power estimates. Furthermore, there is significant segregation (at the same level for both classes at each alternative by construction), and the cell-specific tests are also significant for the right-sided alternatives. Furthermore, $\mathscr{X}_C$ has high power estimates indicating significant deviation in the self column and Z_C has high power for the right-sided alternative, indicating self correspondence in the NN structure. The power estimates for these tests increase from H^1_{IV} to H^3_{IV} and they also increase as r decreases from (a) to (c) at each (S_1, S_2) combination. Hence the power estimates increase as the levels of segregation increases.

Case V: In this case, first, we generate $X_i \stackrel{iid}{\sim} \mathscr{U}((0,1)\times(0,1))$ and then generate Y_j as $Y_j = X_i + r(\cos T_j, \sin T_j)^t$ where $r \in (0,1)$ and $T_j \sim \mathscr{U}(0, 2\pi)$. In the pattern generated, appropriate choices of r will cause Y_j and X_i more associated; that is, a Y point will be more likely to be the NN of an X point, and vice versa. The three values of r we consider constitute the three association alternatives;

$$H^1_V : r = 1/4, \quad H^2_V : r = 1/7, \text{ and } H^3_V : r = 1/10. \tag{17}$$

These are also the association alternatives considered for Monte Carlo simulations in Ceyhan (2010).

The empirical power estimates under $H_V^1 - H_V^3$ are presented in Table 9. Notice that $\mathscr{X}_C$ has high power estimates indicating significant deviations in the self column, and the cell-specific tests have high power estimates for the left-sided alternatives indicating presence of significant association of the classes. Furthermore, Z_C has high power for the left-sided alternative indicating that there is significant mixed correspondence in the NN structure. The power estimates for these tests increase as r decreases.

4.2.2. Empirical Power Analysis for Three Classes

For the three classes, we consider two cases. We generate $n_1 = n_2 = n_3 = 40$ points from classes X, Y and Z.

Case 1: For this class of alternatives, we generate X and Y points as in Case III of power analysis for two classes of Section 4.2.1, and Z points as Y points in Case I of Section 4.2.1. We consider the following two alternatives:

$$H_1^1 : s = 1/6, \sigma = 1/5, \quad \text{and } H_1^2 : s = 1/4, \sigma = 2/15. \tag{18}$$

The classes 1 and 2 (i.e., X and Y) are segregated with shifted supports and class 3 is clustered around $(1/2, 1/2)$. Furthermore, by construction a higher level of niche specificity for Z points exists around the center of the unit square compared to X and Y points, which in turn implies segregation of Z points from X and Y points as well.

The empirical power estimates under the alternatives, H_1^1 and H_1^2, with $n_1 = n_2 = n_3 = 40$ are presented in Table 11, where $\widehat{\beta}_{\mathscr{X}_D}$ is power estimate for Dixon's overall test of segregation; $\widehat{\beta}_{Z_{33}}$ is for the cell-specific test for cell $(3,3)$ (for segregation), the other notation is as in Table 9. Under the case 1 alternatives, the power estimates increase as σ decreases and s increases. In particular, Dixon's overall test and the self column test, $\mathscr{X}_C$ have high power estimates, and the right-sided cell-specific tests for cells $(1,1)$, $(2,2)$ and $(3,3)$ have high power, which indicate segregation of each class from the others. Also, the right-sided Z test for the sum of the self column, Z_C, has high power, implying self correspondence is operating as well. Notice that the Z_C has the highest power estimates.

Case 2: For this class of alternatives, we again generate X and Y points as in Case III of Section 4.2.1, and Z points as Y points in Case V of Section 4.2.1. We consider the following two alternatives:

$$H_2^1 : s = 1/6, r = 1/7, \quad \text{and } H_2^2 : s = 1/4, r = 1/10. \tag{19}$$

The classes 1 and 2 (i.e., X and Y) are segregated with shifted supports and class 3 is clustered around X and Y points.

Table 11: *The power estimates under the case 1 and 2 alternatives with* $N_{mc} = 10000$, $n_1 = n_2 = n_3 = 40$ *at* $\alpha = .05$. $\widehat{\beta}_{\mathscr{X}_D}$ *is the power estimate for Dixon's overall segregation test,* $\widehat{\beta}_{Z_{33}}$ *is for the cell-specific test for cell* $(3,3)$. *The other notation and superscripting for "<" and ">" are as in Table 9.*

Power estimates under						
case 1 alternatives						
	$\widehat{\beta}_{\mathscr{X}_D}$	$\widehat{\beta}_{\mathscr{X}_C}$	$\widehat{\beta}^{>}_{Z_C}$	$\widehat{\beta}^{>}_{Z_{11}}$	$\widehat{\beta}^{>}_{Z_{22}}$	$\widehat{\beta}^{>}_{Z_{33}}$
H_1^1	.3297	.4453	.6453	.5186	.5254	.1951
H_1^2	.9527	.9809	.9958	.9606	.9570	.6985
case 2 alternatives						
	$\widehat{\beta}_{\mathscr{X}_D}$	$\widehat{\beta}_{\mathscr{X}_C}$	$\widehat{\beta}^{>}_{Z_C}$	$\widehat{\beta}^{>}_{Z_{11}}$	$\widehat{\beta}^{>}_{Z_{22}}$	$\widehat{\beta}^{<}_{Z_{33}}$
H_2^1	.2620	.2289	.0539	.1877	.1834	.2954
H_2^2	.6514	.4818	.1032	.3488	.3433	.4099

The empirical power estimates under the alternatives, H_2^1 and H_2^2, with $n_1 = n_2 = n_3 = 40$ are presented in Table 11. Under the case 2 alternatives, the power estimates increase as r decreases and s increases. In particular, Dixon's overall test and the self column test, $\mathscr{X}_C$ have high power, and the right-sided cell-specific tests for cells $(1,1)$ and $(2,2)$, and left-sided test for cell $(3,3)$ have high power, which indicate segregation of X and Y points from other classes, and lack of segregation of Z points from X and Y points which might be association of Z points with one or both of classes X and Y. To determine the specifics one needs to check the off-diagonal cell specific tests in row 3 of the corresponding NNCT. Also, the right-sided Z test for the sum of the self column is mildly significant, implying a mild level of self correspondence is operating as well. Notice also that the Z_C has the lowest power estimates.

In alternative cases I-V the classes are either both segregated or associated (i.e., the direction of the deviation in each diagonal cell is same for both classes). Hence this cumulative effect is better captured by Z_C which has the highest power estimates under all these cases. Similarly, in alternative case 1, by construction, each class is segregated from others (although the type and level of segregation is different for class Z compared to X and Y), hence the direction of the deviation in the self column in CCT (i.e., diagonal cells in NNCT) is same for all classes, thereby rendering Z_C the most powerful test again. However, in alternative case 2, while X and Y are segregated, Z is associated with both classes. Hence direction of deviation in the self column cells are positive for X and Y and negative for Z. So this sign difference tends to nullify the deviations from the null case, which causes Z_C have the lowest power estimates.

5. Real-Life Example Data Set

To illustrate the methodology, we use an example data set with 6 classes: the Lansing Woods data which is available in the spatstat package in R (Baddeley and Turner, 2005).

The Lansing Woods data contains locations of trees (in feet (ft)) and botanical classification of trees according to their species in a 924 ft $\times$ 924 ft (19.6 acre) plot in Lansing Woods, Clinton County, Michigan, USA (Gerrard, 1969). The data set comprises of 2251 trees together with their species as hickories, maples, red oaks, white oaks, black oaks and miscellaneous trees. In our analysis, we consider each species as a class and miscellaneous trees as another class. The scatterplot of these tree locations are presented in Figure 2.

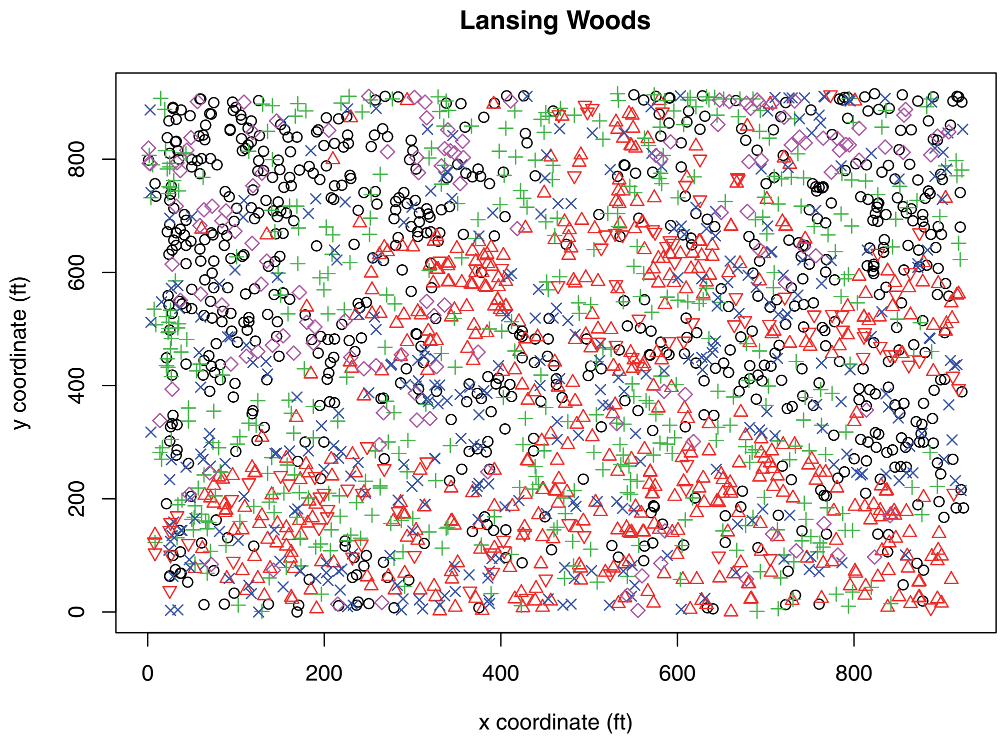

Figure 2: *The scatterplot of the locations of hickories (circles ○), maples (triangles △), white oaks (pluses +), red oaks (crosses ×), black oaks (diamond shapes ⋄), and other species (inverse triangles ▽) in the Lansing Woods, Clinton County, Michigan, USA.*

The CCT for this data is presented in Table 12. Notice that some cell counts in the contingency tables are not integers, since there are ties in the NN relations. For self correspondence, the abundance proportions for the species is hickories:maples:whit oaks:red oaks:black oaks:other $\approx 6 : 70 : 4.90 : 4.27 : 3.30 : 1.29 : 1.00$ and the proportions of the entries in the self column is $\approx 14.14 : 9.70 : 5.50 : 4.20 : 1.08 : 1.00$, which seems to be much different than the abundance proportions, suggesting significant presence of self correspondence.

Table 12: *The CCT for the Lansing Woods data.*

		pair type		
		self	mixed	total
base species	hickory	353.5	349.5	703
	maple	242.5	271.5	514
	white oak	137.5	310.5	448
	red oak	105	241	346
	black oak	27	108	135
	other	25	80	105
	total	890.5	1360.5	2251

Table 13: *The test statistics and the p-values for Lansing Woods data. Z_{ii} are cell-specific tests for cells (i,i) for $i = 1,2,\ldots,6$, $\mathscr{X}_D$ is Dixon's overall test of segregation. Z_C, and $\mathscr{X}_C$ are as defined in the text; TS stands for the test statistic, p_{asy}, p_{mc}, and p_{rand} stand for the p-values based on the asymptotic approximation, Monte Carlo simulation, and randomization of the tests, respectively.*

Test statistics and p-values for Lansing Woods data									
	$\mathscr{X}_D$	$\mathscr{X}_C$	$Z_S^>$	$Z_{11}^>$	$Z_{22}^>$	$Z_{33}^>$	$Z_{44}^>$	$Z_{55}^>$	$Z_{66}^>$
TS	376.8609	325.9750	16.4759	9.4622	11.0934	4.7895	6.3717	5.5085	7.4514
p_{asy}	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$
p_{rand}	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$
p_{mc}	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$	$< .0001$

We compute $Q = 1560$ and $R = 1400$. Again the more appropriate null hypothesis is the CSR independence pattern, since the locations of the tree species can be viewed a priori resulting from different processes (Goreaud and Pélissier, 2003). We present the test statistics and the associated p-values in Table 13, where in this table p_{asy} stands for the p-value based on the asymptotic approximation (i.e., asymptotic critical value), p_{rand} is based on Monte Carlo randomization of the labels on the given locations of the trees 10000 times and p_{mc} is the p-value based on 10000 Monte Carlo replication of the CSR independence pattern in the region plotted in Figure 2. Notice that p_{asy}, p_{rand} and p_{mc} are similar and highly significant for all tests. The cell-specific tests are all significant for the right-sided alternative, and the χ^2 test for the self column, $\mathscr{X}_C$, is significant, implying significant self correspondence for these species, and hence significant segregation of the species (from each other). Similarly, Z_C is significant confirming significant self correspondence for all species combined.

6. Discussion and Conclusions

In this article, we introduce the correspondence in the NN structure pattern for multiple classes/species and tests for it based on a contingency table called correspondence contingency table (CCT) which can also be derived from the associated nearest neighbour contingency table (NNCT). These tests are a χ^2 test of correspondence for the first column of CCT (called self-column), $\mathscr{X}_C$, and a Z test for the sum of the self column of CCT, Z_C. We show that in the two class case, the CCT and the NNCT contain the same information (but in different order in their entries), and the corresponding quadratic test for the self column, $\mathscr{X}_C$ and Dixon's overall test of segregation, $\mathscr{X}_D$, are equivalent. For more than two classes, these tests are different and hence provide different information. On the other hand, regardless of the number of classes, Z_C is different from $\mathscr{X}_C$ and $\mathscr{X}_D$ (i.e., Z_C provides new information not provided by the segregation tests for two or more classes) whereas Z_{S_i} and Z_{ii} are identical (i.e., they always give the same information).

For $k \geq 2$ classes, NNCT is of dimension $k \times k$ and the corresponding CCT is of dimension $k \times 2$, where the entries in the first column (i.e., self column) are the diagonal entries of the NNCT and each entry in the second column (i.e., mixed column) of CCT is the sum of off-diagonal entries at each row of NNCT. Overall segregation test based on NNCT measures any deviation in the entries of the NNCT and a cell-specific test based on NNCT measures the deviation in the corresponding entry of the NNCT (Dixon, 1994, 2002b). On the other hand, the tests based on the CCT are a χ^2 test for the self column and a Z test for the sum of the self column. The former test is based on deviations of the frequencies of the self NN pairs, and the latter is based on the sum of these frequencies. Both tests might indicate presence of self or mixed correspondence which can not be tested directly in the NNCT, hence the need to introduce CCT.

We show that $\mathscr{X}_C$ provides information on the overall deviations jointly in the self column (or in the mixed column) in CCT, Z_C provides information on the abundance of self pairs when all classes are combined. Hence to determine the level and type of correspondence as self or mixed, $\mathscr{X}_C$ should be employed together with the cell-specific tests Z_{ii} (see Equation (5)) so that when $\mathscr{X}_C$ is significant cell-specific tests will provide the direction and significance of the deviations for each diagonal cell in the NNCT (or each cell in the self-column of CCT). If they are all or mostly in the positive (resp. negative) direction, the pattern would be segregation (resp. lack of segregation) for the classes corresponding to the positive (resp. negative) significant Z_{ii} values and self (resp. mixed) correspondence for all classes combined. On the other hand, for Z_C we do not need to confer to the cell-specific tests, as it by itself is sufficient to indicate that the correspondence is of type self or mixed. Another advantage of Z_C is that it is more robust to differences in relative abundances of the classes (i.e., to the class imbalance problem).

Among the tests considered, Z_C is more powerful if all or most classes are segregated. The same holds if all or most class pairs are associated. But if the pattern is mixed (i.e., some classes are segregated while some pairs are associated) the deviations in the self column tend to cancel each other in the sum, rendering Z_C perform rather poorly. In such a case, $\mathscr{X}_C$ (together with the cell-specific tests) provide a more accurate picture of the patterns in the data and are more powerful.

Based on our simulations and example data sets, we recommend to perform both of the tests Z_C and $\mathscr{X}_C$, and if any of them is significant, then the cell-specific tests can be performed (to determine segregation or lack of it at the class/species level). When the cell counts in the self column of CCT are all larger than 10, it is safe to employ $\mathscr{X}_C$ with the asymptotic approximation, and if some cell count is 5 or less, it is better to use Monte Carlo randomized version of the test. If some cell counts are between 5 and 10, both versions (i.e., asymptotic approximation and Monte Carlo randomization) can be used to reach more reliable conclusions. Since Z_C is the sum of the self column, the cell counts are not that relevant as long as column sum is 20 or larger (even 10 or larger seems to work in practice). We recommend randomization version of Z_C if column sum is 10 or less, and for sum between 10 and 20, one can employ both asymptotic approximation and randomization versions for more reliable conclusions.

Throughout this article, we assume the total sample size and class sizes are all fixed. If it is desired to have the sample size be a random variable, we may consider a spatial Poisson point process on the region of interest instead of the binomial process. In fact, this case is also a realistic situation for data collection schemes in plant ecology. That is, in the region of interest, one can examine each subject, determine its species and that of its NN. In this framework, all margins of the NNCT and CCT would be random. The effect of such randomness on the behavior (e.g., distribution), size and power performance of the tests is a topic of prospective research. For the cases where CSR independence is the appropriate benchmark (see Section 3.1), this framework might be more realistic, but for the cases where RL is the appropriate benchmark, then our approach in this article is more realistic.

We have discussed the patterns of segregation and (self and mixed) correspondence mostly in the context of plant ecology. However, the patterns and the associated tests can be applied in other contexts as well. For example, one can apply them in an epidemiological or a social context by using the residences of people as their location. In the epidemiological context, the question of interest could be the distribution (i.e., clustering or lack of it) of a disease. In disease clustering, significant segregation of disease cases can have further implications (e.g., one can then search for the reasons of such clustering which can help in controlling the spread of the disease or curing the diseased people). In the social context of racial distribution of residences, segregation of any particular race would imply their clustering in certain neighbourhoods; self correspondence would mean that all racial groups tend to live in clumps or clusters of same race residents (i.e., there is lack of local diversity in the region) On the other hand, mixed correspondence of racial status of residents would imply that the society is diverse at the local level as people of different races live side by side in a mixed neighbourhood and there is no preference of the residents to live by people of the same race.

In the literature, usually NN relationships are based on the distance metrics. For example, in this article, Euclidean distance in $\mathbb{R}^2$ is the only metric used. The NN relations based on dissimilarity measures is an extension of NN relations based on distance metrics. In such an extension, NN of an object, x, refers to the object with the minimum dissimilarity to x. We assume that the objects (events) lie in a finite or infinite dimensional space satisfying the lack of any inter-dependence which implies lack of self or mixed correspondence in the NN structure. Under RL, the objects' locations are fixed yielding fixed interpoint dissimilarity measures, but the labels are assigned randomly to the objects. Although our correspondence tests are constructed assuming data are in $\mathbb{R}^2$, the extension to higher dimensions is straightforward.

Acknowledgments

I would like to thank an anonymous associate editor and two referees, whose constructive comments and suggestions greatly improved the presentation and flow of the paper. This research was supported by the research agency TUBITAK via Project # 111T767 and by the European Commission under the Marie Curie International Outgoing Fellowship Programme via Project # 329370 titled PRinHDD.

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