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A New Perspective on Moran's Coefficient: Revisited

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Abstract: Moran's I (Moran's coefficient) is one of the most prominent measures of spatial autocorrelation. It is well known that Moran's I has a representation that is similar to a Fourier series and is therefore useful for characterizing spatial data. However, the representation needs to be modified. This paper contributes to the literature by showing the necessary modification and presenting some further results. In addition, we provide the required MATLAB/GNU Octave and R user-defined functions.

Keywords: spatial autocorrelation; Moran's I; linear algebraic graph theory; eigenvector spatial filtering; Geary's c

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1. Introduction

Spatial autocorrelation, which describes the similarity between signals at adjacent vertices, is central to geographical and spatial analysis ([1]). It is also closely related to Tobler's first law of geography ([2]). As listed in [1], many measures of it have been proposed. Among them, Moran's I is one of the most prominent measures. In addition, the popular eigenvector spatial filter (ESF), which was developed by Daniel A. Griffith and his co-authors ([3–10]) is based on Moran's I (see also [11,12]). This paper contributes to the literature by providing new insights into Moran's I.

Dray [13] made an important contribution to the understanding of Moran's I. More specifically, he presented a remarkable representation of it that is similar to a Fourier series. It is an expansion of Moran's I into a linear combination of variables with different degrees of spatial autocorrelation. However, the representation needs to be modified. In this paper, after reviewing Dray's representation, we show the necessary modification. We then present some further results. Specifically, we show that Moran's I is not just a linear combination of variables with different degrees of spatial autocorrelation, but a *weighted average* of such variables. A way to obtain the matrices needed for the modified representation is also provided. In addition, we provide the required MATLAB/GNU Octave and R user-defined functions.

We make four remarks on Moran's I. First, Cliff and Ord [14–17] made today's Moran's I ([18,19]). Second, there exists

$$\begin{cases} \text{positive spatial autocorrelation} & \text{if } I > -\frac{1}{n-1}, \\ \text{no spatial autocorrelation} & \text{if } I = -\frac{1}{n-1}, \\ \text{negative spatial autocorrelation} & \text{if } I < -\frac{1}{n-1}. \end{cases} \tag{1}$$

See [20] (Equation (5)). Third, Moran's I can be regarded as a generalization of some autocorrelation measures, such as Anderson's [21] first circular serial correlation coefficient, Orcutt's [22] first serial correlation coefficient, and Moran's [23] r_{11} ([19]). Thus, our results apply to these as well. Fourth, Anselin [24] developed a spatial autocorrelation coefficient called local Moran's I. In contrast, Moran's I, which is the subject of this paper, is sometimes referred to as global Moran's I.

Two more remarks follow. First, we will refer to Moran's I as Moran's coefficient. The reason for this is that this is what Dray [13] called it. In addition, we will use the same notation as [13] as much as possible. Second, Geary's [25] c is another prominent measure of spatial autocorrelation. Yamada [26,27] provided some results on the coefficient. The current paper can be seen as a companion to [27].

The organization of this paper is as follows. In Section 2, we provide some preliminaries. In Section 3, we briefly review some results in [13]. In Section 4, we present the main results of this paper. In Section 5, we add to the results in Section 4. Section 6 concludes the paper. In Appendices A and B, we provide proofs and MATLAB/GNU Octave and R user-defined functions, respectively.

Some of the Notations

For a matrix $\boldsymbol{A}$, the transpose of $\boldsymbol{A}$ is denoted by $\boldsymbol{A}^\top$. Let $\boldsymbol{x} = [x_1, \ldots, x_n]^\top$, $\boldsymbol{I}_n$ be the identity matrix of order n, $\boldsymbol{1}$ be the n-dimensional column vector of ones, i.e., $\boldsymbol{1} = [1, \ldots, 1]^\top$, and $\boldsymbol{e}_k$ be the k-th column of $\boldsymbol{I}_n$, i.e., $\boldsymbol{I}_n = [\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n]$. Let

$$\boldsymbol{H} = \boldsymbol{I}_n - \boldsymbol{1}(\boldsymbol{1}^\top\boldsymbol{1})^{-1}\boldsymbol{1}^\top = \boldsymbol{I}_n - \frac{1}{n}\boldsymbol{1}\boldsymbol{1}^\top. \tag{2}$$

Then, $\boldsymbol{H}$ is a symmetric and idempotent matrix, such that $\boldsymbol{1}$ belongs to its null space, i.e., $\boldsymbol{H}^\top = \boldsymbol{H}$, $\boldsymbol{H}^2 = \boldsymbol{H}$, and $\boldsymbol{H}\boldsymbol{1} = \boldsymbol{0}$. For an $n \times m$ full column rank matrix $\boldsymbol{A}$, denote the column space of $\boldsymbol{A}$ and its orthogonal complement by $\mathbb{S}(\boldsymbol{A})$ and $\mathbb{S}^\perp(\boldsymbol{A})$, respectively. For a column vector $\boldsymbol{\eta}$, $\|\boldsymbol{\eta}\|^2 = \boldsymbol{\eta}^\top\boldsymbol{\eta}$. Let $\mathrm{cor}(\boldsymbol{\eta}_1, \boldsymbol{\eta}_2)$ denote the correlation coefficient between $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$, i.e.,

$$\mathrm{cor}(\boldsymbol{\eta}_1, \boldsymbol{\eta}_2) = \frac{\boldsymbol{\eta}_1^\top\boldsymbol{H}\boldsymbol{\eta}_2}{\sqrt{\boldsymbol{\eta}_1^\top\boldsymbol{H}\boldsymbol{\eta}_1}\sqrt{\boldsymbol{\eta}_2^\top\boldsymbol{H}\boldsymbol{\eta}_2}}, \tag{3}$$

where $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$ are n-dimensional column vectors that do not belong to $\mathbb{S}(\boldsymbol{1})$, i.e., $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2 \in \mathbb{R}^n \backslash \mathbb{S}(\boldsymbol{1})$.

2. Preliminaries

Following [20], we treat the problem of spatial autocorrelation in terms of a graph (see, for example, [28] for details on linear algebraic graph theory). Let $G = (V, E)$ denote a directed/undirected graph, where $V = \{v_1, \ldots, v_n\}$ is a set of vertices and $E \subset V \times V$ is a set of ordered pairs of distinct vertices. Here, $n \geq 2$ and $E \neq \emptyset$. For $i, j = 1, \ldots, n$, let

$$\begin{cases} w_{i,j} > 0 & \text{if } (v_i, v_j) \in E, \\ w_{i,j} = 0 & \text{otherwise,} \end{cases} \tag{4}$$

and $\boldsymbol{W} = [w_{i,j}] \in \mathbb{R}^{n \times n}$. Here, (v_i, v_j) denotes the directed edge from v_i to v_j. If both (v_i, v_j) and (v_j, v_i) belong to E, then the edge between v_i and v_j is undirected. Given that $(v_i, v_i) \notin E$, $w_{i,i} = 0$ for $i = 1, \ldots, n$, i.e., the diagonal entries of $\boldsymbol{W}$ are all zero. In addition, given that $E \neq \emptyset$, $\sum_{i=1}^n \sum_{j=1}^n w_{i,j} > 0$.

Let x_i denote the realization of a variable on a vertex v_i for $i = 1, \ldots, n$. Here, we exclude the case where $x_1 = \cdots = x_n$. That is, we assume that $\boldsymbol{x} \notin \mathbb{S}(\boldsymbol{1})$. Accordingly, under the assumption, $\sum_{k=1}^n (x_k - \bar{x})^2 > 0$, where $\bar{x} = \frac{1}{n}\sum_{i=1}^n x_i$.

Following [14–17], the Moran's coefficient for $\boldsymbol{x}$, denoted by $MC(\boldsymbol{x})$, is defined by

$$MC(\boldsymbol{x}) = \frac{n}{\sum_{i=1}^n \sum_{j=1}^n w_{i,j}} \frac{\sum_{i=1}^n \sum_{j=1}^n w_{i,j}(x_i - \bar{x})(x_j - \bar{x})}{\sum_{k=1}^n (x_k - \bar{x})^2}. \tag{5}$$

Incidentally, a local Moran's coefficient, [24] (Equation (7)), is

$$MC_i(\boldsymbol{x}) = (x_i - \bar{x}) \sum_{j=1}^{n} w_{i,j}(x_j - \bar{x}), \quad i = 1, \ldots, n. \tag{6}$$

According to this construction, it follows that $\sum_{i=1}^{n} MC_i(\boldsymbol{x}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{i,j}(x_i - \bar{x})(x_j - \bar{x})$, which appears in the numerator of $MC(\boldsymbol{x})$ in (5).

Given that $\boldsymbol{x}^\top \boldsymbol{HWHx} = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{i,j}(x_i - \bar{x})(x_j - \bar{x})$, $\boldsymbol{x}^\top \boldsymbol{Hx} = \sum_{k=1}^{n}(x_k - \bar{x})^2$, and $\boldsymbol{1}^\top \boldsymbol{W1} = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{i,j}$, as shown in, for example, [13,20], $MC(\boldsymbol{x})$ in (5) can be represented in matrix notation as

$$MC(\boldsymbol{x}) = \frac{n}{\boldsymbol{1}^\top \boldsymbol{W1}} \frac{\boldsymbol{x}^\top \boldsymbol{HWHx}}{\boldsymbol{x}^\top \boldsymbol{Hx}}. \tag{7}$$

By definition, $\boldsymbol{W}$ is not necessarily symmetric. However, since $\boldsymbol{\eta}^\top \boldsymbol{W\eta} = (\boldsymbol{\eta}^\top \boldsymbol{W\eta})^\top = \boldsymbol{\eta}^\top \boldsymbol{W}^\top \boldsymbol{\eta}$ for any $\boldsymbol{\eta} \in \mathbb{R}^n$, it follows that

$$\boldsymbol{\eta}^\top \boldsymbol{W\eta} = \boldsymbol{\eta}^\top \boldsymbol{\mathcal{W}\eta}, \tag{8}$$

where $\boldsymbol{\mathcal{W}} = \frac{\boldsymbol{W}+\boldsymbol{W}^\top}{2}$. Note that $\boldsymbol{\mathcal{W}}$ is symmetric even if $\boldsymbol{W}$ is not symmetric. Accordingly, as is well known, $MC(\boldsymbol{x})$ in (7) can be represented with a symmetric matrix $\boldsymbol{\mathcal{W}}$ as

$$MC(\boldsymbol{x}) = \frac{n}{\boldsymbol{1}^\top \boldsymbol{\mathcal{W}1}} \frac{\boldsymbol{x}^\top \boldsymbol{H\mathcal{W}Hx}}{\boldsymbol{x}^\top \boldsymbol{Hx}}. \tag{9}$$

3. Brief Review of a Closely Related Study

In this section, we briefly review some results in [13].

Let $\boldsymbol{z} = [z_1, \ldots, z_n]^\top$, where $z_i = \frac{x_i - \bar{x}}{s}$ for $i = 1, \ldots, n$. Here, $s = \sqrt{\frac{1}{n} \sum_{k=1}^{n}(x_k - \bar{x})^2}$. Then, given that $s = \sqrt{\frac{1}{n}\boldsymbol{x}^\top \boldsymbol{Hx}}$, $\boldsymbol{z}$ can be represented in matrix notation as

$$\boldsymbol{z} = \frac{1}{\sqrt{\frac{1}{n}\boldsymbol{x}^\top \boldsymbol{Hx}}} \boldsymbol{Hx}. \tag{10}$$

Accordingly, it follows that

$$MC(\boldsymbol{x}) = \frac{1}{\boldsymbol{1}^\top \boldsymbol{\mathcal{W}1}} \frac{\boldsymbol{x}^\top \boldsymbol{HH\mathcal{W}HHx}}{\frac{1}{n}\boldsymbol{x}^\top \boldsymbol{Hx}} = \frac{\boldsymbol{z}^\top \boldsymbol{H\mathcal{W}Hz}}{\boldsymbol{1}^\top \boldsymbol{\mathcal{W}1}}. \tag{11}$$

Here, we note that the first equality in (11) follows because $\boldsymbol{H}$ is a symmetric and idempotent matrix.

Given that $\boldsymbol{H\mathcal{W}H}$ is a real symmetric matrix, it can be spectrally decomposed as

$$\boldsymbol{H\mathcal{W}H} = \boldsymbol{U\Lambda U}^\top, \tag{12}$$

where $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ and $\boldsymbol{U} = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n]$ is an orthogonal matrix (e.g., [29] (page 342)). Here, $(\lambda_k, \boldsymbol{u}_k)$ denotes an eigenpair of $\boldsymbol{H\mathcal{W}H}$ for $k = 1, \ldots, n$ such that $\lambda_1, \ldots, \lambda_n$ are in descending order, i.e., $\lambda_1 \geq \cdots \geq \lambda_n$. Incidentally, the ESF is a spatial analysis that uses a submatrix of $\boldsymbol{U}$ (for more details, see, for example, [30] (Section 7)).

From (9), (11), and (12), Dray [13] derived

$$MC(\boldsymbol{x}) = \frac{n}{\boldsymbol{1}^\top \boldsymbol{\mathcal{W}1}} \frac{\sum_{k=1}^{n} \lambda_k \boldsymbol{x}^\top \boldsymbol{u}_k \boldsymbol{u}_k^\top \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{Hx}}, \tag{13}$$

$$MC(\boldsymbol{x}) = \frac{\sum_{k=1}^{n} \lambda_k \boldsymbol{z}^\top \boldsymbol{u}_k \boldsymbol{u}_k^\top \boldsymbol{z}}{\boldsymbol{1}^\top \boldsymbol{\mathcal{W}1}}. \tag{14}$$

(13) and (14), respectively, correspond to Equations (3) and (4) of [13]. In addition, Dray [13] demonstrated that

$$MC(\boldsymbol{x}) = \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}} \mathbf{1}} \sum_{k=1}^{n} \lambda_k \mathrm{cor}^2(\boldsymbol{u}_k, \boldsymbol{z}), \tag{15}$$

$$\mathrm{cor}^2(\boldsymbol{u}_k, \boldsymbol{z}) = \frac{\beta_k^2}{n}, \quad k = 1, \ldots, n, \tag{16}$$

where $\beta_k = \arg\min_{\phi_k} \|\boldsymbol{z} - \phi_1 \boldsymbol{u}_1 - \cdots - \phi_n \boldsymbol{u}_n\|^2 = \arg\min_{\phi_k} \|\boldsymbol{z} - \phi_k \boldsymbol{u}_k\|^2$. Among them, (15) corresponds to [13] (Equation (5)). Finally, by combining (15) and the result given by

$$MC(\boldsymbol{u}_k) = \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}} \mathbf{1}} \lambda_k, \quad k = 1, \ldots, n, \tag{17}$$

from [20], [3] (Equation (3)), [31] (Equation (5)), and [6] (page 1200), Dray [13] derived

$$MC(\boldsymbol{x}) = \sum_{k=1}^{n} MC(\boldsymbol{u}_k) \mathrm{cor}^2(\boldsymbol{u}_k, \boldsymbol{z}), \tag{18}$$

which corresponds to [13] (Equation (6)).

Although (18) as well as (17) are remarkable results, they need to be modified. This is because $\mathbf{1}$ belongs to the null space of $\boldsymbol{H\mathcal{W}H}$, i.e., $\boldsymbol{H\mathcal{W}H}\mathbf{1} = \mathbf{0} = 0 \cdot \mathbf{1}$. Accordingly, when the nullity (the dimension of the null space) of $\boldsymbol{H\mathcal{W}H}$ is one, $\frac{1}{\sqrt{n}}\mathbf{1}$ or $-\frac{1}{\sqrt{n}}\mathbf{1}$ must be one of the normalized eigenvectors of $\boldsymbol{H\mathcal{W}H}$. Denote such normalized eigenvectors by $\boldsymbol{u}_*$. Then, both $MC(\boldsymbol{u}_*)$ and $\mathrm{cor}^2(\boldsymbol{u}_*, \boldsymbol{z})$ cannot be defined because $\boldsymbol{u}_*^\top \boldsymbol{H} \boldsymbol{u}_* = 0$. Even in the case where the nullity is greater than one, to avoid such a situation, care must be taken to ensure that $\boldsymbol{u}_*$ is not selected as one of the normalized eigenvectors. In the next two sections, we present a way to avoid this problem.

Example 1. *We provide a simple* $\boldsymbol{\mathcal{W}}$ *such that the nullity of* $\boldsymbol{H\mathcal{W}H}$ *is one. It is* $\boldsymbol{\mathcal{W}} = \boldsymbol{J}_n + \boldsymbol{J}_n^\top$*, where* $\boldsymbol{J}_n = [\boldsymbol{e}_2, \ldots, \boldsymbol{e}_n, \boldsymbol{e}_1]$*. This* $\boldsymbol{\mathcal{W}}$ *is the binary adjacency matrix of a cycle graph with n vertices. The right side of Figure 1 shows a cycle graph with six vertices. In this case, it follows that*

$$\mathrm{rank}(\boldsymbol{H\mathcal{W}H}) = n - 1, \tag{19}$$

unless n is a multiple of 4*. A proof of* (19) *is provided in Appendix A.1.*

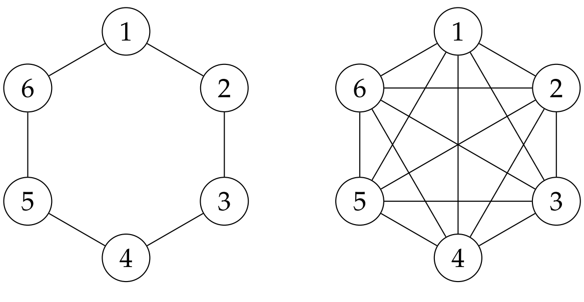

Figure 1. A cycle graph with 6 vertices (**left**). A complete graph with 6 vertices (**right**).

4. Main Results

In this section, we present the main results of this paper.

Let

$$\boldsymbol{H\mathcal{W}H} = \boldsymbol{PQP}^\top, \tag{20}$$

be another spectral decomposition of $\boldsymbol{H\mathcal{W}H}$, where $\boldsymbol{Q} = \mathrm{diag}(q_1, \ldots, q_n)$ and $\boldsymbol{P} = [\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n]$ is an orthogonal matrix. Here, $(q_k, \boldsymbol{p}_k)$ denotes an eigenpair of $\boldsymbol{H\mathcal{W}H}$ for $k = 1, \ldots, n$. As stated, given that $\boldsymbol{H\mathcal{W}H}\mathbf{1} = \mathbf{0}$, $\left(0, \frac{1}{\sqrt{n}}\mathbf{1}\right)$ is an eigenpair of $\boldsymbol{H\mathcal{W}H}$, we let $(q_1, \boldsymbol{p}_1) = \left(0, \frac{1}{\sqrt{n}}\mathbf{1}\right)$. For the other eigenvalues, we suppose that $q_2, \ldots, q_n$ are in descending order, i.e., $q_2 \geq \cdots \geq q_n$. Let $\boldsymbol{Q}_2 = \mathrm{diag}(q_2, \ldots, q_n)$ and $\boldsymbol{P}_2 = [\boldsymbol{p}_2, \ldots, \boldsymbol{p}_n]$. We present the way to obtain $\boldsymbol{P}_2$ as well as $\boldsymbol{Q}_2$ from $\boldsymbol{\mathcal{W}}$ in Section 5.

Given that $\boldsymbol{p}_1 = \frac{1}{\sqrt{n}}\mathbf{1}$ and $\boldsymbol{P} = [\boldsymbol{p}_1, \boldsymbol{P}_2]$ is an orthogonal matrix, $\boldsymbol{H}$ can be represented by $\boldsymbol{P}_2$ as

$$\boldsymbol{H} = \boldsymbol{I}_n - \boldsymbol{p}_1(\boldsymbol{p}_1^\top \boldsymbol{p}_1)^{-1}\boldsymbol{p}_1^\top = \boldsymbol{P}_2(\boldsymbol{P}_2^\top \boldsymbol{P}_2)^{-1}\boldsymbol{P}_2^\top. \tag{21}$$

See Appendix A.2 for details on (21). In addition, $\mathbb{S}(\boldsymbol{P}_2)$ is identical to $\mathbb{S}^\perp(\mathbf{1})$. (In [20] $\mathbb{S}(\mathbf{1})$ and $\mathbb{S}^\perp(\mathbf{1})$ are, respectively, represented as $\mathbb{R}_c$ and $\mathbb{R}_c^+$). That is, $\boldsymbol{H}$ is the orthogonal projection matrix onto $\mathbb{S}^\perp(\mathbf{1})$. Accordingly, given that $\boldsymbol{p}_1 \in \mathbb{S}(\mathbf{1})$ and $\boldsymbol{p}_k \in \mathbb{S}^\perp(\mathbf{1})$ for $k = 2, \ldots, n$, it follows that

$$\boldsymbol{H}\boldsymbol{p}_k = \begin{cases} \mathbf{0}, & k = 1, \\ \boldsymbol{p}_k, & k = 2, \ldots, n. \end{cases} \tag{22}$$

Moreover, we note that the smallest eigenvalue is negative, i.e.,

$$q_n < 0. \tag{23}$$

This is because, as shown in, for example, [32] (page 4),

$$\begin{aligned} \sum_{k=2}^{n} q_k = \sum_{i=1}^{n} q_k &= \mathrm{tr}(\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}) = \mathrm{tr}(\boldsymbol{\mathcal{W}}\boldsymbol{H}) = \mathrm{tr}(\boldsymbol{\mathcal{W}}) - \frac{1}{n}\mathrm{tr}(\boldsymbol{\mathcal{W}}\mathbf{1}\mathbf{1}^\top) \\ &= -\frac{1}{n}\mathrm{tr}(\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}) = -\frac{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}}{n} = -\frac{\sum_{i=1}^n \sum_{j=1}^n w_{i,j}}{n} < 0. \end{aligned} \tag{24}$$

Here, note that $\mathrm{tr}(\boldsymbol{\mathcal{W}}) = \mathrm{tr}\left(\frac{\boldsymbol{W}+\boldsymbol{W}^\top}{2}\right) = 0$ because $\mathrm{tr}(\boldsymbol{W}) = \mathrm{tr}(\boldsymbol{W}^\top) = 0$. If $q_n \geq 0$, then it follows that $\sum_{k=2}^n q_k \geq 0$, which contradicts (24). (Although λ_n is negative, λ_2 is not necessarily positive. See Examples 3 and 5).

Given that $\boldsymbol{p}_k \in \mathbb{S}^\perp(\mathbf{1})$ for $k = 2, \ldots, n$, we can consider

$$\mathrm{cor}(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{\boldsymbol{p}_k^\top \boldsymbol{H}\boldsymbol{z}}{\sqrt{\boldsymbol{p}_k^\top \boldsymbol{H}\boldsymbol{p}_k}\sqrt{\boldsymbol{z}^\top \boldsymbol{H}\boldsymbol{z}}}, \quad k = 2, \ldots, n. \tag{25}$$

Then, given that $\boldsymbol{H}\boldsymbol{z} = \boldsymbol{z}$, $\boldsymbol{p}_k^\top \boldsymbol{H}\boldsymbol{p}_k = \boldsymbol{p}_k^\top \boldsymbol{p}_k = 1$ for $k = 2, \ldots, n$, and $\boldsymbol{z}^\top \boldsymbol{H}\boldsymbol{z} = \boldsymbol{z}^\top \boldsymbol{z} = n$, we obtain

$$\mathrm{cor}(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{\boldsymbol{p}_k^\top \boldsymbol{z}}{\sqrt{n}}, \quad k = 2, \ldots, n. \tag{26}$$

Given that $\boldsymbol{H}$ is a symmetric and idempotent matrix and $\boldsymbol{P}$ is an orthogonal matrix, $MC(\boldsymbol{x})$ in (7) can be represented as

$$MC(\boldsymbol{x}) = \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}} \frac{\boldsymbol{x}^\top \boldsymbol{H}\boldsymbol{P}\boldsymbol{Q}\boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{H}\boldsymbol{P}\boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{x}}. \tag{27}$$

Let $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_n]^\top = \boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{x}$. Then, from (22), α_k for $k = 1, \ldots, n$ are

$$\alpha_k = \boldsymbol{p}_k^\top \boldsymbol{H}\boldsymbol{x} = \begin{cases} 0, & k = 1, \\ \boldsymbol{p}_k^\top \boldsymbol{x}, & k = 2, \ldots, n. \end{cases} \tag{28}$$

Accordingly, $MC(\boldsymbol{x})$ in (27) can be represented as follows:

$$MC(\boldsymbol{x}) = \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}} \frac{\boldsymbol{\alpha}^\top \boldsymbol{Q}\boldsymbol{\alpha}}{\boldsymbol{\alpha}^\top \boldsymbol{\alpha}} = \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}} \frac{\sum_{k=2}^n q_k \alpha_k^2}{\sum_{l=2}^n \alpha_l^2}. \tag{29}$$

Here, we note that $\boldsymbol{\alpha}$ is

$$\boldsymbol{\alpha} = \boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{x} \in \mathbb{S}^\perp(\boldsymbol{e}_1)\backslash\{\mathbf{0}\} \tag{30}$$

and $\frac{\boldsymbol{\alpha}^\top \boldsymbol{Q}\boldsymbol{\alpha}}{\boldsymbol{\alpha}^\top \boldsymbol{\alpha}}$ in (29) is a Rayleigh quotient because $\boldsymbol{Q}$ is symmetric and $\boldsymbol{\alpha} \neq \mathbf{0}$. For a proof of (30), see Appendix A.3.

Now, consider $MC(\boldsymbol{p}_k)$ for $i = 1, \ldots, n$. Among them, $MC(\boldsymbol{p}_1)$ cannot be defined. This is because $\boldsymbol{p}_1^\top \boldsymbol{H}\boldsymbol{p}_1 = 0$. For $k = 2, \ldots, n$, given that $\boldsymbol{p}_k^\top \boldsymbol{H}\boldsymbol{P}\boldsymbol{Q}\boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{p}_k = \boldsymbol{p}_k^\top \boldsymbol{P}\boldsymbol{Q}\boldsymbol{P}^\top \boldsymbol{p}_k = \boldsymbol{e}_k^\top \boldsymbol{Q}\boldsymbol{e}_k = q_k$ and $\boldsymbol{p}_k^\top \boldsymbol{H}\boldsymbol{P}\boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{p}_k = \boldsymbol{p}_k^\top \boldsymbol{P}\boldsymbol{P}^\top \boldsymbol{p}_k = \boldsymbol{e}_k^\top \boldsymbol{e}_k = 1$, it follows that

$$MC(\boldsymbol{p}_k) = \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}} q_k, \quad k = 2, \ldots, n. \tag{31}$$

Hence, from the inequalities given by $q_2 \geq \cdots \geq q_n$, it follows that

$$MC(\boldsymbol{p}_2) \geq \cdots \geq MC(\boldsymbol{p}_n). \tag{32}$$

In addition, from (23), it follows that $MC(\boldsymbol{p}_n) < 0$ and from (24), it follows that

$$\begin{aligned} \frac{1}{n-1} \sum_{k=2}^n MC(\boldsymbol{p}_k) &= \frac{1}{n-1} \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}} \sum_{k=2}^n q_k \\ &= \frac{1}{n-1} \frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}} \times \left(-\frac{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}}{n} \right) = -\frac{1}{n-1}. \end{aligned} \tag{33}$$

If $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n) = \mu$, then $\mu = -\frac{1}{n-1}$ from (33). In addition, $MC(\boldsymbol{x}) = \sum_{k=2}^n \psi_k MC(\boldsymbol{p}_k) = \mu \sum_{k=2}^n \psi_k = \mu$. Accordingly, if $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$, then $MC(\boldsymbol{x}) = -\frac{1}{n-1}$. Hence, if $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$, then, given (1), there is always no spatial autocorrelation measured by Moran's coefficient.

Combining (29) and (31), we obtain

$$\begin{aligned} MC(\boldsymbol{x}) &= \frac{\sum_{k=2}^n \left(\frac{n}{\mathbf{1}^\top \boldsymbol{\mathcal{W}}\mathbf{1}} q_k \right) \alpha_k^2}{\sum_{l=2}^n \alpha_l^2} = \frac{\sum_{k=2}^n MC(\boldsymbol{p}_k) \alpha_k^2}{\sum_{l=2}^n \alpha_l^2} \\ &= \sum_{k=2}^n MC(\boldsymbol{p}_k) \left(\frac{\alpha_k^2}{\sum_{l=2}^n \alpha_l^2} \right) = \sum_{k=2}^n \psi_k MC(\boldsymbol{p}_k), \end{aligned} \tag{34}$$

where

$$\psi_k = \frac{\alpha_k^2}{\sum_{l=2}^n \alpha_l^2}, \quad k = 2, \ldots, n. \tag{35}$$

Here, given that $(\boldsymbol{p}_k^\top \boldsymbol{p}_k)^{-1} = 1$ and $\boldsymbol{p}_k^\top \boldsymbol{p}_l = 0$ if $k \neq l$, α_k in (35), such that

$$\alpha_k = \boldsymbol{p}_k^\top \boldsymbol{x} = \arg\min_{\phi_k} \|\boldsymbol{x} - \phi_k \boldsymbol{p}_k\|^2 = \arg\min_{\phi_k} \|\boldsymbol{x} - \phi_1 \boldsymbol{p}_1 - \cdots - \phi_n \boldsymbol{p}_n\|^2. \tag{36}$$

In addition, from (35), it immediately follows that $\psi_k \geq 0$ for $k = 2, \ldots, n$ and $\sum_{k=2}^n \psi_k = 1$. Moreover, concerning ψ_k, we have the following result.

Lemma 1. *It follows that*

$$\mathrm{cor}^2(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{\alpha_k^2}{\sum_{l=2}^n \alpha_l^2}, \quad k = 2, \ldots, n. \tag{37}$$

Proof of Lemma 1. See Appendix A.4. □

The next proposition summarizes the abovementioned results.

Proposition 1. *(a) $MC(\boldsymbol{x})$ can be represented as $\sum_{k=2}^{n} \psi_k MC(\boldsymbol{p}_k)$, where*

$$\psi_k = \frac{\alpha_k^2}{\sum_{l=2}^{n} \alpha_l^2} = \mathrm{cor}^2(\boldsymbol{p}_k, \boldsymbol{z}), \quad k = 2, \ldots, n. \tag{38}$$

Here, ψ_k for $k = 2, \ldots, n$ are nonnegative and sum to one. (b) It follows that $MC(\boldsymbol{p}_2) \geq \cdots \geq MC(\boldsymbol{p}_n)$, $MC(\boldsymbol{p}_n) < 0$, and $\frac{1}{n-1}\sum_{k=2}^{n} MC(\boldsymbol{p}_k) = -\frac{1}{n-1}$. (c) If $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$, then $MC(\boldsymbol{x}) = -\frac{1}{n-1}$.

Remark 1. *Concerning Proposition 1, we make four remarks.*

(i) *Proposition 1(a) implies that Moran's coefficient in (5) can be represented as a weighted average of $MC(\boldsymbol{p}_2), \ldots, MC(\boldsymbol{p}_n)$. Concerning the weights, ψ_k for $k = 2, \ldots, n$, the larger $|\alpha_k| = |\boldsymbol{p}_k^\top \boldsymbol{x}| = |(\boldsymbol{p}_k^\top \boldsymbol{p}_k)^{-1} \boldsymbol{p}_k^\top \boldsymbol{x}|$ is, the larger ψ_k is. Likewise, for $k = 2, \ldots, n$, the larger $|\mathrm{cor}(\boldsymbol{p}_k, \boldsymbol{z})|$ is, the larger ψ_k is. Recall that, from (26), $\mathrm{cor}(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{\beta_k}{\sqrt{n}}$.*

(ii) *Proposition 1(b) implies that the eigenvectors, $\boldsymbol{p}_2, \ldots, \boldsymbol{p}_n$, are in order of spatial autocorrelation. Accordingly, for example, if $\{\psi_k\}$ is a monotonically decreasing sequence, then $MC(\boldsymbol{x})$ is likely to be positive. Of course, from Proposition 1(c), if $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$, then $MC(\boldsymbol{x}) = -\frac{1}{n-1} < 0$, even if $\{\psi_k\}$ is a monotonically decreasing sequence.*

(iii) *From Lemma 1, it immediately follows that*

$$\sum_{k=2}^{n} \mathrm{cor}^2(\boldsymbol{p}_k, \boldsymbol{z}) = 1. \tag{39}$$

We provide a more direct proof of (39) in Appendix A.5.

(iv) *The MATLAB/GNU Octave and R user-defined functions to compute $\boldsymbol{\psi}_2 = [\psi_2, \ldots, \psi_n]^\top$ (`psi2`) are provided in Appendix B.*

Example 2. *Consider two extreme cases. First, suppose that $\psi_2 = 1$ and $\psi_3 = \cdots = \psi_n = 0$. Then, since ψ_2 is the coefficient of $MC(\boldsymbol{p}_2)$, which is larger or equal to $MC(\boldsymbol{p}_k)$ for $k = 3, \ldots, n$, $\boldsymbol{y}$ is considered to be highly positively autocorrelated. Second, suppose that $\psi_2 = \cdots \psi_{n-1} = 0$ and $\psi_n = 1$. Then, since ψ_n is the coefficient of $MC(\boldsymbol{p}_n)$, which is negative and smaller or equal to $MC(\boldsymbol{p}_k)$ for $k = 2, \ldots, n-1$, $\boldsymbol{y}$ is considered to be highly negatively autocorrelated. Note that, as mentioned, these do not hold if $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$.*

Example 3. *We give an example such that $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$. Consider the case where $\boldsymbol{W}(= \boldsymbol{\mathcal{W}}) = \boldsymbol{1}\boldsymbol{1}^\top - \boldsymbol{I}_n$, which is the binary adjacency matrix of the complete graph with n vertices. The left side of Figure 1 shows a complete graph with six vertices. We note that this case is also considered in [32]. Then, it follows that*

$$\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H} = \boldsymbol{H}(\boldsymbol{1}\boldsymbol{1}^\top - \boldsymbol{I}_n)\boldsymbol{H} = -\boldsymbol{H}. \tag{40}$$

Given that $\boldsymbol{H}$ is a symmetric and idempotent matrix whose rank equals $n-1$, its eigenvalues are 0 with multiplicity 1 and 1 with multiplicity $n-1$ (e.g., [29] (page 167)). Then, since $q_2 = \cdots = q_n = -1$, it follows that $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$. Here, it is noteworthy that, in this case, q_2 is not the largest eigenvalue of $\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}$. This is because $q_2 = -1$ is less than $q_1 = 0$.

From Proposition 1, it immediately follows that

$$MC(\boldsymbol{x}) = \sum_{k=2}^{n} \psi_k MC(\boldsymbol{p}_k) \leq \sum_{k=2}^{n} \psi_k MC(\boldsymbol{p}_2) = MC(\boldsymbol{p}_2) \sum_{k=2}^{n} \psi_k = MC(\boldsymbol{p}_2). \tag{41}$$

Likewise, $MC(\boldsymbol{p}_n) \leq MC(\boldsymbol{x})$ follows.

The next corollary summarizes the above results.

Corollary 1. *$MC(\boldsymbol{x})$ belongs to the interval given by $[MC(\boldsymbol{p}_n), MC(\boldsymbol{p}_2)]$.*

Remark 2. *Concerning Corollary 1, we make three remarks.*

(i) *If $MC(\boldsymbol{p}_2) = \cdots = MC(\boldsymbol{p}_n)$, then the interval given by $[MC(\boldsymbol{p}_n), MC(\boldsymbol{p}_2)]$ reduces to a singleton. For example, as stated, if $\boldsymbol{\mathcal{W}} = \boldsymbol{1}\boldsymbol{1}^\top - \boldsymbol{I}_n$, then*

$$MC(\boldsymbol{x}) \in \left\{-\frac{1}{n-1}\right\}. \tag{42}$$

(ii) *De Jong et al. [20] and [32] (Theorem 2.1) showed that*

$$MC(\boldsymbol{x}) \in \left[\frac{n}{\boldsymbol{1}^\top\boldsymbol{\mathcal{W}}\boldsymbol{1}}q_n, \frac{n}{\boldsymbol{1}^\top\boldsymbol{\mathcal{W}}\boldsymbol{1}}q_2\right]. \tag{43}$$

Given (31), Corollary 1 is its equivalent.

(iii) *The MATLAB/GNU Octave and R user-defined functions to compute the bounds of Moran's coefficient (`MoranIbounds`) are provided in Appendix B.*

Let $\boldsymbol{\chi} = \boldsymbol{\chi}_1 + \boldsymbol{\chi}_2$, where $\boldsymbol{\chi}_1 \in \mathbb{S}(\boldsymbol{1})$ and $\boldsymbol{\chi}_2 \in \mathbb{S}(\boldsymbol{x})\backslash\{\boldsymbol{0}\}$. Maruyama [32] discussed that $MC(\boldsymbol{\chi})$ equals $MC(\boldsymbol{x})$. That is, for all $c_1 \in \mathbb{R}$ and $c_2 \in \mathbb{R}\backslash\{0\}$, $MC(c_1\boldsymbol{1} + c_2\boldsymbol{x})$ and $MC(\boldsymbol{x})$ are identical. Given this result, from Proposition 1, we immediately obtain the following extended result.

Corollary 2. *$MC(\boldsymbol{\chi})$ can be represented as $\sum_{k=2}^{n} \psi_k MC(\boldsymbol{p}_k)$, where $\psi_k = \frac{\alpha_k^2}{\sum_{l=2}^{n}\alpha_l^2} = \mathrm{cor}^2(\boldsymbol{p}_k, \boldsymbol{z})$ for $k = 2, \ldots, n$.*

Example 4. *Given that $\boldsymbol{H}\boldsymbol{x} = \boldsymbol{x} - \bar{x}\boldsymbol{1}$, $\boldsymbol{H}\boldsymbol{x}$ is an example of $\boldsymbol{\chi}$. Of course, this result is quite reasonable because $\boldsymbol{H}$ in (7) is a symmetric and idempotent matrix. Accordingly, from Corollary 2, $MC(\boldsymbol{H}\boldsymbol{x})$ can be represented as $\sum_{k=2}^{n} \psi_k MC(\boldsymbol{p}_k)$.*

5. Additional Results

In this section, we add results to those in the previous section. More specifically, we document the useful results for obtaining $\boldsymbol{P}_2 = [\boldsymbol{p}_2, \ldots, \boldsymbol{p}_n]$ as well as $\boldsymbol{Q}_2 = \mathrm{diag}(q_2, \ldots, q_n)$ from $\boldsymbol{\mathcal{W}}$. Recall that $\alpha_k = \boldsymbol{p}_k^\top \boldsymbol{x}$ for $k = 2, \ldots, n$ and the bounds of Moran's coefficient are described with q_2 and q_n. Although $(q_k, \boldsymbol{p}_k)$ for $k = 2, \ldots, n$ are the eigenpairs of $\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}$, it is not easy to obtain them from it. When the nullity of $\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}$ is one, the location of $\left(0, \frac{1}{\sqrt{n}}\boldsymbol{1}\right)$ is unknown. Moreover, when the nullity is greater than one, $\frac{1}{\sqrt{n}}\boldsymbol{1}$ is not necessarily selected as one of the eigenvectors.

Let $\boldsymbol{G} = [\boldsymbol{g}_1, \boldsymbol{G}_2]$, where $\boldsymbol{g}_1 = \frac{1}{\sqrt{n}}\boldsymbol{1}$ and $\boldsymbol{G}_2 = [\boldsymbol{g}_2, \ldots, \boldsymbol{g}_n]$ such that $\{\boldsymbol{g}_2, \ldots, \boldsymbol{g}_n\}$ is an orthonormal basis of $\mathbb{S}^\perp(\boldsymbol{1})$. Accordingly, $\boldsymbol{G}$ is an $n \times n$ orthogonal matrix. In addition, let $\boldsymbol{V} = \boldsymbol{G}^\top\boldsymbol{P}$ and $\boldsymbol{\Xi}$ be an $(n-1) \times (n-1)$ submatrix of $\boldsymbol{V}$ such that

$$\boldsymbol{V} = \begin{bmatrix} v_{1,1} & \boldsymbol{v}_{1,2} \\ \boldsymbol{v}_{2,1} & \boldsymbol{\Xi} \end{bmatrix}. \tag{44}$$

Then, we have the following results:

Proposition 2. *Let $\boldsymbol{\Xi} = [\boldsymbol{\xi}_2, \ldots, \boldsymbol{\xi}_n]$. Then, $(q_k, \boldsymbol{\xi}_k)$ for $k = 2, \ldots, n$ are the eigenpairs of $\boldsymbol{G}_2^\top\boldsymbol{\mathcal{W}}\boldsymbol{G}_2$. In addition, $\boldsymbol{P}_2$ is equal to $\boldsymbol{G}_2\boldsymbol{\Xi}$.*

Proof. See Appendix A.6. □

Remark 3. *Concerning Proposition 2, we make two remarks.*

(i) *The candidates for $\boldsymbol{G}_2$ are numerous. One of them is the following $n \times (n-1)$ matrix:*

$$\boldsymbol{E}_2 = \sqrt{\frac{2}{n}} \begin{bmatrix} \cos\{(2-1)\theta_1\} & \cdots & \cos\{(n-1)\theta_1\} \\ \cos\{(2-1)\theta_2\} & \cdots & \cos\{(n-1)\theta_2\} \\ \vdots & & \vdots \\ \cos\{(2-1)\theta_n\} & \cdots & \cos\{(n-1)\theta_n\} \end{bmatrix}, \tag{45}$$

where $\theta_i = \frac{(i-0.5)\pi}{n}$ for $i = 1, \ldots, n$. Here,

$$\boldsymbol{E} = \left[\frac{1}{\sqrt{n}} \mathbf{1}, \boldsymbol{E}_2 \right] \tag{46}$$

is the matrix used for the discrete cosine transform ([33] and [34]). The following $n \times (n-1)$ matrix is another candidate:

$$\boldsymbol{F}_2 = \boldsymbol{\Gamma}^{-1} \begin{bmatrix} 1 & \cdots & \cdots & 1 \\ -1 & \ddots & & \vdots \\ 0 & -2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & -(n-1) \end{bmatrix}, \tag{47}$$

where $\boldsymbol{\Gamma} = \mathrm{diag}(\sqrt{1 \cdot 2}, \ldots, \sqrt{(n-1) \cdot n})$. (The use of $\boldsymbol{F}_2$ is inspired by [32]). Here,

$$\boldsymbol{F} = \left[\frac{1}{\sqrt{n}} \mathbf{1}, \boldsymbol{F}_2 \right] \tag{48}$$

is a Helmert orthogonal matrix ([35]).

(ii) *The MATLAB/GNU Octave and R user-defined functions to compute $\boldsymbol{Q}_2$ and $\boldsymbol{P}_2$ (`Q2P2`) and $\boldsymbol{E}$ (`Emat`) are provided in Appendix B.*

Example 5. *We provide an example of the use of user-defined function `Q2P2`. Consider the case such that*

$$\boldsymbol{\mathcal{W}} = \boldsymbol{J}_4 + \boldsymbol{J}_4^\top = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}, \tag{49}$$

which is the binary adjacency matrix of a cycle graph with $four$ vertices. In this case, as shown in Appendix A.1, the spectrum of $\boldsymbol{\mathcal{W}}$ is as follows:

$$\left\{ 2, 2\cos\left(\frac{\pi}{2}\right), 2\cos(\pi), 2\cos\left(\frac{3\pi}{2}\right) \right\} = \{2, 0, -2, 0\}. \tag{50}$$

In addition, again from Appendix A.1, the spectrum of $\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}$ is $\{0, 0, -2, 0\}$. By applying `Q2P2`, we obtain the corresponding $\boldsymbol{P}_2$ as

$$\begin{bmatrix} 0.3607 & -0.6082 & -0.5000 \\ 0.6082 & 0.3607 & 0.5000 \\ -0.3607 & 0.6082 & -0.5000 \\ -0.6082 & -0.3607 & 0.5000 \end{bmatrix}, \tag{51}$$

from which it is easy to see that all column vectors of $\boldsymbol{P}_2$ belong to $\mathbb{S}^\perp(\mathbf{1})$ and are orthogonal to each other.

6. Concluding Remarks

In this paper, we contributed to the literature by showing that the Moran's coefficient can be represented as a weighted average of $MC(\boldsymbol{p}_2), \ldots, MC(\boldsymbol{p}_n)$. Here, $MC(\boldsymbol{p}_2), \ldots, MC(\boldsymbol{p}_n)$ are in descending order, and thus $\boldsymbol{p}_{i+1}$ is more positively autocorrelated than or equal to $\boldsymbol{p}_k$ for $k = 2, \ldots, n-1$. Therefore, the representation is somewhat similar to a Fourier series. This is useful because we can characterize spatial data based on it. We then presented the theory of how to obtain the matrices, such as $\boldsymbol{P}_2 = [\boldsymbol{p}_2, \ldots, \boldsymbol{p}_n]$, and provided MATLAB/GNU Octave and R user-defined functions for analysis. The theoretical results we obtained are summarized in Propositions 1 and 2 and Corollaries 1 and 2.

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Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A. Proofs

In this section, we provide some proofs.

Appendix A.1. Proof of (19)

Proof of (19). The spectrum of $\boldsymbol{\mathcal{W}} = \boldsymbol{J}_n + \boldsymbol{J}_n^\top$ is $\{\gamma_1, \ldots, \gamma_n\}$, where $\gamma_k = 2\cos\{\frac{2\pi}{n}(k-1)\}$ for $k = 1, \ldots, n$ (see, for example, [36,37]). Denote a normalized eigenvector of $\boldsymbol{\mathcal{W}}$ associated with γ_k by $\boldsymbol{\nu}_k$ for $k = 1, \ldots, n$. Given that $\gamma_1 = 2\cos(0) = 2$ and $\boldsymbol{\mathcal{W}}\mathbf{1} = 2 \cdot \mathbf{1}$, it follows that $\boldsymbol{\mathcal{W}}\mathbf{1} = \gamma_1\mathbf{1}$, and thus we may let $\boldsymbol{\nu}_1 = \frac{1}{\sqrt{n}}\mathbf{1}$. In addition, given that $\boldsymbol{\mathcal{W}}$ is symmetric and $\gamma_k \neq \gamma_1$ for $k = 2, \ldots, n$, $\boldsymbol{\nu}_k \in \mathbb{S}^\perp(\mathbf{1})$ for $k = 2, \ldots, n$. Accordingly, the eigenvectors are such that

$$\boldsymbol{H}\boldsymbol{\nu}_k = \begin{cases} \mathbf{0}, & k = 1, \\ \boldsymbol{\nu}_k, & k = 2, \ldots, n. \end{cases} \tag{A1}$$

Consequently, it immediately follows that $\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}\boldsymbol{\nu}_1 = \mathbf{0} = 0 \cdot \boldsymbol{\nu}_1$, from which $(0, \boldsymbol{\nu}_1)$ is an eigenpair of $\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}$. In addition, it also follows that

$$\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}\boldsymbol{\nu}_k = \boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{\nu}_k = \boldsymbol{H}(\gamma_k\boldsymbol{\nu}_k) = \gamma_k\boldsymbol{\nu}_k, \quad k = 2, \ldots, n. \tag{A2}$$

Therefore, $(\gamma_k, \boldsymbol{\nu}_k)$ for $k = 2, \ldots, n$ are also eigenpairs of $\boldsymbol{H}\boldsymbol{\mathcal{W}}\boldsymbol{H}$. Finally, $\gamma_k \neq 0$ for $k = 2, \ldots, n$, unless n is a multiple of 4. □

Appendix A.2. Proof of (21)

Proof of (21). The first equality follows from $\boldsymbol{p}_1(\boldsymbol{p}_1^\top\boldsymbol{p}_1)^{-1}\boldsymbol{p}_1^\top = \frac{1}{\sqrt{n}}\mathbf{1}\left(\frac{1}{n}\mathbf{1}^\top\mathbf{1}\right)^{-1}\frac{1}{\sqrt{n}}\mathbf{1}^\top = \mathbf{1}(\mathbf{1}^\top\mathbf{1})^{-1}\mathbf{1}^\top$. Next, since $\boldsymbol{P}$ is nonsingular, it follows that $\boldsymbol{P}(\boldsymbol{P}^\top\boldsymbol{P})^{-1}\boldsymbol{P}^\top = \boldsymbol{I}_n$. In addition, since $\boldsymbol{p}_1^\top\boldsymbol{P}_2 = \mathbf{0}$, $\boldsymbol{P}^\top\boldsymbol{P}$ is a block diagonal matrix, we then have

$$\boldsymbol{P}(\boldsymbol{P}^\top\boldsymbol{P})^{-1}\boldsymbol{P}^\top = \boldsymbol{p}_1(\boldsymbol{p}_1^\top\boldsymbol{p}_1)^{-1}\boldsymbol{p}_1^\top + \boldsymbol{P}_2(\boldsymbol{P}_2^\top\boldsymbol{P}_2)^{-1}\boldsymbol{P}_2^\top. \tag{A3}$$

Combining these results proves the second equality. □

Appendix A.3. Proof of (30)

Proof of (30). Given that $\boldsymbol{x} \notin \mathbb{S}(\mathbf{1})$ by assumption, $\boldsymbol{x}$ can be represented by $\boldsymbol{p}_1\zeta_1 + \boldsymbol{P}_2\boldsymbol{\zeta}_2$, where $\zeta_1 \in \mathbb{R}$ and $\boldsymbol{\zeta}_2 \in \mathbb{R}^{n-1}\backslash\{\mathbf{0}\}$. Then, from (22), it follows that $\boldsymbol{H}\boldsymbol{x} = \boldsymbol{H}(\boldsymbol{p}_1\zeta_1 + \boldsymbol{P}_2\boldsymbol{\zeta}_2) = \boldsymbol{P}_2\boldsymbol{\zeta}_2$, which results in

$$\boldsymbol{a} = \boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{x} = \begin{bmatrix} \boldsymbol{p}_1^\top \boldsymbol{P}_2\boldsymbol{\zeta}_2 \\ \boldsymbol{P}_2^\top \boldsymbol{P}_2\boldsymbol{\zeta}_2 \end{bmatrix} = \begin{bmatrix} 0 \\ \boldsymbol{\zeta}_2 \end{bmatrix} \in \mathbb{S}^\perp(\boldsymbol{e}_1)\backslash\{\mathbf{0}\}. \tag{A4}$$

□

Appendix A.4. Proof of Lemma 1

Proof of Lemma 1. From (10), (22), and (26), it follows that

$$\mathrm{cor}(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{\boldsymbol{p}_k^\top \boldsymbol{z}}{\sqrt{n}} = \frac{1}{\sqrt{n}} \frac{\boldsymbol{p}_k^\top \boldsymbol{H}\boldsymbol{x}}{\sqrt{\frac{1}{n}\boldsymbol{x}^\top \boldsymbol{H}\boldsymbol{x}}} = \frac{\boldsymbol{p}_k^\top \boldsymbol{x}}{\sqrt{\boldsymbol{x}^\top \boldsymbol{H}\boldsymbol{x}}}, \quad k = 2, \ldots, n. \tag{A5}$$

Here, $\alpha_k = \boldsymbol{p}_k^\top \boldsymbol{x}$ for $k = 2, \ldots, n$ and $\boldsymbol{x}^\top \boldsymbol{H}\boldsymbol{x} = \boldsymbol{x}^\top \boldsymbol{H}\boldsymbol{P}\boldsymbol{P}^\top \boldsymbol{H}\boldsymbol{x} = \sum_{l=2}^n \alpha_l^2$. Thus, we obtain

$$\mathrm{cor}(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{\alpha_k}{\sqrt{\sum_{l=2}^n \alpha_l^2}}, \quad k = 2, \ldots, n, \tag{A6}$$

which results in (37). □

Appendix A.5. Proof of (39)

Proof of (39). From (26), it follows that $\sum_{k=2}^n \mathrm{cor}^2(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{1}{n}\sum_{k=2}^n (\boldsymbol{p}_k^\top \boldsymbol{z})^2$. In addition, $\boldsymbol{p}_1^\top \boldsymbol{z} = \frac{1}{\sqrt{n}}\mathbf{1}^\top \boldsymbol{H}\boldsymbol{z} = 0$. Combining these yields

$$\sum_{k=2}^n \mathrm{cor}^2(\boldsymbol{p}_k, \boldsymbol{z}) = \frac{1}{n}\sum_{k=1}^n (\boldsymbol{p}_k^\top \boldsymbol{z})^2. \tag{A7}$$

Here, we have $\sum_{k=1}^n (\boldsymbol{p}_k^\top \boldsymbol{z})^2 = \boldsymbol{z}^\top \boldsymbol{P}\boldsymbol{P}^\top \boldsymbol{z} = \boldsymbol{z}^\top \boldsymbol{z} = n$. Therefore, $\sum_{k=2}^n \mathrm{cor}^2(\boldsymbol{p}_k, \boldsymbol{z})$ is equal to one. □

Appendix A.6. Proof of Proposition 2

Proof of Proposition 2. The following equalities hold:

$$\boldsymbol{G}^\top \boldsymbol{H}\mathcal{W}\boldsymbol{H}\boldsymbol{G}\boldsymbol{V} = \boldsymbol{G}^\top \boldsymbol{H}\mathcal{W}\boldsymbol{H}\boldsymbol{G}\boldsymbol{G}^\top \boldsymbol{P} = \boldsymbol{G}^\top \boldsymbol{P}\boldsymbol{Q}\boldsymbol{P}^\top \boldsymbol{G}\boldsymbol{G}^\top \boldsymbol{P} = \boldsymbol{V}\boldsymbol{Q}. \tag{A8}$$

The first equality immediately follows from the definition of $\boldsymbol{V}$, i.e., $\boldsymbol{V} = \boldsymbol{G}^\top \boldsymbol{P}$. The second equality follows from (20). The third equality follows from the definition of $\boldsymbol{V}$ and both $\boldsymbol{G}$ and $\boldsymbol{P}$ are orthogonal matrices.

Given that $\boldsymbol{g}_1 = \boldsymbol{p}_1$, it follows that $v_{1,1} = \boldsymbol{g}_1^\top \boldsymbol{p}_1 = 1$, $\boldsymbol{v}_{1,2} = \boldsymbol{g}_1^\top \boldsymbol{P}_2 = \mathbf{0}$, and $\boldsymbol{v}_{2,1} = \boldsymbol{G}_2^\top \boldsymbol{p}_1 = \mathbf{0}$, which results in

$$\boldsymbol{V} = \boldsymbol{G}^\top \boldsymbol{P} = \begin{bmatrix} \boldsymbol{g}_1^\top \boldsymbol{p}_1 & \boldsymbol{g}_1^\top \boldsymbol{P}_2 \\ \boldsymbol{G}_2^\top \boldsymbol{p}_1 & \boldsymbol{G}_2^\top \boldsymbol{P}_2 \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Xi} \end{bmatrix}. \tag{A9}$$

Here, $\boldsymbol{\Xi}$ is an orthogonal matrix because $\boldsymbol{V}\boldsymbol{V}^\top = \boldsymbol{G}^\top \boldsymbol{P}\boldsymbol{P}^\top \boldsymbol{G} = \boldsymbol{I}_n$. In addition, given that $\boldsymbol{H}\boldsymbol{G} = [\mathbf{0}, \boldsymbol{G}_2]$, it follows that

$$\boldsymbol{G}^\top \boldsymbol{H}\mathcal{W}\boldsymbol{H}\boldsymbol{G} = \begin{bmatrix} 0 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{G}_2^\top \mathcal{W}\boldsymbol{G}_2 \end{bmatrix}. \tag{A10}$$

Then, from (A9) and (A10), (A8) can be represented as

$$\begin{bmatrix} 0 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{G}_2^\top \boldsymbol{\mathcal{W}} \boldsymbol{G}_2 \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \Xi \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \Xi \end{bmatrix} \begin{bmatrix} q_1 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{Q}_2 \end{bmatrix}, \tag{A11}$$

from which we obtain

$$\boldsymbol{G}_2^\top \boldsymbol{\mathcal{W}} \boldsymbol{G}_2 \Xi = \Xi \boldsymbol{Q}_2. \tag{A12}$$

Here, recall that Ξ is an orthogonal matrix and $\boldsymbol{Q}_2$ is a diagonal matrix. In addition, given that $\boldsymbol{G}$ is an orthogonal matrix, premultiplying (A9) by $\boldsymbol{G} = [\boldsymbol{g}_1, \boldsymbol{G}_2]$ yields

$$[\boldsymbol{p}_1, \boldsymbol{P}_2] = \boldsymbol{P} = \boldsymbol{G}\boldsymbol{V} = [\boldsymbol{g}_1, \boldsymbol{G}_2] \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \Xi \end{bmatrix} = [\boldsymbol{g}_1, \boldsymbol{G}_2 \Xi], \tag{A13}$$

which yields $\boldsymbol{P}_2 = \boldsymbol{G}_2 \Xi$. □

Appendix B. User-Defined Functions

In this section, we provide the MATLAB/GNU Octave and R user-defined functions to compute $\boldsymbol{\psi}_2 = [\psi_2, \ldots, \psi_n]^\top$ (`psi2`), the bounds of Moran's coefficient (`MoranIbounds`), $\boldsymbol{Q}_2$, $\boldsymbol{P}_2$ (`Q2P2`), and $\boldsymbol{E}$ (`Emat`). Of the input arguments, `x` is an n-dimensional column vector and `W` is an $n \times n$ matrix. Of the output arguments, `Psi2` is an $(n-1)$-dimensional column vector.

Appendix B.1. MATLAB/GNU Octave Functions

```
function [Psi2]=psi2(x,W)
   [Q2,P2]=Q2P2(W);
   c=(P2'*x).^2;
   Psi2=c/sum(c);
end
```

```
function [Ilb,Iub]=MoranIbounds(W)
   W=(W+W')/2; n=size(W,1); m=sum(sum(W));
   [Q2,P2]=Q2P2(W);
   Iub=(n/m)*Q2(1,1); Ilb=(n/m)*Q2(n-1,n-1);
end
```

```
function [Q2,P2]=Q2P2(W)
   W=(W+W')/2; n=size(W,1);
   G=Emat(n); G2=G(:,2:n); A=G2'*W*G2;
   [X,L]=eig((A+A')/2);
   [l,ind]=sort(diag(L),'descend');
   Q2=diag(l); Xi=X(:,ind);
   P2=G2*Xi;
end
```

```
function [E]=Emat(n)
   E=zeros(n,n);
   E(:,1)=ones(n,1)/sqrt(n);
   for i=1:n
      for j=2:n
         E(i,j)=sqrt(2/n)*cos((j-1)*(i-0.5)*pi/n);
      end
   end
end
```

Note that `(A+A')/2` in `Q2P2` is to ensure symmetry. In addition, `G=Emat(n)` in `Q2P2` can be replaced by `G=Fmat(n)`, where `Fmat` is a function to make $\boldsymbol{F}$ and is provided in [27].

Appendix B.2. R Functions

```
psi2=function(x,W){
   Q2P2_result=Q2P2(W)
   c=(t(Q2P2_result$P2)%*%x)^2
   Psi2=c/sum(c)
   return(Psi2)
}
```

```
MoranIbounds=function(W){
   W=(W+t(W))/2; n=dim(W)[1]; m=sum(W)
   Q2P2_result=Q2P2(W); Q2=Q2P2_result$Q2; P2=Q2P2_result$P2
   Iub=(n/m)*Q2[1,1]; Ilb=(n/m)*Q2[n-1,n-1]
   return(list(Ilb=Ilb,Iub=Iub))
}
```

```
Q2P2=function(W){
   W=(W+t(W))/2; n=nrow(W)
   G=Emat(n); G2=G[,2:n]; A=t(G2)%*%W%*%G2
   eig_result=eigen((A+t(A))/2)
   l=eig_result$values; ind=order(l,decreasing=TRUE)
   Q2=diag(l[ind]); Xi=eig_result$vectors[,ind]
   P2=G2%*%Xi
   return(list(Q2=Q2,P2=P2))
}
```

```
Emat=function(n){
   E=matrix(0,n,n)
   E[,1]=rep(1/sqrt(n),n)
   for (i in 1:n){
      for (j in 2:n){
         E[i,j]=sqrt(2/n)*cos((j-1)*(i-0.5)*pi/n)
      }
   }
   return(E)
}
```

Note that `(A+t(A))/2` in `Q2P2` is to ensure symmetry.

References

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