Spatial Pattern in Residuals and Spatial Autocorrelation Tests with Moran's I and local I_i

Outline:

- What is spatial autocorrelation
- Definition of the global and local link matrices
- Definition of coding schemes
- Why autocorrelation in regression residuals?
- Motivating example: Italian Fertility
- General structure of global Moran's I and its distribution under spatial independence.
- Eigen-spectrum of the link matrix and bounds of global Moran's I
- Test under randomization.
- Local Moran's I_i (forthcoming)

What is Spatial Autocorrelation

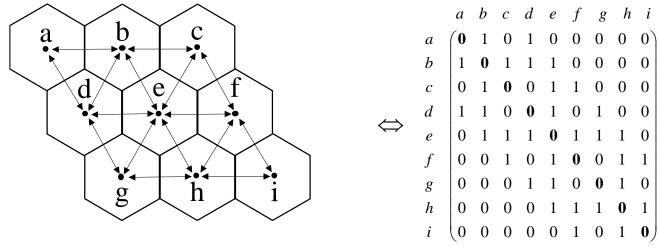
 The concept of an *internal spatial relationship* (order) is trickier than in the time-series situation, where the order comes naturally (the future depends on the past)

- In spatial analysis, the relationships among the observations are [a] multidirectional, [b]
 multilateral and [c] not equally spaced.
 - There are also more observations at the **edge of the study area** and factors like **spatial extend of the regions** and **underlying densities** become important.
- Geographical theories provide many concepts of spatial relationships within a single variable.
 For instance:
 - simple distances between points or representative points of areas
 - neighborhood relationships between areas (rook's or queen's specification in square tessellations, higher order neighborhood relationship of regions several neighbors apart)
 - traffic flows or migration patterns
 - spatial hierarchies (hub and spokes)
 - diffusion processes etc.

The Spatial Link Matrix

- The spatial connectivity matrix operationalizes the underlying structure of the potential spatial relationships among the observations
- For potential distance relationships we have the distance matrix (known from road atlases, perhaps using spherical distances)
- For potential neighborhood relationships we must use a binary spatial connectivity matrix





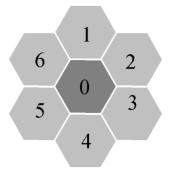
Spatial tessellation of 9 hexagonal cells with underlying connectivity structure

Binary 9×9 spatial connectivity matrix **B**

- An element $b_{ij} = 1$ denotes that the tiles i and j are **adjacent** and an element $b_{ij} = 0$ signifies that the tiles i and j are not common neighbors
- The spatial connectivity matrix **B** is *symmetric*
- A tile is not connected to itself. Thus all *diagonal* elements are zero
- For study areas with a *large number* n of individual regions the generation of the connectivity matrix \mathbf{B} (or distance matrix) must be left to a GIS program. The connectivity matrix has $n \times n$ elements
- Problems occur if we have island and holes in our study area. Usually machine generated connectivity matrices must be polished manually.
- Most of the elements are zero. There are efficient storage modes for sparse matrices. For empirical map patterns an area in the interior has on average 6 neighbors.

Local and Global Spatial Link Matrices

- Each global link matrix can be decomposed into a set of *n* local link matrices. *Vice versa*, a set of local link matrices can be aggregated into a global link matrix.
- Example: The hexagonal spatial tessellation has the global link matrix:



$$\mathbf{B} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

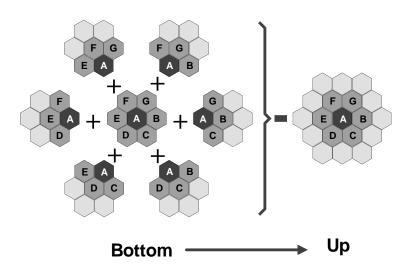
The *local link matrices* are:

- The local link matrices are star-shaped and associate the satellites to the reference cell i.
- The local link matrices satisfy the additive condition:

$$\mathbf{B} = \frac{1}{2} \cdot \sum_{i=0}^{6} \mathbf{B}_{i}$$

The adjustment factor $\frac{1}{2}$ is required because each matrix cell in the summation is counted twice.

This decomposition allows to *relate* local spatial statistics to their global counterpart **Local Global**



Coding schemes

- The spatial link matrix needs to be standardized in order to control for the increase in the overall linkage a as the number of spatial objects n in the tessellation increases.
- In irregular tessellations each interior cell has on average 6 neighbors (see Euler's Theorem).
- Three coding schemes to standardize the global link matrix are commonly in use.
- Each coding scheme has its specific properties and it is based either on the linkage degree vector.
- Note that edge cells on the boundary usually have fewer neighbors.

- These coding scheme are based on the linkage degree of each cell, which reflect *edge effects* and *spatial heterogeneity*.
- Three coding schemes:
 - The globally standardized C-coding scheme uses the overall linkage degree:

$$\mathbf{C} = \frac{n}{a} \cdot \mathbf{B} = \frac{7}{24} \cdot \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

The number of how many objects are neighbors

Implication: The variance of cells with large linkage degree is larger than for cells with a smaller number of neighbors.

 The row-sum standardized W-coding scheme uses the degree vector and divides each row to the link matrix by the linkage degree of that row:

$$\mathbf{W} \equiv \begin{pmatrix} \frac{1}{d_0} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{d_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{d_2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{d_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{d_4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{d_5} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{d_6} \end{pmatrix} \cdot \mathbf{B} = \begin{pmatrix} 0 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 \end{pmatrix}$$

This standardized link matrix is no longer symmetric. The row-sums are constant one. Implication: Cells with a low linkage degree have a larger variance.

 The variance stabilizing S-coding scheme used the square root of the linkage degree and a global scaling constant:

- The coded spatial link matrix is asymmetric
 Implication: The variance of each spatial object is approximately identical.
- The sums over all cells in a coded spatial link matrix is equal to n.
- These coding scheme and others can be specified an a unified equation defining the family of coding schemes:

$$\mathbf{V}_{[q]} = \frac{n}{\sum_{i=1}^{n} d_i^{q+1}} \cdot \begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_n \end{pmatrix}^{q} \cdot \mathbf{B}$$

with

$$q = \begin{cases} 0 & C\text{-coding scheme} \\ -1/2 & S\text{-coding scheme} \\ -1 & W\text{-coding scheme} \end{cases}$$

- ullet With the exception of ${\bf V}_{[0]}$, i.e., the C-coding scheme, none of the other transformed link matrices are symmetric.
- **Spatial econometrics** prefers the row-sum standardized coding scheme and denotes the standardized link matrix by **W**. In contrast, geo-statistics usually works with standardized interpoint distance matrices.

Excursion: Spatial Regression Residuals

• In general terms, the residuals can be expressed by the projection matrix

$$\mathbf{M} = \mathbf{I} - \mathbf{X} \cdot (\mathbf{X}^{T} \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^{T}$$
with
$$\mathbf{e} = \mathbf{M} \cdot \mathbf{y}$$

$$= (\mathbf{I} - \mathbf{X} \cdot (\mathbf{X}^{T} \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^{T}) \cdot \mathbf{y}$$

$$= \mathbf{y} - \mathbf{X} \cdot (\mathbf{X}^{T} \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^{T} \cdot \mathbf{y}$$

$$\mathbf{b}$$

- where X is the matrix of the exogenous variables including the constant unity vector for the regression intercept.
- If we measure only the variation of the dependent variables around its mean then the projection matrix reduces to $\mathbf{M}_{(1)} = \mathbf{I} \mathbf{1} \cdot (\mathbf{1}^T \cdot \mathbf{1})^{-1} \cdot \mathbf{1}^T$

$$\mathbf{M}_{(1)} \equiv \begin{pmatrix} 1 - \frac{1}{n} & -\frac{1}{n} & \cdots & -\frac{1}{n} \\ -\frac{1}{n} & 1 - \frac{1}{n} & \cdots & -\frac{1}{n} \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{n} & -\frac{1}{n} & \cdots & 1 - \frac{1}{n} \end{pmatrix}.$$

• This gives
$$\mathbf{e} = \begin{pmatrix} y_1 - \overline{y} \\ y_2 - \overline{y} \\ \vdots \\ y_n - \overline{y} \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{n} & -\frac{1}{n} & \cdots & -\frac{1}{n} \\ -\frac{1}{n} & 1 - \frac{1}{n} & \cdots & -\frac{1}{n} \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{n} & -\frac{1}{n} & \cdots & 1 - \frac{1}{n} \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_1 \\ \vdots \\ y_n \end{pmatrix}$$

• Due to the projection matrix the residuals are always slightly correlated, that is, $Cov(\mathbf{e} \cdot \mathbf{e}^T) = \sigma^2 \cdot \mathbf{M}$.

Why autocorrelation in regression residuals?

- Regression residuals e capture the unexplained part of the regression model
- They are usually assumed to relate to population disturbances that are $\mathbf{\epsilon} \sim N(0, \sigma^2 \cdot \mathbf{I})$. The following reasons lead to spatial autocorrelation
 - o (1) Misspecification Rational: if we are missing relevant variables in **X** that exhibit a spatial pattern, their spatial pattern will spill over into the regression residuals **e**.
 - (2) Spatial Process Rational: The spatial objects exhibit some spatial exchange relationships, e.g.,
 - interaction flows,
 - competition effects or
 - agglomerative advantages
 - then they will become spatially autocorrelated.
 These exchange relationships cannot be captured by the regression matrix X but

manifest in a *covariance* matrix $\Omega(\rho)$ with $\mathbf{\epsilon} \sim N(0, \sigma^2 \cdot \Omega(\rho))$ where ρ is the *autocorrelation level* and measuring the strength of the spatial process. For

$$\rho = \begin{cases} > 0 & \text{postive autocorrelation} \\ 0 & \text{spatial independence} \\ < 0 & \text{negative autocorrelation} \end{cases}$$

Moran's I is tailored to work best for Gaussian spatial processes with

$$\boldsymbol{\Omega}(\rho) = \begin{cases} \text{simultaneous autoregressive spatial process} \\ \text{conditional autoregressive spatial process} \\ \text{moving average spatial process} \end{cases}$$

- All these processes dependent on the *coded* spatial link matrix V among the spatial objects, which reflects the spatial relationships and that is derived from the binary links B.
- (3) Spatial Aggregation Rational: If areal objects are split into parts and these split parts are merged with adjacent areal objects then these aggregated objects share parts of the information that they inherited from the split objects.

This induces spatial autocorrelation among adjacent spatial objects.

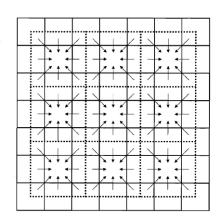
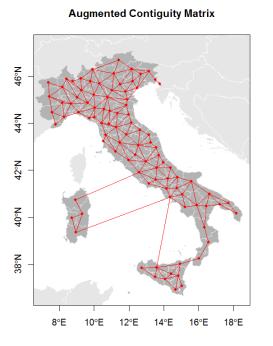


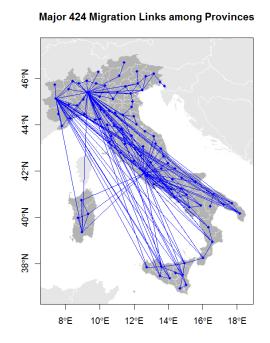
Fig. 4.2. Non-hierarchical aggregation of elemental spatial objects defined by a rectangular 7×7 tessellation into a rectangular 3×3 tessellation

Implication: One needs to get the spatial scale of analysis right.

Motivating Example: Fertility in Italy

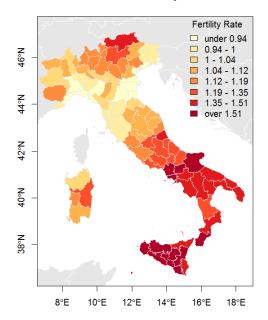
• Several spatial link matrices are conceivable:





- ullet The spatial relationships can be captured in the spatial link matrix ${f V}$
- The map pattern of the observed dependent variable **Total Period Fertility** and the autocorrelation of the regression residuals around the mean is $e_i = y_i \bar{y}$:

Provinical Total Fertility Rate 1994



Global Moran's I for regression residuals

Moran I statistic standard deviate = 12.7804, p-value < 2.2e-16

alternative hypothesis: greater

sample estimates:

Observed Moran's I Expectation Variance 0.853201213 -0.010638298 0.004568551

• The applied *regression model* to explain the Total Fertility Rate is

lm(formula = TOTFERTRAT ~ FEMMARAGE9 + DIVORCERAT + log(ILLITERRAT) +
 TELEPERFAM, data = prov.df)

Residuals:

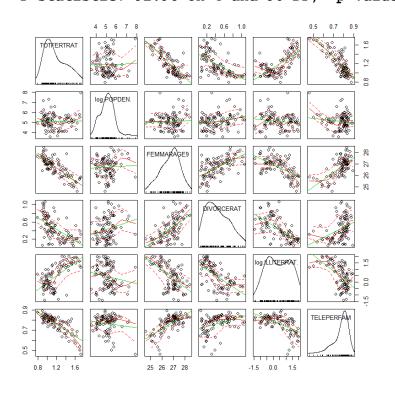
Min 1Q Median 3Q Max -0.19958 -0.05474 -0.01284 0.05272 0.42922

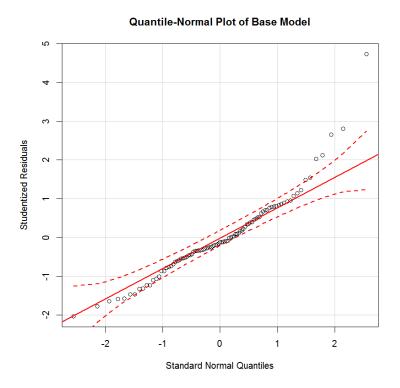
Coefficients:

log(ILLITERRAT) 0.03072 0.01707 1.799 0.0753 .
TELEPERFAM -1.28499 0.18078 -7.108 2.69e-10 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

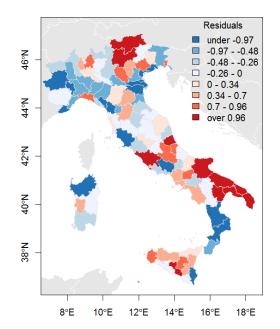
Residual standard error: 0.1047 on 90 degrees of freedom Multiple R-squared: 0.8051, Adjusted R-squared: 0.7965 F-statistic: 92.96 on 4 and 90 DF, p-value: < 2.2e-16





• The map pattern of the residuals $e_i = y_i - \hat{y}_i$ and their autocorrelation level are





Global Moran's I for regression residuals

sample estimates:

Observed Moran's I Expectation Variance 0.276027992 -0.032044882 0.004244308

Notes:

- Accounting for the exogenous variables has substantially reduced the autocorrelation level (⇒misspecification perspective).
- \circ The **expectation** and **variance** of Moran's I dependent on the regression matrix **X**.
- Residuals are best mapped by a bipolar map theme.

General structure of Moran's I and its distribution

The observed value of Moran's I

• Moran's I is defined to measure the strength of spatial autocorrelation in regression residuals $\mathbf{e} = \mathbf{M} \cdot \mathbf{y}$ with

$$\mathbf{e} = \begin{cases} \mathbf{y} - \mathbf{1} \cdot \bar{\mathbf{y}} & \text{if } [\mathbf{I} - \mathbf{1} \cdot (\mathbf{1}^T \cdot \mathbf{1})^{-1} \cdot \mathbf{1}^T] \cdot \mathbf{y} \\ \mathbf{y} - \hat{\mathbf{y}} & \text{if } [\mathbf{I} - \mathbf{X} \cdot (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T] \cdot \mathbf{y} \end{cases}$$

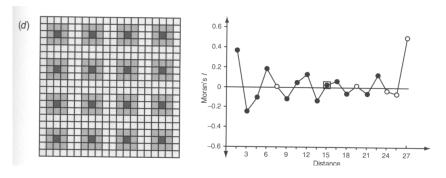
ullet Its observed value I^{obs} has the formal structure of a $\it ratio\ of\ \it quadratic\ \it forms$ in the random variable ${f y}$

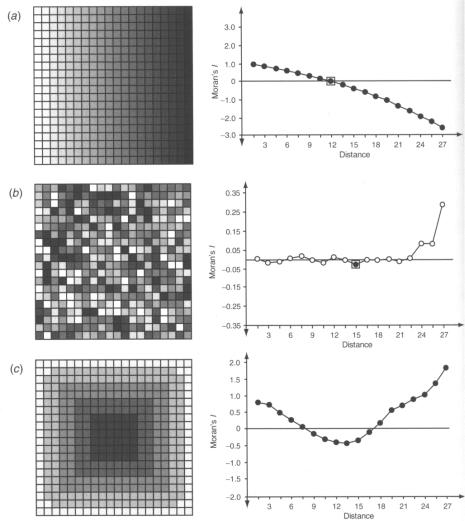
$$I^{obs} = \frac{\mathbf{y}^T \cdot \mathbf{M} \cdot \frac{1}{2} \cdot (\mathbf{V} + \mathbf{V}^T) \cdot \mathbf{M} \cdot \mathbf{y}}{\mathbf{y}^T \cdot \underbrace{\mathbf{M} \cdot \mathbf{M}}_{=\mathbf{M}} \cdot \mathbf{y}} = \frac{\mathbf{e}^T \cdot \frac{1}{2} \cdot (\mathbf{V} + \mathbf{V}^T) \cdot \mathbf{e}}{\mathbf{e}^T \cdot \mathbf{e}}$$

The denominator is simply the residual sum of squares: $RSS = \sum_{i=1}^{n} e_i^2 = \mathbf{e}^T \cdot \mathbf{e}$

- Besides the spatial autocorrelation pattern in the dependent *random variable* y through $\varepsilon \sim N(0, \Omega)$ the observed value of Moran's I also depends on the *exogenous* variables X through the projection matrix M and the *exogenous* spatial link matrix V.
- The spatial link matrix \mathbf{V} is *symmetrized* by the transformation $\frac{1}{2} \cdot (\mathbf{V} + \mathbf{V}^T)$. While the observed value I^{obs} is invariant under this transformation, the evaluation of its distribution requires a symmetric structure.

- Global Moran's I can be evaluated for different specification so the link matrix $\frac{1}{2} \cdot (\mathbf{V} + \mathbf{V}^T)$ such as higher order lags which leads to the correlogram or directional correlogram:
- The number of point pairs depends again on the spatial order of the spatial lag.
- Example correlograms:

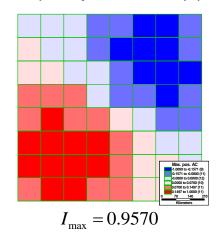


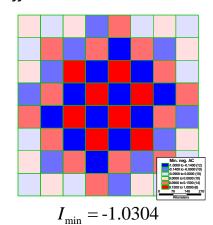


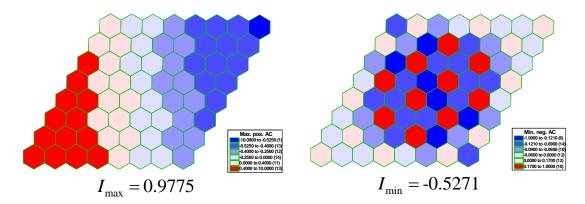
Extreme Values of Moran's I

- The *largest and smallest possible values* of Moran's I can be determined by the largest eigenvalue λ_1 and smallest eigenvalue λ_n of the matrix $\mathbf{M} \cdot \frac{1}{2} \cdot (\mathbf{V} + \mathbf{V}^T) \cdot \mathbf{M}$.
- The associate eigenvectors \mathbf{v}_i show a distinctive map pattern. These eigenvectors build the foundation for the spatial filtering methodology.
- Note that the possible value range of Moran's I does not necessarily need to be $I \in [-1,1]$ such as for the Pearson's correlation coefficient.

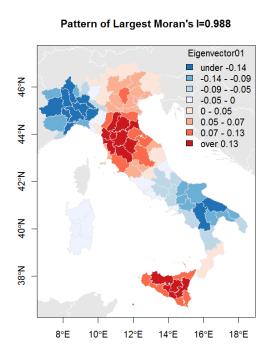
Examples of extreme map patterns for different tessellations:

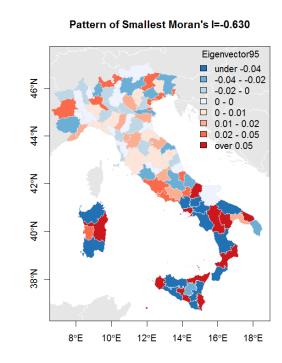






• Most *extreme possible spatial map patterns* and their autocorrelation levels for the tessellation of the 95 Italian provinces for the *S*-coding scheme:



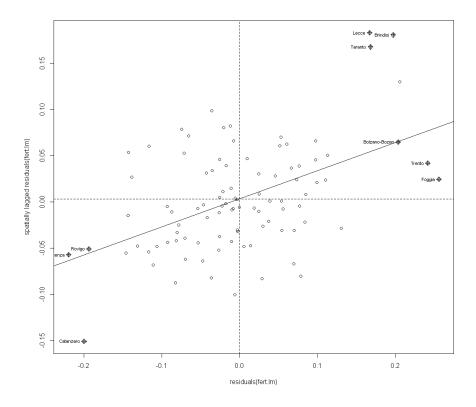


Test under the Assumption of Spatial Independence

Exploratory visualization:

• The observed residuals e_i can be plotted against the average values of their neighboring values e_i^{avg} using the "Moran's scatterplot".

For the row-sum standardized link matrix \mathbf{V} these averages are given by $\mathbf{e}^{avg} = \mathbf{V} \cdot \mathbf{e}$.



Under the assumption of $\varepsilon \sim N(0, \sigma^2 \cdot \mathbf{I})$:

• Assuming that the population disturbances are independently identically distributed with $\mathbf{\epsilon} \sim N(0, \sigma^2 \cdot \mathbf{I})$ the moments of Moran's I can be evaluated directly through the matrix terms:

$$E(I|H_0) = \frac{tr[\mathbf{M} \cdot \mathbf{V}]}{n - K}$$

$$Var(I|H_0) = \frac{tr[\mathbf{M} \cdot \mathbf{V} \cdot \mathbf{M} \cdot \mathbf{V}^T] + tr[\mathbf{M} \cdot \mathbf{V} \cdot \mathbf{M} \cdot \mathbf{V}] + (tr[\mathbf{M} \cdot \mathbf{V}])^2}{(n - K) \cdot (n - K + 2)} - [E(I|H_0)]^2$$

• For sufficiently *large number* of spatial objects n and "well-behaved" link matrices V one can use the normal approximation to evaluate the distribution of I^{obs} :

$$\frac{I^{obs} - E(I|H_0)}{\sqrt{Var(I|H_0)}} \sim N(0,1)$$

- This expression is frequently used in software implementations.
- However, those implementations frequently use incorrectly the projections matrix ${f M}_{(1)}={f I}-{f 1}\cdot ({f 1}^T\cdot {f 1})^{-1}\cdot {f 1}^T$
- To evaluate the exact significance values of an observed value of Moran's I^{obs} numerical integration or the saddle-point approximation need to be employed.

Under the assumption of $\varepsilon \sim N(0, \sigma^2 \cdot \Omega(\rho))$:

• Again, these conditional distribution functions $F(I|\mathbf{X}, \mathbf{\Omega}(\rho))$ of Moran's I can be evaluated by numerical integration.

Under the assumption of $\varepsilon \sim i$. i. d with unknown distribution:

- In case the distribution of the residuals is unknown randomization needs to be employed to evaluated the significance of the observed Moran's I^{obs} .
- Underlying idea:
 - Any observed spatial association of the residuals e is broken up by randomly distributing these residuals to different areas.
 - \circ This random assignment generates a map pattern under the assumption H_0 : $\mathbf{e} \sim spatial \ independent$
 - \circ This random assignment is repeated R-times (say R=999) and for each random pattern r the associated Moran's I^r is calculated.
 - \circ These random Moran's I^r are sorted ascendingly and their distribution is plotted. This is the distribution under the null hypothesis H_0 : $\mathbf{e} \sim spatial \ independent$.
 - o If the observed Moran's I^{obs} falls into a tail of this distribution (either lowest or highest ranking I^r 's, then the observed pattern exhibits significant spatial autocorrelation. Otherwise, it is spatially independent.

