A C T A U N I V E R S I T A T I S L O D Z I E N S I S
FOLIA OECONOMICA 252, 2011

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THE METHOD OF COMPUTING THE LOG-JACOBIAN OF THE VARIABLE TRANSFORMATION FOR SPATIAL MODELS – TEST AND COMMENTS

Abstract. One of the most important problems in spatial econometrics is the computation of the log of the Jacobian of variable transformations in models with spatial interactions. The computation is necessary in ML estimation and Bayesian analysis of models with spatial dependence (Smirnov and Anselin 2009).

The effectiveness of the implementation of ML depends on computing effectiveness of the log-determinant of a matrix, especially for sparse and large matrices.

The second problem is the numerical accuracy of computation of the log-determinant using different methods as it was shown by Walde et al. (2008). These issues provoked a search of new methods of estimation for spatial models. One of them is GMM being easier but more restrictive for computation than ML (Lee 2004, 2007). Another solution is to make some simplifications based on regular grids or band matrices (Rue, Held 2005).

In the paper we test and comment the method of computing the log-Jacobian of the variable transformation for models with spatial interactions, suggested by Smirnov and Anselin (2009), for some practical case studies.

1. INTRODUCTION

Describing an object with a precise spatial location is a specific property of the data used in economic geography and the Regional Science. Standard methods (both statistical and econometric) have a little use for the analysis of such data, because they do not take into account the spatial aspect. Moreover, the use of spatial data for modelling the various processes by classical methods of econometrics can lead to false conclusions based on the test.

The space may be one of the factors that influencing on investigated phenomena and processes in different locations by the presence of so-called spatial effects. The classical methods and econometric models do not include the existence of such effects. Therefore, since the `50s of the XX century began researches to develop new methods and models, which in the `70s were placed in the domain of a new scientific discipline - spatial econometrics.

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The general linear spatial model used in many papers (e.g. Anselin [1988]) is usually presented in the form:

$$\begin{aligned} &\mathbf{y} = \rho \mathbf{W}_1 \mathbf{y} + \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \\ &\boldsymbol{\varepsilon} = \lambda \mathbf{W}_2 \boldsymbol{\varepsilon} + \boldsymbol{\mu} \\ &\boldsymbol{\mu} \sim \mathrm{N}(\mathbf{0}, \mathbf{V}),\ v_{ii} = h_i(\mathbf{z'}\boldsymbol{\alpha}),\ h_i > 0 \end{aligned} \quad . \tag{1}$$

The symbols in these equations mean, respectively: $\mathbf{y}$ - dependent k x 1 variable vector, $\boldsymbol{\beta}$ - k x 1 vector of parameters exogenous variables, $\mathbf{X}$ - n x k matrix of exogenous variables are coefficients for the autoregressive dependent variable and spatially lagged error term. Matrices $\mathbf{W}_1$, $\mathbf{W}_2$ are square matrices of size n. The vector of unknown parameters of this spatial model:

$$\boldsymbol{\theta}' = \left(\rho, \boldsymbol{\beta}', \lambda, \sigma^2, \boldsymbol{\alpha}'\right), \tag{2}$$

where: $\boldsymbol{\beta}$ has k elements, and $\boldsymbol{\alpha}$ contains p elements. Thus, the vector composed k+p+3 of unknown model parameters.

It is often assumed that random error $\boldsymbol{\mu}$ is normally distributed with zero expectation and some covariance matrix $\mathbf{V}$. In the above formulation the model could be used in the case of homoscedasticity (additional assumption are needed) as well as heteroscedasticity case situation**.**

A few known spatial model structures result when subvectors of the parameter vector are set to zero. Specifically, the following situations correspond to the four traditional spatial autoregressive models discussed in the literature (Anselin [1988], Griffith [2003], Arbia [2006], Bivand [1984]):

1) The classical linear regression model:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},\ \rho = \lambda = 0,\ \boldsymbol{\alpha} = 0, \tag{3}$$

2) The mixed regressive-spatial autoregressive model

$$\mathbf{y} = \rho \mathbf{W}_1 \mathbf{y} + \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},\ \lambda = 0,\ \boldsymbol{\alpha} = 0, \tag{4}$$

3) The spatial error model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},\ \boldsymbol{\varepsilon} = \lambda \mathbf{W}_2 + \boldsymbol{\mu},\ \rho = 0,\ \boldsymbol{\alpha} = 0. \tag{5}$$

The two N x N matrices $\mathbf{W}_1$ and $\mathbf{W}_2$ are standardized or unstandardized spatial weight matrices, respectively associated with a spatial autoregressive process in the dependent variable and in the error term. This allows two different spatial processes. Estimation of model parameters 1) is usually a classical method of least squares (OLS). Parameter estimators are consistent, unbiased and most efficient.

As shown in Anselin [1988], in the presence of:

C1) lagged dependent variable, OLS estimator is biased and inconsistent,

C2) spatial residual autocorrelation, OLS estimator is inefficient, due to non-diagonal structure of disturbance variance matrix.

For the cases C1) and C2), to estimate the parameters of spatial autoregressive model and spatial error model the OLS method should be replaced by another. The most common method used method is the maximum likelihood (ML). The maximum likelihood estimators and discussion on their properties can be found in numerous works of Cliff and Ord [1981], Ripley [1981] and Anselin [1988]. This is not the only method of estimating the parameters of models with spatial dependence. For the spatial error model, the estimators are derived based on the GLS (Generalised Least Squares). In turn, Haining [1978] and Bivand [1984] suggested the use of instrumental variables (IV) to estimate the spatial models. There are used also generalised method of moments and Bayesian approach.

For the general spatial model, the maximum likelihood estimates are obtained from a maximization following log-likelihood function with respect to parameters $\boldsymbol{\beta}$, $\boldsymbol{\alpha}$, and λ.

$$L = -\frac{n}{2}\ln\pi - \frac{1}{2}\ln|\boldsymbol{\Omega}| + \ln|\mathbf{A}| + \ln|\mathbf{B}| - \frac{1}{2}(\mathbf{Ay} - \mathbf{X}\boldsymbol{\beta})'\mathbf{B}'\boldsymbol{\Omega}^{-1}\mathbf{B}(\mathbf{Ay} - \mathbf{X}\boldsymbol{\beta}), \quad (6)$$

where:

$\mathbf{A} = \mathbf{I} - \rho\mathbf{W}$, $\mathbf{B} = \mathbf{I} - \lambda\mathbf{W}$.

For the mixed regressive autoregressive spatial model we have λ=0, and for the linear regression with spatially dependent error terms we have ρ=0.

From computational point of view one of the important problems is the calculation of log-Jacobians $\ln|\mathbf{I} - \rho\mathbf{W}|$ and $\ln|\mathbf{I} - \lambda\mathbf{W}|$.

The computation is necessary in ML estimation and Bayesian analysis of models with spatial dependence (Smirnov and Anselin [2009]). The effectiveness of the implementation of ML depends on computing effectiveness of the log-determinant of a matrix, especially for sparse and large matrices.

The second problem is the numerical accuracy of computation of the log-determinant using different methods as it was shown by Walde et al. [2008]. These issues provoked to a search for the new methods of estimation for spatial models. One of them is GMM being easier but more restrictive for computation than ML (Lee [2004], [2007]). Another solution can be some simplifications based on regular grids or band matrices (Rue and Held 2005).

In the paper we test and comment the method of computing the log-Jacobian of the variable transformation for models with spatial interactions, suggested by Smirnov and Anselin [2009], for some practical case studies.

2. METHODS

Spatial weights matrix is defined as a formal expression of spatial dependencies between units of observation (Anselin [1988]). It defines a spatial neighborhood structure, and measures the strength of potential interactions. There is no convincing view about how the store should be a spatial neighborhood structure. Therefore, the literature has already identified a number of encoding spatial weights matrix elements.

The simplest spatial weights matrix is a binary matrix of the immediate vicinity of **C -** the weights will take values 1 for close neighbours, and 0 otherwise. The neighborhood is generally understood as a fact of having a common border. There are two types of such a neighborhood: a) rook - where individuals contiguous borders with non-zero length, b) queen - is taken into the neighborhood through a point. The matrix **C** is a symmetric matrix which elements are lying on the principal diagonal under the convention are zero. Standardizing the immediate vicinity of the matrix **C** by the formula:

$$w_{ij} = \frac{c_{ij}}{\sum_{j=1}^{n} c_{ij}}, \tag{7}$$

we obtain a matrix in which the sum of the elements in each row is 1. This is the most common used definition of spatial weights matrix. Tiefelsdorf, Griffith and Boots [1998] noted that in the row standardized matrix too much weight are assigned to units with a small number of neighbors, for example, located on the border area under consideration.

In addition to these definitions of the matrix of spatial scales, to the most popular encoding schemes can be classified as (Getis and Aldstadt [2004]): a) the inverse of the distance between the observations raised to the power, 2) the length of their common border, divided by the parameter, 3) the distance not greater than the distance to the n-th neighbor, 4) ordered distance, 5) distance limited to constant, 6) all centroids to the critical distance d, 7) *n* nearest neighbors, 8) based on local statistics.

Now let us comment properties of the above defined matrices in matricial and topological language (following Smirnov and Anselin [2009]). Let N be the size of the spatial dataset. The spatial weights matrix $\mathbf{W} = (w_{ij})$ is obtained from a symmetric nonnegative matrix **C** by its row-standardization, i.e. $\mathbf{W} = \mathbf{D}^{-1}\mathbf{C}$, where **D** is the diagonal N x N matrix of positive row-sums. Thus the matrix **W** is generally non-symmetric, but the matrix $\mathbf{W}_s$, obtained by the similarity transformation:

$$\mathbf{W}_s = \mathbf{D}^{1/2}\mathbf{W}\,\mathbf{D}^{-1/2}, \tag{8}$$

is symmetric (symmetry of **C** follows from the property of distance function or contiguity), which implies that the set of eigenvalues of **W** and $\mathbf{W}_s$ coincides and determinants are equal. So:

$$\ln\left|\mathbf{I}-\rho\mathbf{W}_s\right| = \ln\left|\mathbf{I}-\rho\mathbf{W}\right| . \tag{9}$$

The matrix **C**, and in consequence, matrix **W** are usually sparse non-negative matrices for large *N*. The proportional number of non-zero elements decreases while *N* is increasing. It would be convenient from mathematical point of view to have spatial weights matrices equivalent to band matrices. But in fact it is not true - spatial weights matrices generally are not equivalent to band matrices even cannot be approximated by a band matrix (Rue and Held [2005]). The level of reducibility of given sparse matrix to band matrix depends on Hausdorff dimension, as it was described by Anselin and Smirnov (1996). They used the spatial weights matrix to define topological distance *D(i,j)* between *i-th* and *j-th* locations. On the basis of the *D(i,j)* they defined the topological circle of radius *r* for the location *i* as the set of points with topological distance $S^r(i)$ from *i* of *r* or less: $(t \in S^r(i)) \Leftrightarrow (D(i,j) \leq r)$.

It is obvious that the size of set $S^r(i)$ is monotonically increasing with radius *r* and the level of growth rate depends on location.

The Hausdorff dimension *d* of the spatial dataset in the *R*-vicinity of each location is a positive real number for which for all locations specified in matrix **W**:

$$\frac{\left|S^r(i)\right|}{\left|S^1(i)\right|} \leq \mathcal{O}(r^d),\ r \in \{1,2,\ldots, R\}, \tag{10}$$

where **|.|** denotes the number of elements of the set and *R* is a finite positive integer number.

Although Hausdorff dimension is defined on the infinite datasets, Smirnov and Anselin [2009] extended the notion of the topological dimension to a finite dataset. Specifically, they used the smallest *d* for which (10) is satisfied to determine the Hausdorff dimension in the vicinity of each location. If the Hausdorff dimension is finite, *d* indicates the topological dimension of the spatial dataset. Finally, Smirnov and Anselin [2009] came to conclusion that most geo-spatial data have finite Hausdorff dimension.

The topological dimension of the spatial dataset "describes" the structure of non-zero elements in the spatial weights matrix **W**. For the case *d =1* we have single-dimensional spatial dataset and there exists such order of elements with the corresponding spatial weights matrix being a band matrix. In this case the band is finite and it is independent of the size of the dataset. The crucial (the most problematic for calculation) situation is when the spatial dataset has topological dimension *d = 2* because the spatial weights matrix cannot be transformed by row and column permutation into a matrix with a fixed band. Unfortunately, most of geo-spatial data have dimension two, which leads us to corresponding spatial weights matrices with a band that increases with matrix size. It implies that band matrix techniques would be a poor choice for solving spatial problems.

The numerical method presented by Smirnov and Anselin [2009] delivered an $O(N)$ method for the spatial datasets with a finite and constant topological dimension. The assumption of the method is mostly satisfied for practical spatial samples. The theoretical base for the method is described below.

The log-determinant of a positive definite matrix $\ln|\mathbf{I}-\rho\mathbf{W}|$ is given by:

$$\ln|\mathbf{I}-\rho\mathbf{W}| = \sum_{i=1}^{N}\ln(1-\rho\omega_i), \tag{11}$$

where ω_i are eigenvalues of the matrix **W** (Anselin, 1988; Ord, 1975).

Since the matrix **W** is symmetrizable via transformation (8), its eigenvalues are real, but their computation is impractical if not impossible for large **W** because of lack of numerical methods for computing all eigenvalues. Using following notation for the non-central moment of the set of eigenvalues of the matrix: $\Omega^j = \sum_{i=1}^{N}\omega_i^j$, we get:

$$\ln|\mathbf{I}-\rho\mathbf{W}| \ = \ \sum_{i=1}^{N}\ln(1-\rho\omega_i) = -\lim_{n\to\infty}\sum_{j=1}^{N}\frac{1}{j}\rho^j\Omega^j \ . \tag{12}$$

It is important to note that the formula (12) holds for any real matrix **W** obtained by the similarity transformation (81) because the latter preserves its eigenvalues. Numerical approximation with chosen m

$$\ln|\mathbf{I}-\rho\mathbf{W}| \ = \ -\sum_{j=1}^{m}\frac{1}{j}\rho^j\Omega^j - R_m(\rho), \tag{13}$$

where $R_m(\rho)$ is a generally positive with zeros only in the absence of spatial dependence.

The key component of the efficient computation relies on the following

$$\Omega^j \ = \ tr(\mathbf{W}^j) \ = \ tr(\mathbf{W}^j\mathbf{I}) \ = \ tr(\mathbf{W}^j\sum_{j=1}^{N}\boldsymbol{\eta}_i\boldsymbol{\eta}_i') \ = \sum_{j=1}^{N}\boldsymbol{\eta}_i'\mathbf{W}\boldsymbol{\eta}, \tag{14}$$

where $\boldsymbol{\eta}_i$ is the N x 1 vector that has only one non-zero element equal to 1 on the i-th position.

Below we present steps of the algorithm proposed by Smirnov and Anselin [2009] based on formulas mentioned above.

Efficient method for computation of $\Omega^j = 0,\ j=1,\dots,m$**:**

set $\Omega^j = 0,\ j=1,\dots,m$
for $i \in \{1, 2, \dots, N\}$ do
initialize $\boldsymbol{\eta} = \boldsymbol{\eta}_i$
j:=2
repeat
$\boldsymbol{\zeta} := \mathbf{W}\boldsymbol{\zeta}$
$\Omega^{j-1} := \Omega^{j} + \boldsymbol{\zeta}'\boldsymbol{\eta}$
$\Omega^{j} := \Omega^{j} + \boldsymbol{\zeta}'\boldsymbol{\zeta}$
$\boldsymbol{\eta} = \boldsymbol{\zeta}$
j:=j+2
until $j > m$
end *for*

3. DATA

Typical spatial systems used in geographical analysis, are those based on the basic units of territorial division of the country. A characteristic feature of this type of spatial systems is a relatively large number of their constituent units, usually a few thousands. In this paper the method proposed by Smirnov and Anselin was used to calculate the log-Jacobian for quite large three datasets. We analysed:

1) Poland (communes – Polish name: *gminy*) 2478 spatial units,
2) Slovakia (communes – Slovakian name: *obce*) 2920 spatial units,
3) Czech Republic (communes – Czech name: *obce*) 6249 spatial units.

Below we present maps of this three cases showing borders of spatial units.

Fig. 1. Map of administrative units in Poland (gminy - communes)

Source: developed by the authors.

Fig. 2. Map of administrative units in Slovakia (obce - communes)

Source: developed by the authors.

Fig. 3. Map of administrative units in Czech Republic (obce - communes)

Source: developed by the authors.

4. RESULTS AND DISCUSSION

The method of calculating the log-Jacobian proposed by Smirnov and Anselin [2009] was used for the three previous sets of data. Its numerical performance has been tested on a typical PC equipped with 2.4GHz Intel processor, running on Windows Vista. The algorithm of calculation of the logarithm of the determinant was developed and launched in Matlab 7.9 R2009b.

In the first step the first-order neighborhood matrices for Poland, Slovakia and the Czech Republic administrative units were constructed, and then their row-standardized versions were calculated. The matrices were characterized by a high degree of sparseness. The matrix constructed for Polish has 14214 non-zero (on figures noted by "nz") elements, which constitute 0.23% of all its elements. For Slovakia, the matrix has 17104 nonzero elements, or 0.2%, and for the Czech Republic was 37012 nonzero elements, i.e. 0.09%. Analyzed weighting matrices are given in Figure 4-6. It is easy to observe that their structures are far from regular.

Fig. 4. Spy matrix – Poland

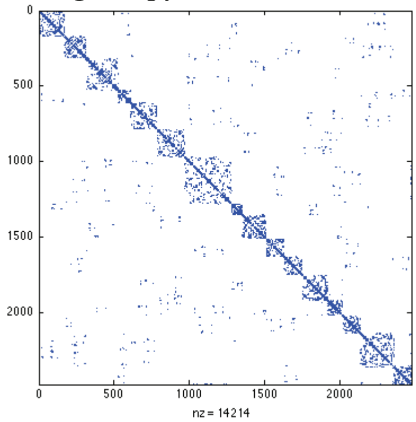


Fig. 5. Spy matrix – Slovakia

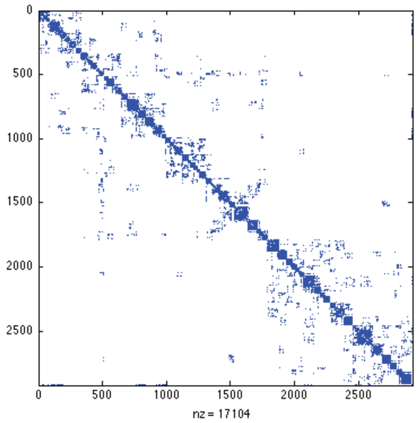
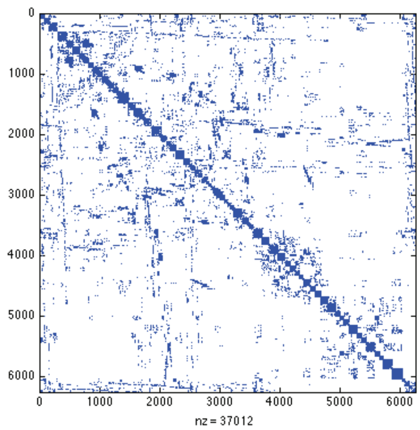


Fig. 6. Spy matrix – Czech Republic



Source: developed by the authors.

In the next step the algorithm calculating value of lower moments of eigenvalues of the matrix **W** and logarithm of the determinant of a matrix ($\mathbf{I}-\rho\mathbf{W}$) was running. Due to the fact that the series expansion of the logarithm of the determinant is theoretically infinite sum, it was essential to establish criteria to stop the algorithm. It is the value of *m* beyond which the logarithm will be stopped. The rule of stopping the algorithm was adopted arbitrarily for such even value of m, for which the calculated value of the logarithm of the determinant does not differ from that calculated for *m*-1 and *m*-2 to the nearest fourth decimal place.

Positive definiteness of the matrix ($\mathbf{I}-\rho\mathbf{W}$) requires that ρ should be contained in the interval $\left(\frac{1}{\omega_{\min}}, \frac{1}{\omega_{\max}}\right)$, which also guarantees existence of the limit (12). In the paper, similarly as in Smirnov and Anselin [2009], we took ρ=0.5.

The calculated values $\Omega^j = 0$, j=1,…, m and the subsequent approximations of the logarithm of the determinant are given in Tables 1-3. For the Polish case the logarithm of the determinant of the value stabilized at a level -76.1353, for *m*=18, for Slovakia it was -83.3156 for *m*=20, and for Czech Republic value was -176.7591 with *m*=20. It is worth noting that the value of the logarithm of the determinant for Slovakia did not change at the fourth decimal place already for m = 15, and for Rep. Czech m = 19, but in both cases the value of *m* was odd (*m* is required to be even).

Tab. 1. Results of log-Jacobian computation for Poland

m	Ω^j	$\ln\lvert\mathbf{I}-\rho\mathbf{W}\rvert$
1	0,0000	0,0000
2	527,8508	-65,9808
3	140,6423	-71,8410
4	193,3311	-74,8617
5	121,1219	-75,6188
6	127,7235	-75,9514
7	98,0888	-76,0608
8	91,5162	-76,1055
9	79,6153	-76,1228
10	74,7609	-76,1301
11	67,0151	-76,1331
12	62,5022	-76,1343
13	57,6532	-76,1349
14	54,3728	-76,1351
15	50,7052	-76,1352
16	47,9883	-76,1353
17	45,2621	-76,1353
18	43,1204	-76,1353

Source: developed by the authors.

Tab. 2. Results of log-Jacobian computation for Slovakia

m	Ω^j	$\ln\lvert\mathbf{I}-\rho\mathbf{W}\rvert$
1	0,0000	0,0000
2	566,3908	-70,7989
3	180,4263	-78,3166
4	221,7587	-81,7816
5	148,8706	-82,7120
6	146,7932	-83,0943
7	118,9219	-83,2270
8	108,1242	-83,2798
9	96,0125	-83,3007
10	88,5236	-83,3093
11	80,6016	-83,3129
12	74,5767	-83,3144
13	69,3046	-83,3151
14	64,9274	-83,3153
15	60,9180	-83,3155
16	57,4529	-83,3155
17	54,3786	-83,3155
18	51,6544	-83,3156
19	49,1747	-83,3156
20	46,9441	-83,3156

Source: developed by the authors.

Tab. 3. Results of log-Jacobian computation for Czech Republic

m	Ω^j	$\ln\lvert\mathbf{I}-\rho\mathbf{W}\rvert$
1	0,0000	0,0000
2	1205,9002	-150,7327
3	377,3803	-166,4575
4	457,9719	-173,6145
5	306,1114	-175,5320
6	300,5133	-176,3093
7	241,8057	-176,5814
8	218,5798	-176,6792
9	193,1210	-176,7315
10	177,6003	-176,7437
11	160,8189	-176,7519
12	148,4907	-176,7551
13	137,3276	-176,7562
14	128,4723	-176,7572
15	120,0194	-176,7581
16	113,0403	-176,7588
17	106,5926	-176,7591
18	101,1308	-176,7591
19	95,9583	-176,7591
20	91,4894	-176,7591

Source: developed by the authors.

The effectiveness of the Smirnov-Anselin algorithm may be measured over time, after which a satisfactory approximation of values of $\ln|\mathbf{I}-\rho\mathbf{W}|$ is received. The time required for obtaining approximations is included in Table 4.

Tab. 4. The time needed to computation the log-detrminant

Data	***N***	***m***	**Time (*s*)**
Poland	2478	18	357.12
Slovakia	2920	20	653.25
Czech Republic	6249	20	6448.76

Source: developed by the authors.

Commenting the results let us note that there is difference in the time needed to obtain approximations for Slovakia and the Czech Republic, as both cases required m=20. In the case of Slovakia, this time was 653.25 [*s*], with N=2920, while in the case of the Czech Republic was 6,448.76 [s] for N=6249. The proportion of sample size for Slovakia to sample size of the Czech Republic number is approximately equal to k=2.14. The appropriate ratio for the length of calculation time is 9.87, which is close to k^3=9.80. Thus, k fold increase in sample size implies approximately k^3 fold increase in operating time of the algorithm for a fixed m.

5. CONCLUSION

The *O(N)* parallel method of computing the log-Jacobian of the variable transformation for models with spatial interaction presented by Smirnov and Anselin [2009] is extremely effective for 3.0 GHz dual-processor with quad core - as was proved in the paper. It turned out sufficiently effective (due to the time of computation) even for standard PC for relatively big set of data typically used in geographical analysis. Thus the aforementioned method can be used in typical research without advanced hardware and software calculation support.

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METODA OBLICZANIA LOGARYTMU JAKOBIANU TRANSFORMACJI ZMIENNYCH W MODELACH PRZESTRZENNYCH - TEST I KOMENTARZE

Jednym z najważniejszych problemów w ekonometrii przestrzennej jest obliczenie logarytmu jakobianu transformacji zmiennych w modelach z interakcją przestrzenną. Wyznaczenie tego logarytmu jest konieczne przy estymacji modeli metodą największej wiarogodności i analizie Bayesowskiej modeli zależności przestrzennej (Smirnov i Anselin [2009]). Efektywność implementacji metody największej wiarogodności (ML) zależy od efektywności obliczeniowej logarytmu wyznacznika macierzy, w szczególności dla dużych i rzadkich macierzy. Drugim problemem jest dokładność obliczeń numerycznych logarytmu wyznacznika macierzy przekształcenia przy użyciu różnych metod, co wykazano w pracy Walde i in. [2008]. Problemy te spowodowały poszukiwania nowych metod szacowania modeli przestrzennych. Jedną z nich jest prostsza obliczeniowo uogólniona metoda momentów, ale bardziej restrykcyjna niż metoda największej wiarogodności (Lee [2004], [2007]). Innym rozwiązaniem jest dokonanie pewnych uproszczeń w oparciu o regularne kraty lub band matrices (Rue i Held [2005]).

W artykule przetestowano i skomentowano metodę obliczania logarytmu jakobianu przekształcenia zmiennych w modelach interakcji przestrzennych, zaproponowane przez Smirnova i Anselina [2009], na kilku praktycznych przykładach.