THE RIMINI CENTRE FOR ECONOMIC ANALYSIS

WP 10-22

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SENSITIVITY ANALYSIS OF SAR ESTIMATORS: A SIMULATION STUDY

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Sensitivity analysis of SAR estimators: A numerical approximation

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Abstract

The estimation of a spatial autoregressive (SAR) model depends on the spatial correlation parameter ρ in a highly non-linear way, and the least squares (LS) estimators for ρ cannot be computed in closed form. In this paper, we propose two simple LS estimators and we compare them by distance and covariance properties in order to study the local sensitivity behavior of these estimators. Using matrix derivatives we calculate the Taylor approximation of the least squares estimator in the spatial auto-regression (SAR) model up to the second order. In a next step we compare the covariance structure of the two estimators by Kantorovich inequalities and we derive efficiency comparisons by upper bounds. Finally, we explore the quality of our new approximations by a Monte Carlo simulation study. The simulation results show significant computation time reductions and a good approximation behavior of the SAR LS estimator in the neighborhood of $\rho = 0$, when using a non-spatial LS estimator. The results are encouraging and can be used for further developments, like quick diagnostic tools to explore the sensitivity of spatial estimators w.r.t. the size of the spatial correlation.

Key words: Spatial Autoregressive Models, Least-Squares Estimators, Sensitivity analysis, Taylor Approximations, Kantorovich Inequality.
JEL: C11, C15, C52, E17, R12.

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1 Introduction

Spatial auto-regression (SAR) models for the error covariance structure have been studied and applied to a wide range of areas in e.g. economics, demography, geography, biology, epidemiology, statistics and scientific modeling. See e.g. Anselin (1988, 1999), LeSage (1997), LeSage and Pace (2004, 2009), and LeSage and Polasek (2008). In recent years, sensitivity analysis for least-squares (LS) estimators have been developed for several models. One of the approaches to get such results is to use Taylor series to approximate the proposed estimator, as used e.g. in a repeated multivariate sampling model by Wang et al. (1994). To our knowledge, however, a sensitivity analysis for LS estimators in spatial models has not been reported.

In recent years, spatial models have become popular in applications, but little is known as how computations should be done. Classical estimators even for a simple SAR model can suffer from numerical computation problems, especially for large dimensional problems. For large cross sections the introduction of a spatial lag requires the inversion of the large spread matrix $R = I_n - \rho W$ (see below), which is of the dimension n, the number of observations. Thus it would be desirable to explore if simple approximations of spatial estimators can be found without inverting the spread matrix. Furthermore, such approximations can be useful for a Bayesian estimation with MCMC , like if we need a proposal density for a Metropolis step.

Popular estimators for the SAR model, that are available in the literature, are the maximum likelihood, the ordinary LS and the two-stage LS (2SLS) estimators. It was shown that the LS estimator is asymptotically consistent and efficient for row-normalized dense spatial matrices. The two-stage LS estimator proposed by Kelejian and Prucha (1998) is asymptotically consistent and computationally simple. LeSage and Pace (2009) give a good review on recent advances in the computation of spatial estimators, like the maximum likelihood and Bayesian estimators.

In this paper, we consider estimators for the SAR(1) model, i.e. a spatial model of order 1 and we are interested in the sensitivity analysis of the LS estimators in this model. The idea is to use a Taylor approximation with respect to the spatial correlation parameter ρ, similar to the approach of the repeated sampling model with unequal sample size that was studied by Wang et al. (1994). The variance matrix of the LS estimator of the SAR model is a non-linear function of the spatial autocorrelation parameter ρ. In this respect the SAR models are different from the repeated sampling model, where the LS estimator is a linear function of the correlation parameter. A numerical draw-back in the estimation of SAR models is that the spread matrix R (which is a function of the large spatial neighborhood matrix W) depends on ρ and needs to be inverted, which can be computationally challenging and time consuming. The question is if the matrix inversion can be avoided and do good approximations exist, and if so, what type of estimators and what approaches should be used?

First we propose the 'pseudo' LS estimator and we show that be expanded in a Taylor series around the non-spatial LS estimator of a linear regression model. Then we discuss how to measure the distance between the LS estimator and the first or second order Taylor approximation of the pseudo LS estimator. Finally, we show how the covariance matrix of these estimators can be evaluated by the Kantorovich inequality.

The structure of the paper is as follows. In section 2 we introduce the SAR model and the possible estimators. We continue with making sensitivity analysis and efficiency comparisons in section 3. The Taylor approximations of the estimators are established in section 4. The results are illustrated by a Monte Carlo simulation study in section 5. Finally we make some concluding remarks in section 6.

2 LS estimators in the SAR model

Let us consider here the following notation for SAR models, i.e. for the $n \times 1$ cross-sectional observations y of the form

$$y = \rho W y + X\beta + u, \quad u \sim N[0, \sigma^2 I_n], \tag{1}$$

where ρ is the spatial autocorrelation parameter (a scalar), W is a $n \times n$ spatial weight matrix normalized with row sums 1, β is a $n \times 1$ parameter vector, I_n is a $n \times n$ identity matrix, u is a $n \times 1$ error vector and follows a normal distribution with a $n \times 1$ mean vector centered at 0 and a $n \times n$ variance matrix $\sigma^2 I_n$.

The SAR model (1) can be written for known spatial autocorrelation ρ in the spatial filter (SF) form

$$Ry = X\beta + u, \quad u \sim N(0, \sigma^2 I_n). \tag{2}$$

By inversion of the spread matrix $R = I_n - \rho W$ we get the reduced form (RF) of the SAR model

$$y = R^{-1} X\beta + R^{-1} u = Z\beta + v, \quad v \sim N[0, \sigma^2 \Sigma(\rho) = \sigma^2 (R'R)^{-1}], \tag{3}$$

where the reduced form (RF) can be also written by the following transformed variables of the SAR model:

$$Z = R^{-1}X, \quad v = R^{-1}u. \tag{4}$$

The RF implies a heteroskedastic model with covariance matrix $Cov(y) = Cov(v) = \sigma^2\Sigma(\rho) = \sigma^2(R'R)^{-1}$. Obviously, the variance matrix of the reduced form $\Sigma = \Sigma(\rho)$ is a non-linear function of the spatial correlation parameter ρ. In the following we list the LS estimators for the β coefficients in the SAR models, which follow from the different ways of looking at the SAR model.

1. First, there is the ordinary LS (OLS) estimator of β if we set $\rho = 0$ in the SAR model (1). Thus, a $SAR(\rho = 0)$ model with no correlation is just the linear regression model $y = X\beta + u$ and is given by

$$b_0 = (X'X)^{-1}X'y. \tag{5}$$

The covariance matrix of this LS estimate is the same as in the ordinary regression model.

$$\begin{aligned} Cov(b_0) &= Cov[(X'X)^{-1}X'y] \\ &= \sigma^2(X'X)^{-1}X'Cov(y)X(X'X)^{-1} \\ &= \sigma^2(X'X)^{-1}. \end{aligned} \tag{6}$$

2. Second, conditionally on a known $\rho \in (-1, 1)$ and for row-normalized W, we find the spatial filter (SF) form (2) also known as the SF model $Ry \sim N[X\beta, \sigma^2 I_n]$ and we obtain the LS estimator b_r for β or in brief the SF-LS estimator

$$b_r = (X'X)^{-1}X'Ry. \tag{7}$$

This estimator b_r differs from the OLS estimator b_0 only by the spatial filter transformation Ry, which replaces the dependent variable y. The covariance matrix of this estimator is

$$\begin{aligned} Cov(b_r) &= Cov[(X'X)^{-1}X'Ry] \\ &= (X'X)^{-1}X'Cov(Ry)X(X'X)^{-1} \\ &= \sigma^2(X'X)^{-1}X'RR'X(X'X)^{-1} \end{aligned} \tag{8}$$

Note that $b_r = b_r(\rho)$ also reduces to the OLS estimator $b_0 = b_r(0)$ for $\rho = 0$, because $R = I_n$.

3. Third, we consider a 'pseudo' LS estimator b_z of β for the reduced form model (3). We estimate the model by LS but we ignore the covariance structure

$$b_z = (Z'Z)^{-1}Z'y = H^{-1}h \tag{9}$$

with the transformed (spatially filtered) regressors $Z = R^{-1}X$ (but untransformed y) and we define the two components

$$H = Z'Z = X'(RR')^{-1}X, \quad h = Z'y = X'R'^{-1}y. \tag{10}$$

The covariance matrix of this 'pseudo' LS estimator is

$$\begin{aligned} Cov(b_z) &= Cov[(Z'Z)^{-1}Z'y] \\ &= (Z'Z)^{-1}Z'Cov(y)Z(Z'Z)^{-1} \\ &= \sigma^2(Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1}, \end{aligned} \tag{11}$$

where we have used the correct covariance $Cov(y) = \sigma^2\Sigma$. In case of $\Sigma = I_n$ we have the result

$$Cov(b_z) = \sigma^2(Z'Z)^{-1}.$$

Note that $b_z = b_z(\rho)$ also reduces to b_0 for $\rho = 0$.

In addition, for the reduced form (RF) model (3) the correct GLS estimator b_{GLS} of β is given by

$$\begin{aligned} b_{GLS} &= (Z'\Sigma^{-1}Z)^{-1}Z'\Sigma^{-1}y = [Z'(R'R)Z]^{-1}Z'(R'R)y \\ &= (X'X)^{-1}X'Ry \\ &= b_r, \end{aligned} \tag{12}$$

which is the same as the LS of the SF model in (7). The covariance matrix of the GLS estimator is therefore

$$\begin{aligned} Cov(b_{GLS}) &= Cov(b_r) = \sigma^2(X'X)^{-1} \\ &= \sigma^2(Z'\Sigma^{-1}Z)^{-1}. \end{aligned} \tag{13}$$

Thus, it follows that ρ plays an important role for spatial modeling and estimation. The behavior of the estimators when the value of ρ changes around zero or the relationship between the estimators should be important information for spatial models. Therefore the sensitivity of the estimators with respect to ρ is studied in the next section.

3 Local SAR sensitivity analysis

For the local sensitivity analysis for the SAR models we will use the following estimators, which we summarize with their corresponding regression models:

- $b_0 = b_{OLS}$ is the LS estimator in the model $y = X\beta + u,\ u \sim N[0, \sigma^2 I_n]$. The covariance matrix is $Cov(b_0) = \sigma^2(X'X)^{-1}$.
- b_1 is the LS estimator in the spatial lag-1 model $Wy = X\beta + u,\ u \sim N[0, \sigma^2 I_n]$, the basic linear regression model explaining the spatial lag Wy. The covariance matrix is the same as before: $Cov(b_1) = \sigma^2(X'X)^{-1}$.
- b_r is the LS (or SF-LS) estimator in the spatial filter (SF) model $Ry = X\beta + u,\ u \sim N[0, \sigma^2 I_n]$, the linear regression model explaining the spatial filter Ry, where y is 'filtered' by the spread matrix $R = I_n - \rho W$. The covariance matrix is $Cov(b_r) = \sigma^2(X'X)^{-1}$.
- b_z is the 'pseudo' LS estimator in the reduced form (RF) model $y = Z\beta + v$ with $Z = R^{-1}X$ and instead of $v \sim N[0, \sigma^2\Sigma]$ we impose the uncorrelated error matrix $\Sigma = I_n$. The covariance matrix of the pseudo LS estimator is $Cov(b_z) = \sigma^2(Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1} = \sigma^2(Z'Z)^{-1}$.

3.1 Sensitivity analysis for the spatial filter estimator b_r

For the spatial filter (SF-LS) estimator b_r we find a simple linear relationship, which shows the difference to the LS estimator b_0.

Theorem 1 (The SF-LS estimator b_r) *The spatial filter (SF) estimator in the SAR model (conditional on ρ) is a linear combination of two simpler LS estimators*

$$b_r = b_0 - \rho(X'X)^{-1}X'Wy = b_0 - \rho b_1, \tag{14}$$

and therefore the squared distance of SF estimator b_r to the LS estimator b_0 is given by

$$||b_r - b_0||^2 = \rho^2 b_1' b_1 = \rho^2 y'W'X(X'X)^{-2}X'Wy. \tag{15}$$

Proof 1 *For the estimator b_r we can make the following substitutions*

$$\begin{aligned} b_r &= (X'X)^{-1}X'Ry \\ &= (X'X)^{-1}X'(I_n - \rho W)y \\ &= (X'X)^{-1}X'y - \rho(X'X)^{-1}X'Wy \\ &= b_0 - \rho(X'X)^{-1}X'Wy = b_0 - \rho b_1. \end{aligned}$$

We see that the difference between the OLS and the SF-LS estimator $b_0 - b_r = \rho b_1$ is proportional to the spatial parameter ρ and the 1^{st} order spatial lag-1 LS estimator b_1. Next, we want to find the derivative of b_r with respect to ρ, which measures actually the sensitivity of b_r upon a small change of ρ. For analytical and mathematical convenience, we use the differential notation which is mathematically equivalent to the derivative. The notation of the matrix calculus follows Magnus and Neudecker (1988/1999).

Theorem 2 (The derivative of the SF estimator b_r) *The derivative of the spatial filter b_r in (7) with respect to ρ is the negative LS estimator in the linear model for explaining the first order spatial lag:*

$$\partial b_r/\partial\rho = -(X'X)^{-1}X'Wy = -b_1. \tag{16}$$

Proof 2 *Using the result $b_r = b_0 - \rho b_1$ in (14), we get the differential of the b_r estimator with respect to ρ:*

$$db_r = -b_1 d\rho = -(X'X)^{-1}X'Wy d\rho.$$

By rearranging terms, we establish the derivative.

We can interpret this remarkable result that the direction of the first order correction is the OLS estimator with respect to the spatial neighbors. This results follows from the presence of the spread matrix R in the b_r estimator. The spread matrix can be interpreted as a correction of the identity matrix with respect to the neighborhood structure W of the cross section model. It is the direction of this 'covariance correction' that we get as the result of the differencing operation. Thus, a spatial lag-1 model explains the direction of the correction in a SAR model and is estimated by b_1. The spatial ρ is just the length of this direction.

For the pseudo LS estimator b_z we cannot get results that can be presented in a similar simple way. However, we will use the matrix differential technique and the Taylor approximation to get a similar result, as it is shown in the next subsection.

3.2 First order sensitivity analysis for the estimator b_z

This section gives the sensitivity of the pseudo LS estimator of the reduced form of the SAR model (3).

Theorem 3 (Sensitivity analysis of the pseudo LS estimator b_z) *The derivative of b_z with respect to ρ takes into account the transformed variables of the estimator*

$$\begin{aligned}\partial b_z/\partial\rho &= H^{-1}[\partial h/\partial\rho - (\partial H/\partial\rho)b_z)] \\ &= H^{-1}[X'R'^{-1}W'R'^{-1}y - (X'R'^{-1}(W'R'^{-1} + R^{-1}W)R^{-1}X)b_z] \\ &= H^{-1}[h_r - H_r b_z] \\ &= P \end{aligned} \tag{17}$$

with H given in (10) and we define the two auxiliary quantities

$$\begin{aligned} h_r &= X'R'^{-1}W'R'^{-1}y \quad \text{and} \\ H_r &= X'R'^{-1}(W'R'^{-1} + R^{-1}W)R^{-1}X. \end{aligned}$$

Proof 3 *For the sensitivity analysis of $b_z = H^{-1}h$, we need the differential of b_z with respect to ρ:*

$$\begin{aligned} d\ b_z &= (d\ H^{-1})h + H^{-1}(d\ h) \\ &= -H^{-1}(d\ H)H^{-1}h + H^{-1}d\ h \\ &= H^{-1}[d\ h - H^{-1}(dH)H^{-1}h] \end{aligned} \tag{18}$$

where we used differentials and partial derivatives that are given by

$$\begin{aligned} dR &= -W d\rho \\ dR^{-1} &= R^{-1}WR^{-1}d\rho \\ dR'^{-1} &= R'^{-1}W'R'^{-1}d\rho \\ dH &= d(X'R'^{-1}R^{-1}X) = X'(dR'^{-1})R^{-1}X + X'R'^{-1}(dR^{-1})X \\ &= X'R'^{-1}(W'R'^{-1} + R^{-1}W)R^{-1}X d\rho \\ \partial H/\partial\rho &= X'R'^{-1}(W'R'^{-1} + R^{-1}W)R^{-1}X \\ dh &= X'R'^{-1}W'R'^{-1}y d\rho \\ \partial h/\partial\rho &= X'R'^{-1}W'R'^{-1}y \end{aligned} \tag{19}$$

with the spread matrix $R = I_n - \rho W$.

Next we evaluate the derivatives at $\rho = 0$. Because the spread matrix $R(\rho = 0) = I_n$ reduces to the identity matrix, we get $H(\rho = 0) = X'X$ and

$$\begin{aligned} h_r(\rho = 0) &= X'R'^{-1}W'R'^{-1}y = X'W'y = h_0^r \\ H_r(\rho = 0) &= X'R'^{-1}(W'R'^{-1} + R^{-1}W)R^{-1}X = X'(W' + W)X = H_0^r. \end{aligned}$$

Note that $W' + W$ is symmetric and takes the role of a precision matrix.

Corollary 1 *For $\rho = 0$ we get the derivative for the uncorrelated case, denoted by $P(\rho = 0) = P_0$, which leads to the following expression:*

$$\begin{aligned} P_0 &= H^{-1}[h_r - H_r b_z] \\ &= (X'X)^{-1}[X'W'y - X'(W' + W)Xb_0]. \end{aligned} \tag{20}$$

Theorem 4 (Distance between the pseudo LS b_z and b_0 estimator) *The distance between the pseudo LS estimator b_z and the OLS estimator b_0 is given by*

$$||b_z - b_0||^2 = y'Vy, \tag{21}$$

where we have used the estimators $b_z = Z^+ y$, $b_0 = X^+ y$, *and the matrices* $V = Z'^+ Z^+ + X'^+ X^+ - Z'^+ X^+ - X'^+ Z^+$, $Z^+ = (Z'Z)^{-1} Z'$, *and* $X^+ = (X'X)^{-1} X'$.

Proof 4 *This follows by simplifications using the definitions of the estimators* b_z *in (9) and* b_0.

3.3 Second order sensitivity analysis for b_z

The second order local sensitivity derivative of the pseudo LS estimator (9) of the reduced form of the SAR model (3) is given in the next theorem.

Theorem 5 (The 2nd order sensitivity of the pseudo LS estimator b_z**)** *For the pseudo LS estimator* $b_z = H^{-1}h$ *in the reduced form model (3) we find*

$$\begin{aligned}
Q = & \partial^2 b_z/\partial\rho^2 \\
= & -H^{-1}(\partial H/\partial\rho)H^{-1}[\partial h/\partial\rho - (\partial H/\partial\rho)b_z] \\
& +H^{-1}[(\partial^2 h/\partial\rho^2) - (\partial^2 H/\partial\rho^2)b_z - (\partial H/\partial\rho)(\partial b_z/\partial\rho)] \\
= & -H^{-1}(\partial H/\partial\rho)H^{-1}[\partial h/\partial\rho - (\partial H/\partial\rho)b_z] \\
& +H^{-1}[(\partial^2 h/\partial\rho^2) - (\partial^2 H/\partial\rho^2)b_z] \\
& +H^{-1}(\partial H/\partial\rho)H^{-1}[(\partial H/\partial\rho)b_z - \partial h/\partial\rho] \\
= & -H^{-1}H_r H^{-1}[h_r - H_r b_z] \\
& +H^{-1}[h_{rr} - H_{rr} b_z] \\
& +H^{-1}H_r H^{-1}[H_r b_z - h_r]
\end{aligned} \tag{22}$$

with the second order derivatives $h_{rr} = \partial^2 h/\partial\rho^2$ *and* $H_{rr} = \partial^2 H/\partial\rho^2$.

Proof 5 *We compute the first differential* db_z *(of the pseudo LS estimator* $b_z = H^{-1}h$*) in (9) of Theorem 3 and get*

$$\begin{aligned}
d^2 b_z = & -H^{-1}(dH)H^{-1}[(dh) - (dH)H^{-1}h] \\
& +H^{-1}[(d^2 h) - (d^2 H)H^{-1}h - (dH)db_z] \\
= & -H^{-1}(dH)H^{-1}[(dh) - (dH)b_z] \\
& +H^{-1}[(d^2 h) - (d^2 H)b_z] \\
& +H^{-1}(dH)H^{-1}[(dH)b_z - (dh)].
\end{aligned} \tag{23}$$

From the differentials in (23), dh, dH *and* db, *we establish the derivative results using* $h_r = \partial h/\partial\rho$ *and* $H_r = \partial H/\partial\rho$ *as given above. Now we find*

$$
\begin{aligned}
\partial^2 h/\partial\rho^2 &= 2X'W'^2R'^{-2}y \\
&= h_{rr}, \\
\partial^2 H/\partial\rho^2 &= 2X'[W'^2R'^{-3}R^{-1} + W'R'^{-2}R^{-2}W + R'^{-1}R^{-3}W^2]X \\
&= H_{rr},
\end{aligned} \tag{24}
$$

where the last two equalities are obtained by using the differentials dh and dH, which are given in (19) above.

A simpler version of the second derivative for the case $\rho = 0$ is found in the following way: We compute the simplified second derivatives in (24) by

$$
\begin{aligned}
h_{rr}(\rho = 0) &= 2X'W'^2y \\
H_{rr}(\rho = 0) &= 2X'[W'^2 + W'W + W^2]X \\
&= 2X'W^{\oplus}X
\end{aligned} \tag{25}
$$

with the extended 'second order' weight matrix $W^{\oplus} = W'^2 + W'W + W^2$, which is symmetric.

Corollary 2 *With the simplified first order derivatives in (20) we get*

$$
\begin{aligned}
Q_0 &= Q(\rho = 0) \\
&= -H^{-1}H_rH^{-1}[h_r - H_rb_z] \\
&\quad +H^{-1}[h_{rr} - H_{rr}b_z] \\
&\quad +H^{-1}H_rH^{-1}[H_rb_z - h_r] \\
&= H^{-1}[h_{rr} - H_{rr}b_z] \\
&\quad +H^{-1}H_rH^{-1}[-h_r + H_rb_z + H_rb_z - h_r] \\
&= H^{-1}[h_{rr} - H_{rr}b_z] \\
&\quad +2H^{-1}H_rH^{-1}[H_rb_z - h_r] \\
&= (X'X)^{-1}[h_{rr} - H_{rr}b_0] \\
&\quad +2(X'X)^{-1}H_r(X'X)^{-1}[H_rb_0 - h_r] \\
&= 2(X'X)^{-1}[X'W'^2y - X'W^{\oplus}Xb_0] \\
&\quad +2(X'X)^{-1}X'(W' + W)X(X'X)^{-1}[X'(W' + W)Xb_0 - X'W'y].
\end{aligned} \tag{26}
$$

3.4 Efficiency comparisons

The results of the next theorem allow to obtain the main result for the comparison between the estimators b_z and b_r.

Theorem 6 (Kantorovich inequality for the b_z and b_r estimators) *The covariance matrices of the pseudo LS estimator b_z in (9) and the SF estima-*

tor b_r in (8) can be compared and establish the efficiency of b_z in terms of the covariance matrix of the b_r estimator: The difference-type bounds for the covariance matrices of the pseudo LS and the SF-LS estimators can be found for the following comparisons:

(1) For bounding the covariance matrix of the pseudo LS estimator b_z we find

$$Cov(b_r) \leq Cov(b_z) \leq k_1 Cov(b_r), \quad k_1 = \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1\lambda_n}; \tag{27}$$

(2) For bounding the difference of covariance matrices of the pseudo LS estimator b_z and the SF-LS estimator b_r we find

$$\Sigma_D = Cov(b_z) - Cov(b_r) \leq k_2\sigma^2(Z'Z)^{-1}, \quad k_2 = (\sqrt{\lambda_1} - \sqrt{\lambda_n})^2; \tag{28}$$

(3) For the determinant of the 'ratio of the covariance matrices:

$$|Cov(b_z)[Cov(b_r)]^{-1}| \leq k_3, \quad k_3 = \prod_{j=1}^{n} \frac{(\lambda_j + \lambda_{n-j+1})^2}{4\lambda_j\lambda_{n-j+1}}; \tag{29}$$

(4) For the trace of the 'ratio' of the covariance matrices:

$$tr\ Cov(b_z)[Cov(b_r)]^{-1} \leq k_4, \quad k_4 = \sum_{j=1}^{n} \frac{(\lambda_j + \lambda_{n-j+1})^2}{4\lambda_j\lambda_{n-j+1}}, \tag{30}$$

where $\lambda_1 \geq ... \geq \lambda_n > 0$ are the eigenvalues of the covariance matrix $R'R$.

k_1 is the covariance bound of the pseudo LS estimator, while k_2 is a "difference inefficiency" bound for the pseudo LS estimator. Alternatively, the constant k_1 can be interpreted as the least squares inefficiency bound, since it compares the reduced form estimator with the SAR spatial filter model, and k_2 is the upper bound for the difference between the two covariance matrices of b_z and b_r.
The constant k_3 is the determinant-ratio constant as it is the upper bound for the ratio of determinants, while k_4 is a trace-ratio constant since it is a bound for the trace of the 'ratio' of covariance matrices.

Proof 6 *The covariance matrices of the two estimators are given by $Cov(b_z) = \sigma^2(Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1}$ as in (11) and $Cov(b_r) = \sigma^2(Z'\Sigma^{-1}Z)^{-1}$ as in (8), where the transformed variables of the reduced form are given in (3). Comparing them we find $Cov(b_r) \leq Cov(b_z)$ due to the Cauchy-Schwarz inequality*

$$(Z'\Sigma^{-1}Z)^{-1} \leq (Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1},$$

and $Cov(b_z) \leq k_1 Cov(b_r)$ *due to the Kantorovich inequality*

$$(Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1} \leq k_1(Z'\Sigma^{-1}Z)^{-1},$$

where the constant k_1 *is given in (27). This constant* k_1 *was derived by using* $V = Z(Z'Z)^{-1/2}$ *and* $V'\Sigma V \leq k_1(V'\Sigma^{-1}V)^{-1}$*, for* $V'V = I$*; see e.g. Proposition 1 of Liu (1995, p. 48).*

$$\begin{aligned}
Cov(b_z) - Cov(b_r) &= \sigma^2(Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1} - \sigma^2(Z'\Sigma^{-1}Z)^{-1} \\
&= \sigma^2(Z'Z)^{-1/2}[(Z'Z)^{-1/2}Z'\Sigma Z(Z'Z)^{-1/2} \\
&\quad -((Z'Z)^{-1/2}Z'\Sigma^{-1}Z(Z'Z)^{-1/2})^{-1}](Z'Z)^{-1/2} \\
&\leq M = k_2\sigma^2(Z'Z)^{-1}
\end{aligned}$$

and the constant k_2 *is obtained from* $V'\Sigma V - (V'\Sigma^{-1}V)^{-1} \leq k_2 I$*, because* $V'V = I$ *with* $V = Z(Z'Z)^{-1/2}$*, see Liu and Neudecker (1994). Note that the difference is non-negative definite and the upper bound comes with* k_2*.*
The 2 'ratio'-constants k_3 *and* k_4 *are obtained in the following way:*

$$\begin{aligned}
Cov(b_z)[Cov(b_r)]^{-1} &= (Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1}Z'\Sigma^{-1}Z, \\
|Cov(b_z)[Cov(b_r)]^{-1}| &= |(Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1}Z'\Sigma^{-1}Z| \\
&= |(Z'Z)^{-1/2}Z'\Sigma Z(Z'Z)^{-1}Z'\Sigma^{-1}Z(Z'Z)^{-1/2}| \\
&\leq k_3, \qquad (31) \\
trCov(b_z)[Cov(b_r)]^{-1} &= tr(Z'Z)^{-1}Z'\Sigma Z(Z'Z)^{-1}Z'\Sigma^{-1}Z \\
&= tr(Z'Z)^{-1/2}Z'\Sigma Z(Z'Z)^{-1}Z'\Sigma^{-1}Z(Z'Z)^{-1/2} \\
&\leq k_4. \qquad (32)
\end{aligned}$$

The results of the inequalities (31) and (32) rely on the following inequalities $|V'\Sigma VV'\Sigma^{-1}V| \leq k_3$ *and* $tr(V'\Sigma VV'\Sigma^{-1}V) \leq k_4$*, for* $V'V = I$*, and these inequalities were shown e.g. in Theorem 1 in Liu (2000).*

Furthermore, we can derive an inequality for the difference of the covariance matrices for the point predictions of the pseudo LS and ordinary LS estimator, i.e. $y_z = Zb_z$ and $y_r = Zb_r$:

$$Cov(Zb_z) - Cov(Zb_r) \leq k_2\sigma^2 Z(Z'Z)^{-1}Z' \leq k_2\sigma^2 I_n.$$

Interestingly, k_2 is the same constant as given above and $Z(Z'Z)^{-1}Z' \leq I$ is known from linear regression theory. Thus, the increase in uncertainty or efficiency loss also turns over to the same type of efficiency loss if it comes to predictions with the pseudo LS or the SF estimator that are based on the SAR model.
Note that the constants k_1 and k_2 depend on the minimum and maximum eigenvalues of $R'R$, and therefore on the spread matrix R, which implies on ρ

and the neighborhood matrix W. The dependence on W increases if the eigenvalues of W start dominating the size of ρ. In fact, the constant k_1 depends on $(c+1)^2/4c$, where $c = \lambda_1/\lambda_n$ is the condition number of $R'R$.

Therefore any $R'R$ matrix that increases the condition number will increase the constant k_1. We see that the covariance matrix of the pseudo b_z estimator can be almost as good as the one of b_r (and therefore b_z can be 'almost as good' as b_r) if k_1 is close enough to one. In particular, the variances on the main diagonal of $\text{Cov}(b_z)$ have upper bounds by k_1 times the variances on the main diagonal of $\text{Cov}(b_r)$:

$$Var(b_z(i)) \leq k_1 Var(b_r(i)) \quad \text{for} \quad i = 1, ..., k, \tag{33}$$

where $b_z(i)$ and $b_r(i)$ are the elements of the vectors b_z and b_r.

Furthermore, we conclude that the covariance matrix of the pseudo LS estimator b_z can be almost as good as the b_r SF-LS estimator if the constant k_2 is close enough to zero. In particular, the differences of the variances on the main diagonal of $\text{Cov}(b_z)$ and $\text{Cov}(b_r)$ are upper bounded by k_2 times the main diagonal of $(Z'Z)^{-1}$ (apart from σ^2). Equivalently, the main diagonal of the difference of $\text{Cov}(Zb_z)$ and $\text{Cov}(Zb_r)$ is upper bounded by k_2, apart from σ^2. In other words, the efficiency loss of the point predictors is measured by the covariance matrices of the predictors and is at most k_2. Thus, k_2 can be interpreted as 'predictive efficiency loss' constant.

Since the difference is positive for all type of comparisons we conclude that the pseudo LS estimator comes (necessarily) with more uncertainty than the SF-LS estimator in the spatial filter model. Knowing that ρ can reduce the uncertainty of all the estimated regression coefficients, the result is independent of the way efficiency comparison is made. The unknown ρ blows up the correlation structure of the residuals, and this property creates additional heteroskedasticity and does not reduce the uncertainty in the covariance matrix.

We are interested how the above findings of the approximate SAR estimators can translate into the questions as how good are predictions that are made by approximate SAR estimators. Let z be a vector of known regressor values where we make the prediction with the estimator b of β by $\hat{y} = z'b$ then we have $Var(\hat{y}) = Var(z'b) = z'Cov(b)z$, and we look at the difference of the covariance matrices of the predictions made by b_z and b_r

$$\begin{aligned} Cov(z'b_z) - Cov(z'b_r) &= z'Cov(b_z)z - z'Cov(b_r)z \\ &= z'[Cov(b_z) - Cov(b_r)]z \\ &\leq z'Mz, \end{aligned} \tag{34}$$

where $M = k_2\sigma^2(Z'Z)^{-1}$ is the upper bound matrix of the difference $\Sigma_D = Cov(b_z) - Cov(b_r)$.

3.5 SAR-IV: LS estimation with instrumental variables

The instrumental variables (IV) estimator of the SAR model is based on the idea of a two stage least squares (2SLS) estimation of the rho parameter in a SAR based on the instrumental variables matrix $V = [W\hat{u}, W^2\hat{u}]$ with $\hat{u} = y - \bar{y}$. The motivation for the instruments come from the Taylor series expansion for R:

$$R^{-1} = I_n + \rho W + \rho^2 W^2 + ...$$

Using the IV projector $P_V = V(V'V)^{-1}V'$ we can define the SAR-IV estimator as the LS estimator of ρW in the auxiliary model

$$y = \rho P_V W y + u, \quad u \sim N[0, \sigma^2 I_n] \tag{35}$$

leading to the estimator

$$\rho_{IV} = (Z'Z)^{-1}Z'y \quad with \quad Z = [1_n, P_V W y]. \tag{36}$$

A further alternative is to use a biased estimate $\hat{\rho} = y'W'P_V y / y'W'P_V W y$ with $\hat{u} = y - \hat{\alpha} - \hat{\rho} P_V W y$ or to use the implied ρ estimate of Moran's I. A spatial autocorrelation coefficient was defined as ρ_{CO} by Cliff and Ord (1981), while the OLS estimator ρ_{OLS} and Moran's $I : \rho_I$ are defined as

$$\rho_{CO} = (u'Wu)/((u'u) * (u'W'Wu))^{1/2} - (u'Wu)/(u'W'Wu), \tag{37}$$

$$\rho_I = (u'Wu)/(u'u), \tag{38}$$

$$\rho_{OLS} = (u'Wu)/(u'W'Wu), \tag{39}$$

while the ML is adjusted by the Jacobian.

4 Taylor approximation for the SAR estimator

This section develops a Taylor approximation for the SAR estimator. Based on the first and second order derivative results for the pseudo LS estimator b_z of the SAR model from the previous section we develop the Taylor expansion of the pseudo LS estimator around the OLS location $b_0 = b_z(\rho = 0)$ by the mean value theorem of calculus (see Magnus and Neudecker 1988/1999, p. 113). The twice differentiable function is given by

$$\phi(c+u) = \phi(c) + d\phi(c;u) + d^2\phi(c+\theta u;u)/2 \quad \text{for } \; 0<\theta<1,$$

where the first order differential is given by $d\phi(c;u) = (db_z)\rho$ and the second order differential is $d^2\phi(c+\theta u;u) = (d^2b_z)\rho^2$. In our case c in the ϕ function denotes the point of the OLS location ($\rho = 0$) and u denotes the value of the ρ parameter, evaluated around 0.

$$b_z(\rho) = b_0 + (db_z/d\rho)\rho + (d^2b_z/d\rho)\rho^2\theta/2, \quad \text{for } \; 0<\theta<1, \tag{40}$$

and the first and second order differentials, db_z and d^2b_z, are given in Theorems 3 and 5, respectively.

4.1 First and second order Taylor approximation for SAR models

This section develops the Taylor approximation for the SAR model.

Theorem 7 (First and second order Taylor approximation for b_z) *The first order Taylor approximation of the pseudo LS estimator $b_z(\rho)$ around the OLS location $b_0 = \hat{\beta}$ is:*

$$b_z(\rho) = b_0 + P_0\rho + O(\rho^2) \tag{41}$$

with P_0 given in (20). The 2nd order Taylor approximation for the SF-LS estimator b_z around the OLS location $b_0 = \hat{\beta}$ is given by

$$b_z(\rho) = b_0 + P_0\rho + Q_0\rho^2/2 + O(\rho^3), \tag{42}$$

where the vectors P_0 and Q_0 are as given in (20) and (26), respectively. They are the first and second order derivatives (obtained in Theorems 3 and 5), evaluated at the uncorrelated case $\rho = 0$.

Proof 7 *: The result is obtained by plugging (17) and (22) into (40).*

5 Monte Carlo Results

In this section we demonstrate the sensitivity analysis of the spatial filter LS estimator (SF-LS) b_r and the pseudo LS estimator (PLS) b_z in a Monte Carlo study. As these estimators involve the a priori unknown parameter ρ, we use the Moran's I related estimate of this parameter given in equation (38). First, we compare the two introduced estimators to the existing 2SLS estimator of Kelejian and Prucha (1998) and a maximum likelihood estimator using sparse matrix algorithms programmed by LeSage and Pace (2009) in terms of computational time. In a second step, we analyze the distances, derivatives and Kantovorich inequality measures.

For the Monte Carlo experiment, we generated SAR data according to

$$y = \rho W y + \beta X + u, \quad u \sim N[0, \sigma^2 I_n], \tag{43}$$

with I_n being a $n \times n$ identity matrix, and the matrix of explanatory variables X of dimension $n \times 2$ is given by

$$X = (I_n - \phi W)^{-1} u_2,$$

with u_2 being a $n \times 2$ matrix of uniformly distributed random numbers in $U[0, 1]$. We fix the coefficients at $\beta = (1, 2)$ for each run and we draw u_2 once for all replications for a given ϕ value and a fixed W matrix. The correlation between the regressors is set to $\phi = 0.33$ and the R^2 to 0.05. The dependent variable is constructed by

$$y = (I_n - \rho W)^{-1}(X\beta + u_1\sqrt{s})),$$

where u_1 is a $n \times 1$ uniformly distributed random variable, and S is

$$S = (1 - R^2)/R^2 * Var(I_n - \rho W)^{-1} X\beta)^{-1}/Var((I_n - \rho W)^{-1} u).$$

We compare the computation time between the SF-LS, pseudo LS, ML and 2SLS estimators for sample sizes $n = [50, 250, 750, 1500, 3000]$. As a spatial weight matrix W_{11} we use a simple one forward, one behind based neighborhood scheme that has well known properties. The computation time for different sample size n is displayed (in seconds) in Table 1. The computational experiment was done without Monte Carlo runs, so the values in the Table indicate the seconds of an estimation run [1]. In terms of computation time, the spatial filter least squares (SF-LS) estimator performs best followed by the pseudo least squares (PLS) estimator. Comparing the IV estimator to the SF-LS for a sample size of 3,000, the SF-LS only takes only a fraction of 1/500 the time of the IV estimator.

[1] An Intel(R) Core(TM) i5-2410M CPU with 2.30 GHz and 4 GB of RAM was used for computation with Matlab 7.10.

Table 1
Computational time of estimators by sample size (n)

n	IV	ML	pseudo LS	SF-LS
50	0.0780	0.0150	0.0001	0.0001
250	0.0780	0.0150	0.0002	0.0001
750	0.0940	0.0310	0.0003	0.0002
1,500	0.1250	0.0470	0.0008	0.0004
3,000	0.2500	0.0780	0.0009	0.0005

Legend: n denotes the sample size e.g. the number of regions, $W = W_{11}$, $\rho = 0.3$.

Table 2
Computational time of estimators by sparseness, $n = 3,000$

sparseness	IV	ML	pseudo LS	SF-LS
0.99	0.2500	0.0780	0.0009	0.0005
0.98	1.8090	0.5000	0.0826	0.0048
0.90	8.1430	2.0600	0.3577	0.0209
0.80	16.5360	3.9310	1.3782	0.0424

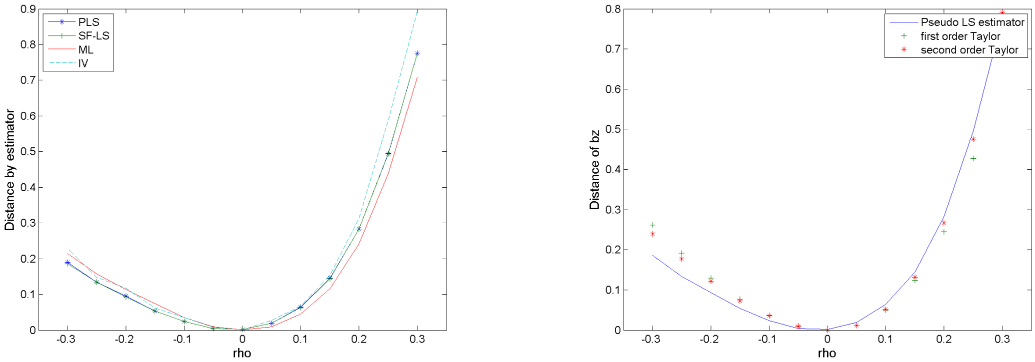
Legend: Sparseness is the number of zero entries in W, $\rho = 0.3$.

Table 1 shows the computational time for $n = 3,000$ samples for different degrees of sparseness of W, i.e. the number of zero entries in W. For the most dense spatial neighborhood we find a fraction of the computational time of the SF-LS estimator compared to the IV of 1/390. The sparse matrix algorithm using ML estimator takes up 92 times the computational time of the SF-LS.

To simulate the distances in (7) and (9) for the estimators, the Kantorovich measures in (27) to (30) and the derivatives of the estimator b_z given in (17), (20), (22) and (26), we varied ρ through an interval of $[-0.3, 0.3]$ in steps of 0.05.

First, we compare the distances of the two estimators in (7) and (9) to the ML and 2SLS estimators, respectively. For this simulation we used the one forward, one behind neighborhood structure (in matrix W_{11}) for a sample of $n = 250$ regions. For each ρ we ran 1,000 replications, took the averages of the beta estimates and computed the distances according to (15) and (21). As can be seen in Figure 1 (right), the bias with respect to the OLS beta estimate increases in ρ and has a asymmetric shape around the origin. The reason for this result is that the spatial dependence in the spread matrix can be expanded in a Neumann series $(I_n - \rho W)^{-1} = \sum_{i=0}^{\infty} \rho^i W$, where even powers of negative ρ's cancel out and creat the bias towards the OLS estimate. The proof for this asymmetric property is given in the Appendix.

Fig. 1. Distances: (left) ML, IV, SF-LS, PLS to β_{OLS}; (right) PLS, 1^{st} and 2^{nd} Taylor



Legend: Mean of 1,000 Monte Carlo trials with $W = W_{11}$.

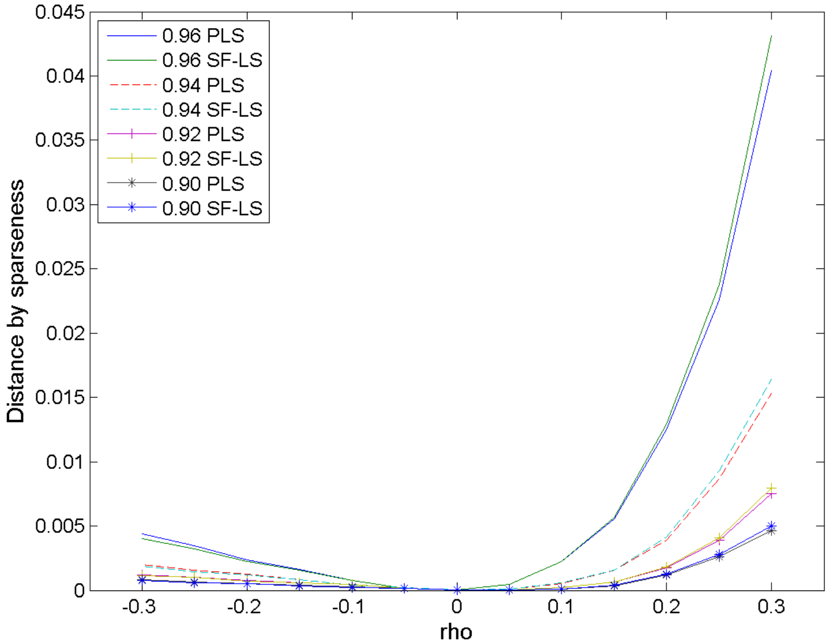
Figure 1(right) shows the distance between the pseudo LS estimator and the first and second order Taylor approximation given in (41) and (42). The PLS estimator and the Taylor series approximations show good approximations to the β_{OLS} estimate in terms of distances. Again, we see the asymmetric shape around the origin.

In a next step, we compare the distances of the b_z and b_r estimators between different degrees of sparseness of the spatial weight matrix. For this exercise, we constructed 4 spatial weight matrices based on the nearest neighborhood (matrices denoted by W_{nn}) concept. For a fixed sample size of $n = 250$ regions, a higher number of neighbors is associated with a denser (and thus less sparse) matrix. We decided for $nn = [10, 15, 20, 25]$ neighbors, corresponding to a share of zeros of $0.96, 0.94, 0.92, 0.90$, respectively. To construct the nearest neighbors based on Euclidian distances, we took geographical coordinates of the Pace and Barry (1997) data set on presidential election in 3,107 US counties. The results are shown in Figure 2. It can clearly be seen that the denser a matrix the lesser the distance of both the SF-LS and the PLS beta estimator to the OLS beta estimate, a result that is in line with Lee (2002).

Next, we analyze the derivatives of the estimator b_z given in (17), (20), (22) and (26). The results of the Monte Carlo experiment with $1,000$ replications is shown in Figures 3 (left) and (right). In Figure 3, the first order derivative, denoted by P, declines as ρ increases. For the case $\beta_2 = 2$, the double value of $\beta_1 = 1$, we see a much steeper decline. The first order derivative evaluated at $\rho = 0$ is shown in Figure 3(right). Again we find a declining pattern as ρ increases. Figures 4 (left) and (right) show the second order derivatives of b_z denoted by Q and Q_0 for the case $\rho = 0$. For the second derivative given in Figure 4, β_2 has an inverse U-shaped pattern as ρ increases. Evaluated at $\rho = 0$ the second order derivative shows a flat decline in increasing ρ.

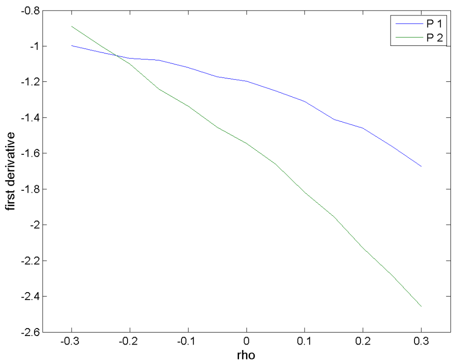
Finally, we examine the the Kantorovich inequality measures for ρ's around

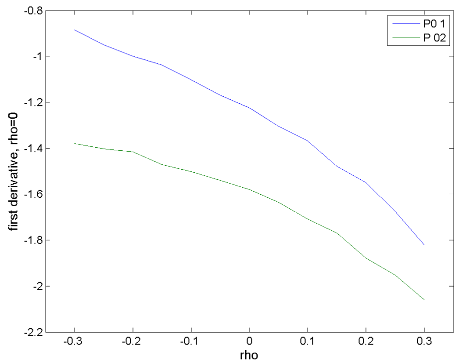
Fig. 2. Pseudo LS and SF-LS distance to β_{OLS} by sparseness ($W_{nn}, nn = [10, 15, 20, 25]$)



Legend: Mean of 1,000 Monte Carlo trials.

Fig. 3. (left) $P_0 : 1^{st}$ order derivative b_z; (right) $P_0 : 1^{st}$ order derivative $b_z, \rho = 0$

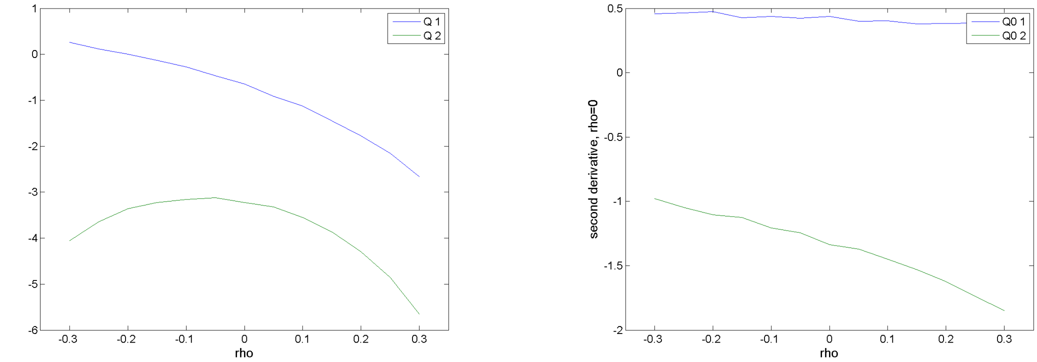




Legend: Mean of 1,000 Monte Carlo trials with $W = W_{11}$.

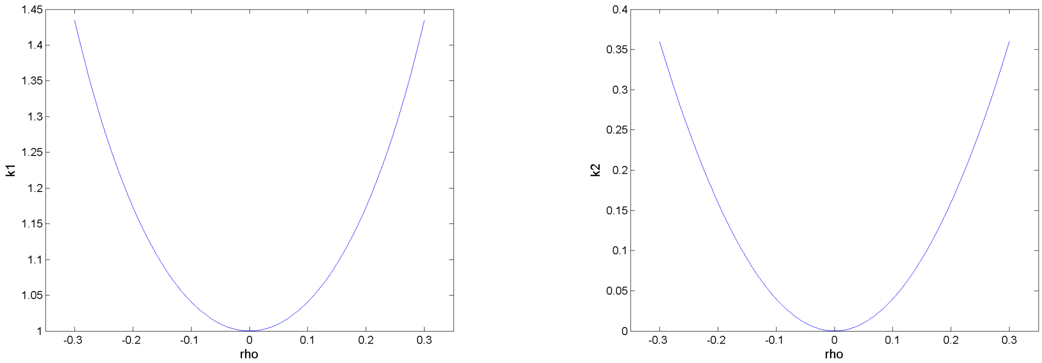
zero. As these measures solely depend on the eigenvalues of the covariance matrix $R'R$, no Monte Carlo (MC) trials are needed. The results are given in Figures (5) to (6). All figures show a symmetric U-shaped pattern, centered around the origin of $\rho = 0$, where the estimators collapse to the OLS estimator.

Fig. 4. (left): Q (2^{nd} derivative) of b_z; (right): Q_0 (2^{nd} derivative) of $b_z, \rho = 0$



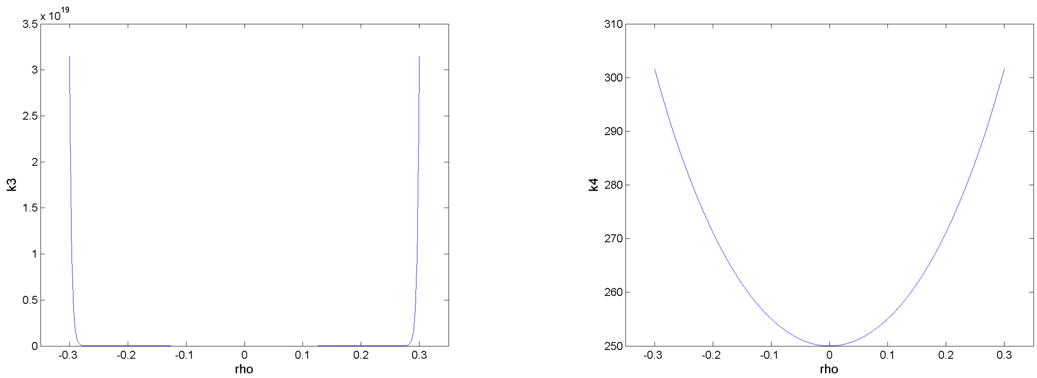
Legend: Mean of 1,000 Monte Carlo trials with $W = W_{11}$.

Fig. 5. (left): k_1-bounds of b_z and b_r; (right): k_2 diff-bounds of b_z and b_r



Remarks: $W = W_{11}$.

Fig. 6. (left): k_3 diff-bounds of b_z and b_r; (right): k_4 cov-trace of b_z and b_r



6 Conclusions

In this paper we have derived several results for the sensitivity analysis of the LS estimators for the spatial autoregressive (SAR) model. We used new results on the Kantorovich inequality to establish the quality of the approximation with respect to the difference of the covariance matrices. The main goal was to find the Taylor approximation with respect to ρ in the SAR model, and to measure the difference of the ordinary LS estimator to the pseudo LS estimator, which is non-linear function in ρ.

In a simulation analysis we have shown that: the Taylor approximation of the LS estimator of the SAR model gives a good approximation results for small ρ's up to ± 0.3. The efficiency loss according to the Kantorovich inequality is about 50%, if ρ approaches the range ± 0.3. These values were found in Monte Carlo simulation study for $n = 250$ and a one forward, one behind neighborhood scheme.

There is an interesting result that needs further research: The approximation results are encouraging since they allow good first step approximations for non-linear LS methods or can be used as a proposal densities in the Metropolis step of a MCMC algorithm. An open question is if other or better approximations can be found for medium or large ρ values.

Acknowledgements

The research was conducted when Wolfgang Polasek visited Shuangzhe Liu at University of Canberra and when Shuangzhe Liu took his OSP leave. The authors are grateful to Matthias Koch, the Editor and the referees for their constructive remarks and suggestions on an early version of the paper.

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APPENDIX: On the asymmetric behavior of the approximation

Let the data generating process defined by

$$Y = \rho_0 WY + X\beta_0 + \epsilon,$$

with ρ_0 and β_0 being the true values. The OLS estimate of β is

$$\hat{\beta}_{OLS} = (X'X)^{-1}X'y$$

and the expectation of $\hat{\beta}_{OLS}$ is

$$\begin{aligned} E[\hat{\beta}_{OLS}] &= \beta_0 + E[\rho_0(X'X)^{-1}X'WY] \\ &= \beta_0 + \rho_0(X'X)^{-1}X'W(I-\rho_0 W)^{-1}X\beta_0. \end{aligned}$$

The difference between β_0 and $\hat{\beta}_{OLS}$ is

$$\begin{aligned} bias(\rho_0) &:= (\beta_0 - \hat{\beta}_{OLS}) \\ &= \rho_0 (X'X)^{-1} X'W(I - \rho_0 W)^{-1} X\beta_0 \\ &= \rho_0 (X'X)^{-1} X'W \sum_{k=0}^{\infty} \rho_0^k W^k X\beta_0, \end{aligned}$$

where a symmetric bias around zero would satisfy

$$|bias(\rho_1) - bias(-\rho_1)| = 0.$$

However, the symmetry of the bias is given by

$$\begin{aligned} |bias(\rho_1) - bias(-\rho_1)| &= |\rho_1 (X'X)^{-1} X'W \sum_{k=0}^{\infty} \rho_1^k W^k X\beta_0 \\ &\quad - \rho_2 (X'X)^{-1} X'W \sum_{k=0}^{\infty} \rho_2^k W^k X\beta_0| \\ &= |\rho_1 (X'X)^{-1} X'W \sum_{k=0}^{\infty} \rho_1^k W^k X\beta_0 \\ &\quad + \rho_1 (X'X)^{-1} X'W \sum_{k=0}^{\infty} (-\rho_1)^k W^k X\beta_0| \\ &= |\rho_1 (X'X)^{-1} X'W \sum_{k=0}^{\infty} (\rho_1^k + (-\rho_1)^k) W^k X\beta_0| \\ &= |\rho_1| |\sum_{k=0}^{\infty} (\rho_1^k + (-\rho_1)^k)(X'X)^{-1} X'WW^k X\beta_0| \\ &= |\rho_1| |\sum_{k=0}^{\infty} (\rho_1^k + (-\rho_1)^k) x_k|, \end{aligned}$$

with $x_k = (X'X)^{-1} X'W^{k+1} X\beta_0$. If $X = \iota_n$ and W ist row-normalized, then $x_k = \beta_0$ and

$$
\begin{aligned}
|bias(\rho_1) - bias(-\rho_1)| &= |\rho_1\beta_0|| \sum_{k=0}^{\infty}(\rho_1^k + (-\rho_1)^k)| \\
&= |\rho_1\beta_0||1 + 1 + \rho_1 - \rho_1 + \rho_1^2 + \rho_1^2 + \rho_1^3 - \rho_1^3 + ...| \\
&= 2|\rho_1\beta_0|| \sum_{k=0}^{\infty} \rho_1^{2k}| \\
&= 2|\rho_1\beta_0|| \sum_{k=0}^{\infty} \rho_1^{2k}| = \frac{2|\rho_1\beta_0|}{1 - |\rho_1^2|}.
\end{aligned}
$$

Thus, the difference between the bias of a ρ and a $-\rho$ is expected to increase by approximately $\frac{2|\rho_1|}{1-|\rho_1^2|}$ with increasing $|\rho|$.