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Lukas Dargel and Christine Thomas-Agnan

Efficient estimation of spatial econometric interaction models for sparse OD matrices

Lukas Dargel ^{1,2} and Christine Thomas-Agnan ¹

¹Toulouse School of Economics, University of Toulouse Capitole, France

²BVA Group, France

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Abstract

In the framework of spatial econometric interaction models for origin-destination flows, we develop an estimation method for the case when the list of origins may be distinct from the list of destinations, and when the origin-destination matrix may be sparse. The proposed model resembles a weighted version of the one of LeSage and Pace (2008) and we are able to retain most of the efficiency gains associated with the matrix form estimation, which we illustrate for the maximum likelihood estimator. We also derive computationally feasible tests for the coherence of the estimation results and present an efficient approximation of the conditional expectation of the flows, marginal effects and predictions.

Keywords: spatial econometric interaction models, zero flow problem

JEL Codes: C21 C51

1 Introduction

Spatial interaction models describe interaction behavior that occurs between a set of origins and a set of destinations. Some typical applications for this model are international trade flows between countries, passenger flows between cities, or geomarketing flows of customers who reside in the districts of a city and who visit the stores of a brand. Traditionally, this type of problem has been formulated in terms of the gravity equation, which assumes the size of the flow to increase in proportion to the mass of the origins and destinations and to decrease in proportion to the distance. Some examples for mass variables are the size of the population, or the surface area of a store. The success of the gravity equation can be explained by its intuitive simplicity and its high ability to explain the observed data in empirical applications. Also the criticism that these models describe macro-level behavior without foundation in individual actions has been overcome (see for example Wilson 1967; Bergstrand 1985). One legitimate concern, however, arises from the fact that most gravity models rely on independently distributed data to provide efficient and unbiased parameter estimates and predictions. In the context of interaction behavior, this independence assumption is usually untenable and has been refuted by empirical evidence in very diverse applications, such as public transport Kerkman, Martens, and Meurs (2018), air-passengers transport Margaretic, Thomas-Agnan, and Doucet (2017), home-to-work commuting Dargel (2021), international trade Fischer and LeSage (2020), migration Chun and Griffith (2011), or social interactions Wang et al. (2018).

LeSage and Pace (2008) propose a spatial econometric interaction model that explicitly models spatial dependence in origin-destination (OD) flows. Their model is particularly appealing because it can be estimated using a matrix representation of the flows, which reduces the dimension of most objects we need to manipulate during the estimation from N to \sqrt{N} , where N represents the number of OD pairs. For spatial econometric models this reduction may be critical in making the difference whether the model is computationally feasible in large data sets or not. However, to attain this efficiency gains the model of LeSage and Pace (2008) relies on two conditions that reduce its applicability to real-world data. The first condition requires that the set of origins coincides with the set of destinations and excludes, for example, geomarketing applications. The second condition requires that we actually observe interaction behavior for all possible OD pairs. This constraint becomes more difficult to satisfy in practice, as data sets with high spatial resolutions are increasingly frequent. Some examples of high resolution flow data sources are GPS tracking, smart-card data for public transport networks, or interactions in social networks. In such data sources the aggregation level is much lower, making the abundance of zero flows more likely, and often the norm. The issue of abundant zero flows has recently been raised again by Laurent, Margaretic, and Thomas-Agnan (2022b), who model bilateral remittances. They solve this issue by restricting the model to a subset of the potential OD pairs. However, they use a vectorized estimation approach, which does not benefit from the efficiency gains of the matrix formulation.

In this article we present a generalization to the matrix form estimator of the spatial econometric interaction model that extends the version of LeSage and Pace (2008) in two ways. The new method applies to cases where the list of origins may be different from the list of destinations, and where the model can be restricted to any subset of all potential OD pairs. To do so, we develop a modeling framework that treats flows as interactions between the nodes of spatial networks, and derive new properties of Kronecker products that allow to include weights in the previous version of the matrix form estimator.

The previously mentioned issue of missing entries in the OD matrix is linked to the well known zero flow problem, as unobserved flows may be considered as implicitly reflecting zero values. When the number of such zeros is large, the normality assumption is clearly violated, and alternative models, such as Tobit or zero inflated Poisson regression, have been proposed

to accommodate the excess zeros. Burger, Oort, and Linders (2009) reviews and compares such methods in the context of international trade flows, but without specific focus on spatial dependence. Krisztin and Fischer (2015) extend the zero inflated Poisson model of trade flows by spatial filtering (Griffith 2003), which addresses the problem of biases in the parameter estimates due to spatial correlation. However, the main drawback of spatial filtering is that spatial dependence is treated as a nuisance, which means that we lose the ability to quantify spillover effects (Pace, Lesage, and Zhu 2013). There exist models that simultaneously account for excess zeros and explicitly model spatial dependence, such as the Tobit models put forward by LeSage and Pace (2009) and Xu and Lee (2015) or the family of models for spatially correlated limited dependent variables developed in Liesenfeld, Richard, and Vogler (2016), but it is clear that computational constraints make these approaches less feasible for big data environments. Unlike the previous methods, the model presented here maintains the hypotheses of gaussian data by only considering the subsample of OD pairs related to observed flows. It is easy to appreciate the computational advantage of this procedure, but we have to be aware that the obtained results do not generalize to the unobserved OD pairs. This would only be possible if the flows were missing at random, which is hard to justify in our context as unobserved flows are most often linked with high distances. While, this is certainly a drawback of the model here, it might be the better compromise if the alternative is ignoring spatial dependence altogether. Moreover, Linders and Groot (2006) find that the omission of zero flows yields results surprisingly similar to those of a model that accounts for sample selection, and much better than Tobit models or gaussian models in which the unobserved values are imputed by a constant.

The structure of the article is as follows: the next section introduces the origin-destination flow problem from the perspective of interactions between networks and develops the generalized version of the model. Section 3 presents the matrix form estimation for the MLE. The final section concludes.

2 A generalized framework for spatial interaction models

In this section we present origin-destination flows from the perspective of pairwise interactions between the nodes of an origin network and those of a destination network. Within this framework we distinguish for the cases of square and rectangular flows. An example of the square case is international trade, where the origin network as well as the destination network correspond to the countries of the world. A typical rectangular example arises when modeling customer flows in geomarketing. Here the origin network contains residential zones and the destination network are the stores of a brand. In addition to the classification into rectangular and square, we differentiate the cartesian from the non-cartesian case, as has been proposed by Laurent, Margaretic, and Thomas-Agnan (2022b). The former applies when all possible interactions are actually observed, implying that the number of OD pairs correspond to the cartesian product of all origins with all destinations. When some of the possible OD pairs are unobserved we are in the non-cartesian case. This additional separation becomes especially relevant if we want to use the efficiency gains provided by the matrix formulation of the model.

Notations and definition of cases

π_o : origin network

π_d : destination network

n_o : number of nodes in the origin network

n_d : number of nodes in the destination network

OW : $n_o \times n_o$ neighborhood matrix of the origin network

DW : $n_d \times n_d$ neighborhood matrix of the destination network

\mathcal{F} : the set of all potential OD pairs $\mathcal{F} = \{(o_j \rightarrow d_i) : j = 1, 2, \dots, n_o, i = 1, 2, \dots, n_d\}$

Γ : the subset of OD pairs that are actually included in the model $\Gamma \subseteq \mathcal{F}$

N : the total number of OD pairs $N = n_o \cdot n_d = \text{card}(\mathcal{F})$, where card is the cardinality

N^* : the number of OD pairs included in the model $N^* = \text{card}(\Gamma)$

Using the above notations we formalize the distinction in our cases. The **square case** treats flows within the same network $\pi_o = \pi_d$, which implies $n_o = n_d$ and $OW = DW$. In the **rectangular case** we treat flows between two distinct networks $\pi_o \neq \pi_d$. The **cartesian case** applies when we model all theoretically possible OD pairs $\Gamma = \mathcal{F}$, yielding $N^* = n_o \cdot n_d = N$. In contrast, the **non-cartesian case**, applies when we model a strict subset of all potential OD pairs $\Gamma \subset \mathcal{F}$, which leads to $N^* < n_o \cdot n_d = N$.

An illustrative example

To illustrate the different cases let us consider two networks π_1 and π_2 , whose number of nodes are n_1 and n_2 . The matrix \mathbf{Y}_\diamond , with dimensions $(n_2 + n_1) \times (n_2 + n_1)$, represents all possible pairwise interactions between nodes that belong to any of the two networks. We may then group these interactions into four sub-matrices

$$\mathbf{Y}_\diamond = \begin{pmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{pmatrix}, \quad (1)$$

where the flows within the network π_1 are represented by $Y_{11}(n_1 \times n_1)$ and those within the network π_2 by $Y_{22}(n_2 \times n_2)$. Similarly, flows that connect the nodes of π_2 with those of π_1 are contained in $Y_{12}(n_1 \times n_2)$, and the flows connecting the nodes both networks in the other direction in $Y_{21}(n_2 \times n_1)$. Hence, if we model a diagonal block in (1) we are in the square case and for the off-diagonal ones we are in the rectangular case. Whether we observe all values in the sub-matrix then defines if the case is cartesian or not.

Differentiating the square from the rectangular case is trivial when the separation of nodes into two distinct subsets of the network set of nodes is already given, but in practice such considerations may be up to the definition of the researcher. Our advise regarding this issue is to consider the potential neighborhood links between all of the observations. Separating origins and destinations into two nodes subsets is appropriate if neighborhood relations within each subset are conceivable but not between the two. Hence, in such a case, the neighborhood matrix of all observations should have the form

$$\mathbf{W}_\diamond = \begin{pmatrix} W_1 & \mathbf{0} \\ \mathbf{0} & W_2 \end{pmatrix}, \quad (2)$$

where the matrices $W_1(n_1 \times n_1)$ and $W_2(n_2 \times n_2)$ capture the neighborhood relations between the nodes the networks π_1 and π_2 . When it is not possible to defend the zero matrices on the off-diagonal blocks in (2) we should probably treat all observations as part of the same network and consider the case as square. In geomarketing applications the separation is apparent from the fact that the origins (residential areas) are conceptually different from the destinations (stores). When this conceptual distinction is not possible we could also use geographical arguments for such a separation as for example when modeling investment flows from the United States to the Chinese provinces.

2.1 The cartesian model

To define the spatial econometric interaction model we need to fix the role of the origin and destination networks. Within the formalism of the previous example this choice corresponds to setting $\pi_o = \pi_j$ and $\pi_d = \pi_i$ for one pair of $i, j = 1, 2$. Given the roles of each network we may extract the part of the interaction matrix we want to model $Y = Y_{ij}$ and define the neighborhood matrix of the origins $OW = W_j$ and that of the destinations $DW = W_i$. These neighborhood matrices OW and DW should have only non-negative entries, a zero diagonal. We further consider them to be similar to a symmetric matrix and have spectral radius, that is the eigenvalues with largest absolute value, of one. In practice, these conditions are met if we use matrices based on pairwise distances or contiguity, and normalize them by row or with respect to their spectral radius. When all OD pairs are included in the model we may use the Kronecker product \otimes to derive three OD neighborhood matrices from the node-level neighborhood matrices.

$$\begin{aligned} W_d &= I_{n_o} \otimes DW & W_o &= OW \otimes I_{n_d} & W_w &= OW \otimes DW \end{aligned} \quad (3)$$

In the model W_o represents origin-based dependence, W_d represents destination-based dependence and W_w represents origin-to-destination dependence. Definition (3) of these three matrices makes clear that if we model interaction within the same network ($\pi_o = \pi_d$), we find that $OW = DW := W$, which recovers the traditional framework of LeSage and Pace (2008). We use these three matrices in conjunction with the three autoregression parameters $\rho = (\rho_d \ \rho_o \ \rho_w)$ to define the spatial filter matrix ($A = I_N - \rho_d W_d - \rho_o W_o - \rho_w W_w$). This matrix can be used to remove spatial autocorrelation from the flow vector $y = \text{Vec}(Y)$, which we obtain by stacking the columns of the flow matrix. If we relate the spatially filtered flows to linear combination of some exogenous variables $Z(N \times K)$ and a gaussian error $\varepsilon \sim \mathcal{N}(0, \sigma^2 I_N)$

$$Ay = Z\delta + \varepsilon \quad (4)$$

we obtain a spatial lag (LAG) model, where we follow the terminology of Elhorst (2010). In Section 3 we present the Z matrix in detail, but for the introduction of the model in its vectorized form the current definition suffices. It is also important to note that the above model is only well defined if the inverse of the filter matrix exists, an issue that will be treated in Section 3.3.

2.2 The non-cartesian model

Model (4) has the disadvantage that we can only use it when we actually observe all values in the flow matrix. In practice, this condition is rarely fulfilled, especially if we want to model flow data with a high spatial resolution. To clarify this issue let us consider an origin network with three nodes $\pi_o = \{o_1, o_2, o_3\}$ and a destination network with two nodes $\pi_d = \{d_1, d_2\}$, where flows from o_1 to d_2 and from o_3 to d_1 are theoretically possible but unobserved.

$$Y = \begin{pmatrix} y_{o_1 \rightarrow d_1} & y_{o_2 \rightarrow d_1} & \times \\ \times & y_{o_2 \rightarrow d_2} & y_{o_3 \rightarrow d_2} \end{pmatrix}, \quad (5)$$

It may be tempting to replace missing entries in the flow matrix by zeros and go on with model (4), but this would introduce a point-mass at zero, invalidating the normality assumption. To avoid this inconsistency, we prefer to drop the unobserved flows and create a truncated flow vector of the form

$$y^* = (y_{o_1 \rightarrow d_1} \quad y_{o_2 \rightarrow d_1} \quad y_{o_2 \rightarrow d_2} \quad y_{o_3 \rightarrow d_2})'. \quad (6)$$

This truncated flow vector only contains the subset of OD pairs we want to include in the model. We then define the part of the spatial filter matrix $A^*(N^* \times N^*)$ and the explanatory variables

$Z^*(N^* \times K)$ that correspond to the same subset of OD pairs to define a model for the truncated sample

$$A^*y^* = Z^*\delta + \varepsilon^*, \quad (7)$$

where the error is supposed to be gaussian $\varepsilon^* \sim \mathcal{N}(0, \sigma^2 I_{N^*})$. We can link the matrices of the above non-cartesian model to those of the cartesian model in (4), by means of the selection operator $S_\Gamma(N \times N^*)$. The effect of this operator on a matrix or vector is to drop the columns or rows at the position of the OD pairs, for which we do not observe interaction data.

$$A^* = S_\Gamma' A S_\Gamma \quad Z^* = S_\Gamma' Z \quad y^* = S_\Gamma' y \quad (8)$$

For the example considered in (5) and (6) the selection operator and the flow vector $y = \text{Vec}(Y)$ would be

$$S_\Gamma = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad y = \begin{pmatrix} y_{o_1 \rightarrow d_1} \\ \times \\ y_{o_2 \rightarrow d_1} \\ y_{o_2 \rightarrow d_2} \\ \times \\ y_{o_2 \rightarrow d_2} \end{pmatrix}.$$

It is easy to verify that the selection operator satisfies $S_\Gamma' S_\Gamma = I_N^*$ and $S_\Gamma S_\Gamma' = R_\Gamma$, where R_Γ replaces the unobserved flows in y with zeros instead of removing them. We can derive this replacement operator explicitly from a binary matrix of the observed flows, which is equal to one if a flow is observed and zero if it is not. Denoting this flow indicator matrix \mathcal{I}_Γ the relationship is $R_\Gamma = \text{Diag}(\text{Vec}(\mathcal{I}_\Gamma))$, where the Diag operator places a vector on the main diagonal of a zero matrix. Below we illustrate these matrices for our previous example.

$$\mathcal{I}_\Gamma = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \quad \text{Vec}(\mathcal{I}_\Gamma) = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \\ 0 \\ 1 \end{pmatrix} \quad R_\Gamma = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

3 Matrix form estimation in the general case

This section derives the matrix form estimator for the non-Cartesian model in (7), where we focus on the maximum likelihood estimator (MLE) for a LAG model. Extensions to a Spatial Durbin Model and to Bayesian Markov-Chain Monte-Carlo or spatial two-stage least squares estimators could be derived without much difficulty, using the arguments of Dargel (2021). The likelihood of the non-cartesian model is

$$\mathcal{L}(\rho, \delta, \sigma^2) = \left(\frac{1}{2\pi\sigma^2} \right)^{N^*/2} \exp \left\{ \frac{1}{2\sigma^2} (A^*y^* - Z^*\delta)' (A^*y^* - Z^*\delta) \right\} |A^*|. \quad (9)$$

In the following four subsections we treat different parts of the estimation problem. The first one deals with methods that allow to efficiently evaluate the quadratic term $RSS(\rho, \delta) = (A^*y^* - Z^*\delta)' (A^*y^* - Z^*\delta)$. The next section deals with the log-determinant term $\log |A^*|$ that appears in the log-likelihood function. In the third subsection we discuss the issue of the feasible parameter space and in the last one we present a computationally efficient way to approximate the conditional expectation of the flows.

3.1 Second order moments matrix calculation

One key to the efficient estimation of the spatial econometric interaction model is to express the quadratic term in the likelihood function in terms of low dimensional moment matrices that are independent of the parameters. In what follows we first present some well-known and some new properties of Kronecker products, that allow to avoid computations with high-dimensional objects. Afterwards, we will treat the three moments that appear after expanding the quadratic term

$$RSS(\rho, \delta) = y^{*'} A^{*'} A^* y^* + \delta' Z^{*'} Z^* \delta - 2\delta' Z^{*'} A^* y^*. \quad (10)$$

We refer to the first part of the RSS term in (10) as uncentered TSS-moment because it offers an analogy to the analysis of variance formula. Using $\tau(\rho)' = (1 \quad -\rho_d \quad -\rho_o \quad -\rho_w)$, and $y_{\bullet} = (R_{\Gamma} y \quad W_d R_{\Gamma} y \quad W_o R_{\Gamma} y \quad W_w R_{\Gamma} y)$, we can factorize the TSS-moment into

$$y^{*'} A^{*'} A^* y^* = \tau(\rho)' y'_{\bullet} R_{\Gamma} y_{\bullet} \tau(\rho). \quad (11)$$

The 4×4 matrix in the middle of the factorization $TSS_{\bullet} = y'_{\bullet} R_{\Gamma} y_{\bullet}$ only depends on the data. Hence, it needs to be computed once and can then be used to quickly reevaluate the term for changing values of ρ . Based on the definition of the OD-level neighborhood matrices in (3) and the properties K1, K2, K4 in Appendix A, we compute the elements of the TSS_{\bullet} matrix for $l, k = 1, 2, 3, 4$ as

$$TSS_{\bullet kl} = \iota'_{n_d} (Y^{(k)} \odot \mathcal{I}_{\Gamma} \odot Y^{(l)}) \iota_{n_o}, \quad (12)$$

where $Y^{(1)} = (\mathcal{I}_{\Gamma} \odot Y)$, $Y^{(2)} = DW(\mathcal{I}_{\Gamma} \odot Y)$, $Y^{(3)} = (\mathcal{I}_{\Gamma} \odot Y)OW'$ and $Y^{(4)} = DW(\mathcal{I}_{\Gamma} \odot Y)OW'$.

The second moment is given by $Z^{*'} Z^* = Z' R_{\Gamma} Z$. For centered data, it is proportional to the variance-covariance matrix of Z^* . To exploit the benefits of the matrix form estimation we have to pay attention to the structure of the variables that are contained in the matrix Z . For our model we suppose that $Z = (\iota_N \quad X_d \quad X_o \quad g)$ is composed of four sets of variables¹, where ι_N is a constant, X_d contains the characteristics of the origins, X_o those of the destinations and g is a vector characteristics for OD-pairs. In classical gravity models, this g vector reflects the geographic distance, but we could use more general measures of separation between origins and destinations, possibly several of them. The variables in Z can be expressed as functions of the network-level data $OX(n_o \times k_o)$, $DX(n_d \times k_d)$ and a matrix representation of the OD-characteristics $G(n_d \times n_o)$.

$$\begin{aligned} \iota_N &= \iota_{n_o} \otimes \iota_{n_d} & X_d &= \iota_{n_o} \otimes DX \\ g &= \text{Vec}(G) & X_o &= OX \otimes \iota_{n_d} \end{aligned} \quad (13)$$

Given the above structure of the matrices in Z and the definition of the replacement operator $R_{\Gamma} = \text{Diag}(\text{Vec}(\mathcal{I}_{\Gamma}))$, we can use the Kronecker product properties developed in Appendix A to derive the elements of the variance moment as

$$Z^{*'} Z^* = \begin{bmatrix} N^* & & & & \\ \bullet & \iota'_{n_o} \mathcal{I}'_{\Gamma} DX & & \iota'_{n_d} \mathcal{I}'_{\Gamma} OX & \iota'_{n_d} (\mathcal{I}'_{\Gamma} \odot G) \iota_{n_o} \\ \bullet & DX' \text{Diag}(\iota'_{n_o} \mathcal{I}'_{\Gamma}) DX & & DX' \mathcal{I}'_{\Gamma} OX & DX' (\mathcal{I}'_{\Gamma} \odot G) \iota_{n_o} \\ \bullet & \bullet & & OX' \text{Diag}(\iota_{n_d} \mathcal{I}_{\Gamma}) OX & OX' (\mathcal{I}'_{\Gamma} \odot G) \iota_{n_d} \\ \bullet & \bullet & & \bullet & \iota'_{n_d} (G \odot \mathcal{I}_{\Gamma} \odot G) \iota_{n_o} \end{bmatrix}. \quad (14)$$

¹Many extensions to the spatial econometric interaction model correspond to additional sets of variables in the matrix Z . We may, for example, use the spatial lags $W_d X_d$ and $W_o X_o$ as additional variables, to extend the LAG model considered in this article to a Spatial Durbin model.

For centered data, the moment $Z'R_\Gamma y_\bullet$ is proportional to the empirical covariances of the explanatory variables and the spatial lags of the flow vector. This moment appears when we factor out the autocorrelation parameters from the third part of the RSS term in (10) using the same notations as in (11) and we get

$$2\delta' Z^{*'} A^* y^* = 2\delta' Z' R_\Gamma y_\bullet \tau(\rho).$$

The result in the above formula is a product of a matrix $Z'R_\Gamma y_\bullet$ of small dimension with the parameter vectors on each side. In the following we reuse definition (12) of $Y^{(t)}$, for $t = 1, 2, 3, 4$ to derive $y^{(t)} = \text{Vec}(Y^{(t)})$, and to compute the elements of each column of the moment $Z'R_\Gamma y_\bullet$ as

$$Z'R_\Gamma y^{(t)} = \begin{bmatrix} \iota_{n_d}(\mathcal{I}_\Gamma \odot Y^{(t)})\iota_{n_o} \\ DX'(\mathcal{I}_\Gamma \odot Y^{(t)})\iota_{n_o} \\ OX'(\mathcal{I}'_\Gamma \odot Y^{(t)})\iota_{n_d} \\ \iota'_{n_d}(G \odot \mathcal{I}_\Gamma \odot Y^{(t)})\iota_{n_o} \end{bmatrix}. \quad (15)$$

3.2 Determinant calculation

In this section we treat the problem of evaluating the determinant term that appears in the likelihood function in (9). Evaluating this term based on classical decomposition methods such as the LU, QR, or Cholesky factorization would require $\mathcal{O}(N^*{}^3)$ operations, which may be prohibitive in large sample applications. This issue is well known in the spatial econometrics literature, and to address it we adapt an existing approximation method to model (7). The underlying idea was first proposed by Martin (1992) and later adjusted to the spatial econometric interaction model by LeSage and Pace (2008) and Fischer and LeSage (2020), who use it in the square and cartesian cases.

The general form of the approximation is derived from a Taylor series expression of the log-determinant term

$$\ln |A^*| = \ln |I_{N^*} - W_F^*| = - \sum_{t=1}^{\infty} \frac{\text{tr}(W_F^{*t})}{t}, \quad (16)$$

where the matrix W_F^* contains the weight matrices and the autoregression parameters. If all eigenvalues of W_F^* are less than one in magnitude the series in (16) converges and we can use the first m terms to approximate the log-determinant.

For the model considered in this article $W_F^* = \rho_d W_d^* + \rho_o W_o^* + \rho_w W_w^*$, which means that we have to compute the trace of t^3 matrix products to evaluate the term t in the series (16). For an approximation of order m this leads to an overall number of $1^3 + 2^3 + \dots + m^3$ matrix products. One big advantage of this approximation is that we can factor the parameters ρ_d, ρ_o and ρ_w out of the traces of the matrix products that emerge from $\text{tr}((\rho_d W_d^* + \rho_o W_o^* + \rho_w W_w^*)^t)$. However, even a single evaluation of the traces of these products of potentially large matrices may significantly augment computational cost and memory requirement of the estimation. This holds especially for high values of t , as the matrix products involved become increasingly dense, even when the original matrices W_d^*, W_o^* and W_w^* are sparse. In Appendix B we simplify the computations for the fourth order approximation of the determinant. These simplifications reduce the number of required matrix products from $1^3 + 2^3 + 3^3 + 4^3 = 120$ down to 10, but their evaluation may remain a computational blocking point for large scale applications.

If we are willing to use the second order approximation the computational issues can be completely overcome. In this case, only the three trace values $\text{tr}(W_d^* W_d^*)$, $\text{tr}(W_o^* W_o^*)$ and $\text{tr}(W_w^* W_w^*)$

are non-zero. By using the links $W_r^* = S'_\Gamma W_r S_\Gamma$, for $r = d, o, w$, and some of the new Kronecker product properties in Appendix A, we obtain these values with only $\mathcal{O}(n_o) + \mathcal{O}(n_d)$ operations

$$\begin{aligned}\text{tr}(W_d^* W_d^*) &= \iota'_{n_d} \{ \mathcal{I}_\Gamma \odot [(DW \odot DW') \mathcal{I}_\Gamma] \} \iota_{n_o} \\ \text{tr}(W_o^* W_o^*) &= \iota'_{n_d} \{ \mathcal{I}_\Gamma \odot [\mathcal{I}_\Gamma (OW \odot OW')] \} \iota_{n_o} \\ \text{tr}(W_w^* W_w^*) &= \iota'_{n_d} \{ \mathcal{I}_\Gamma \odot [(DW \odot DW') \mathcal{I}_\Gamma (OW \odot OW')] \} \iota_{n_o}.\end{aligned}\tag{17}$$

In the cartesian case, we can achieve a similar performance even for higher order approximations. Here we have $W_F^* = \rho_d W_d + \rho_o W_o + \rho_w W_w$. We may then notice that the three matrices W_d , W_o and W_w represent a commuting family, which means that for any matrix product that only involves a subset of these matrices the multiplication order is irrelevant. This allows to compute the values of the traces of W_F^t for $t = 1, 2, \dots, m$ from a multinomial expansion of the form

$$\text{tr}(W_F^t) = \sum_{k_d+k_o+k_w=t} \rho_d^{k_d} \rho_o^{k_o} \rho_w^{k_w} \binom{t}{k_d+k_o+k_w} \text{tr} \left(W_d^{k_d} W_o^{k_o} W_w^{k_w} \right).\tag{18}$$

We may further use the fact that $W_o W_d = W_d W_o = W_w$, allowing to simplify the trace of the matrix products in the above expression by

$$\text{tr}(W_d^{k_d} W_o^{k_o} W_w^{k_w}) = \text{tr}(W_d^{k_d+k_w} W_o^{k_o+k_w}).\tag{19}$$

The Kronecker product structures of $W_d = I_{n_o} \otimes DW$ and $W_o = OW \otimes I_{n_d}$ then allow to express the above trace in terms of the traces of powers of the much smaller node level neighborhood matrices

$$\text{tr}(W_d^{k_d+k_w} W_o^{k_o+k_w}) = \text{tr}(OW^{k_o+k_w}) \text{tr}(DW^{k_d+k_w}).\tag{20}$$

3.3 Considerations about the feasible parameter space

The issue of the feasible parameter space is recurrent in the spatial econometrics literature and relates to the fact that model (7) is incoherent when the spatial filter matrix A^* is singular. This condition imposes constraints on the autoregression parameters. Dargel (2021) discusses this issue in the context of the cartesian and square flows and develops an efficient method to check the coherence of the model. In this subsection we extend this method first to the rectangular and cartesian case and then to the general case.

For the cartesian and rectangular case, the filter matrix is given by $A = I_N - W_F$, with $W_F = \rho_d(I_{n_o} \otimes DW) + \rho_o(OW \otimes I_{n_d}) + \rho_w(OW \otimes DW)$. The necessary and sufficient condition for A to be non singular is that all its eigenvalues are different from zero. As this condition is too hard to work with in practice, we use the sufficient, but more restrictive, alternative that the spectral radius $r(W_F)$ is smaller than one. Using the developments in Appendix C we can write the eigenvalues vector of $\lambda(W_F)$ of W_F in terms of $\lambda(DW)$ and $\lambda(OW)$

$$\lambda(W_F) = \rho_d(\iota_{n_o} \otimes \lambda(DW)) + \rho_o(\lambda(OW) \otimes \iota_{n_d}) + \rho_w(\lambda(OW) \otimes \lambda(DW)).\tag{21}$$

This representation clearly shows that we can test the condition $r(W_F) < 1$ without having to construct W_F explicitly. Furthermore, to infer $r(W_F)$, we do not require to compute the full spectrum of OW and DW , but only their smallest and largest eigenvalue (for more details see

Dargel 2021). We refer to these two extreme eigenvalues as λ_{max} and λ_{min} . When OW and DW are sparse these eigenvalues can be computed with only $\mathcal{O}(n_d) + \mathcal{O}(n_o)$ operations, using for example the implicitly restarted Arnoldi method of Sorensen (1992) or the Krylow-Schur algorithm of Stewart (2002).

It is obvious that equation (21) does not hold in the non-cartesian case, as we loose the Kronecker product structure of the spatial filter matrix A^* . Consequently, the eigenvalues of A^* cannot be directly expressed as a function of those of the matrices OW and DW . However, we can show that the previous test for non-singularity of A still allows to conclude that the non-cartesian model is coherent. To do so, let us first recall the definition of the spatial filter matrix in the non-cartesian case $A^* = I_{N^*} - W_F^*$. We may then note that $W_F^* = S'_\Gamma W_F S_\Gamma$ is a principal sub-matrix of W_F , which is evident from the fact that the indices of the rows and columns removed by the selection operator are identical. When W_F is symmetric, so is W_F^* , which allows us to recursively apply Cauchy's eigenvalue interlacing theorem (see for example Horn and Johnson 2012, page 242) to conclude

$$\lambda_{min}(W_F) \leq \lambda_{min}(W_F^*) \quad \text{and} \quad \lambda_{max}(W_F^*) \leq \lambda_{max}(W_F). \quad (22)$$

In Appendix C.2, we demonstrate that the relations also hold for the case of W_F matrices which are not necessarily symmetric but similar to a symmetric matrix. In particular, this extends to the case of row-normalized symmetric matrices. The inequalities (22) clearly show that constraints placed on the eigenvalues of W_F are more binding than those placed on the eigenvalues of W_F^* . Hence, a condition that ensures the coherence of the cartesian model remains sufficient for the coherence of its non-cartesian versions.

3.4 Expectation, Impacts and Predictions

In this subsection we describe some techniques to efficiently compute the conditional expectation, marginal effects and predictions.

3.4.1 Expectations

Another practical concern is the computation of the conditional expectation of the value of the flows $\mathbb{E}[y^*|Z^*] = A^{*-1}Z^*\delta$. We need this expectation to compute predictions (see for example Goulard, Laurent, and Thomas-Agnan 2017) and to evaluate the impact measures of LeSage and Thomas-Agnan (2015). Since the direct computation of A^{*-1} is often not feasible we will use an approximation based on a series expression of the inverse matrix. For a standard spatial model this approximation is already suggested by LeSage and Pace (2009, page 111) and we will adapt it to the spatial interaction model and derive its matrix form expression.

Let us first recall that the inverse of a matrix may be derived as $A^{*-1} = \sum_{t=0}^{\infty} (I - A^*)^t$, which is a converging series if the spectral radius of A^* is inferior to one. This expression allows to approximate the conditional expectation without the need to compute an inverse.

$$\mathbb{E}[y^*|Z^*] \approx \sum_{t=1}^m (W_F^*)^t Z^* \delta \quad (23)$$

With some further restructuring we can also bypass computing the powers of W_F^* . This is done based on the recursive expression $z_{t+1} = W_F R'_\Gamma z_t$, for $t = 0, 1, \dots, m - 1$ that we derive from

$$\mathbb{E}[y^*|Z^*] \approx \sum_{t=0}^m (S'_\Gamma W_F S_\Gamma)^t S'_\Gamma Z \delta = S'_\Gamma \sum_{t=0}^m z_t, \quad (24)$$

where the starting point of the sequence $z_o = Z\delta$ corresponds to a vectorized representation of the signal. We then denote by \mathcal{Z}_t the matrix version of $z_t = \text{Vec}(\mathcal{Z}_t)$, which entails further dimension reductions of our calculations.

$$\begin{aligned} \text{Vec}(\mathcal{Z}_{t+1}) &= W_F R_\Gamma \text{Vec}(\mathcal{Z}_t) \\ &= (\rho_d W_d + \rho_o W_o + \rho_w W_w) \text{Diag}(\text{Vec}(\mathcal{I}_\Gamma)) \text{Vec}(\mathcal{Z}_t) \\ &= \text{Vec}(\rho_d DW(\mathcal{I}_\Gamma \odot \mathcal{Z}_t) + \rho_o(\mathcal{I}_\Gamma \odot \mathcal{Z}_t)OW' + \rho_d DW(\mathcal{I}_\Gamma \odot \mathcal{Z}_t)OW') \end{aligned} \quad (25)$$

The final approximation is $\mathbb{E}[y^*|Z^*] \approx \sum_{t=0}^m S'_\Gamma \text{Vec}(\mathcal{Z}_t)$, and for a fixed order m its quality depends on the values of the autoregressive parameters. When their magnitude is small the terms of the series will quickly tend to zero and for stronger autocorrelation the higher order terms become more important.

3.4.2 Impacts

We can use the same technique to infer the marginal impact of changes in the explanatory variables. A same variable may enter the model multiple times, for example when using the population and its spatial lag for the origins and the destinations. This fact makes the direct derivative computation with respect to a given variable complex thus we propose the following factorization of the effect of changes in the data on the conditional expectation

$$\frac{\partial \mathbb{E}[y^*|z^*]}{\partial \mathcal{D}} = \frac{\partial \mathbb{E}[y^*|z^*]}{\partial z^*} \cdot \frac{\partial z^*}{\partial \mathcal{D}} = A^{*-1} \Delta_{z^*}, \quad (26)$$

where $\Delta_{z^*} = \frac{\partial z^*}{\partial \mathcal{D}}$ captures how the non-cartesian version of the signal $Z^*\delta$ changes if the input data is altered. From (26), it is fairly simple to compute Δ_{z^*} in practice as we only need to alter the input data and subtract the previous signal from the new one. Given the change in the signal we can use the methods of the previous section to approximate the impact that any variation in the input data has on the flows. Additionally, if these variations only concern few observations the change in signal can be represented by a sparse matrix which accelerates the computations.

As usual for spatial models this impact is different for all observations and to ease the interpretation it is possible to use the summary measures that have been proposed in the literature. For changes in variables that describe OD pairs (e.g. distance, or travel time) we recommend the traditional summaries, that is a total effect which can be decomposed into network effect and direct effect. For variables that describe the origins or the destinations, the summaries as well as their decomposition proposed by LeSage and Thomas-Agnan (2015) and further developed in Laurent, Margaretic, and Thomas-Agnan (2022a) are more adapted.

3.4.3 Predictions

Predictions for spatial autoregressive models have been studied by Goulard, Laurent, and Thomas-Agnan (2017), who use the optimality criterion of Goldberger (1962) to develop the best predictor (BP) for spatial econometric models. In the following we call in sample-predictors those that are feasible based on knowledge of the sample only, and full-sample predictors are those that require knowledge of the neighborhood structure and the explanatory variables for the entire population. At first this seems to be a harsh requirement, but in the case of interaction models it is often met, since most explanatory variables and the neighborhood structure are derived from node-level information. A third family of predictors should be developed for the case of changes in the underlying population, as for example when adding a new shop in a network of stores. However, such an extrapolation requires to anticipate changes in the neighborhood structure of the original population, which is not a topic in the scope of the current article.

For the three in-sample predictors presented in (27) below, Goulard, Laurent, and Thomas-Agnan (2017) have shown the following ranking $\hat{y}^{*BPI} > \hat{y}^{*TS} > \hat{y}^{*TC}$, indicating that \hat{y}^{*BPI} has the smallest and \hat{y}^{*TC} the largest prediction error. The trend corrected predictor \hat{y}^{*TC} corresponds to the conditional expectation $\mathbb{E}(y^*|X)$, whose calculation in matrix form is presented in Section 3.4.1. The predictors \hat{y}^{*TS} and \hat{y}^{*BPI} reduce the prediction error by additionally using information on y for all other observations. When the values of X change, this becomes a problem for \hat{y}^{*TS} because the observed values of y may no longer be valid. The trend-signal predictor \hat{y}^{*TS} goes back to Haining (1990) and the in-sample best predictor \hat{y}^{*BPI} is the one of Goulard, Laurent, and Thomas-Agnan (2017) for the LAG models. It is originally presented as a correction on \hat{y}^{*TC} , that uses additional information contained in the residuals $y - \hat{y}^{*TC}$. The correction term is defined in terms of the precision matrix $Q^* = \frac{1}{\sigma^2}(A^*{}'A^*)$ and the matrix $D_{Q^*} = Q^* \odot I_N$ in which all elements outside the main diagonal of Q^* are zero.

$$\begin{aligned}
\hat{y}^{*TCI} &= \hat{A}^{*-1}Z^*\hat{\delta} \\
\hat{y}^{*TS} &= \hat{\rho}_d W_d^* y^* + \hat{\rho}_d W_d^* y^* + \hat{\rho}_d W_d^* y^* + Z^* \hat{\delta} \\
\hat{y}^{*BPI} &= \hat{y}^{*TC} - D_{Q^*}^{-1}(Q^* - D_{Q^*})(y^* - \hat{y}^{*TC}) \\
&= y^* - D_{Q^*}^{-1} \hat{A}^{*'}(y^* - \hat{y}^{*TS})
\end{aligned} \tag{27}$$

In the last line of (27) we derive an alternative form for \hat{y}^{*BPI} that presents it as a correction on the observed values y^* , involving a residual based on \hat{y}^{*TS} . This has a clear computational advantage since we do not require \hat{y}^{*TC} that is defined in terms of inverse \hat{A}^{*-1} . In Appendix D we show how the matrix formulations for \hat{y}^{*TS} and \hat{y}^{*BPI} can be used to compute them efficiently.

Before entering into the details of the full population predictors we need to define the notions of sample and population more rigorously, as different sets of observations. For the spatial interaction model considered in this article these sets have the following relations $\Gamma_{sample} \subseteq \Gamma_{pop} \subseteq \mathcal{F}$, where all previous results were based on the assumption that the population is entirely observed in our sample $\Gamma = \Gamma_{sample} = \Gamma_{pop}$. If we are only concerned with parameter estimation, and in-sample predictors the distinction between the sample and the population is not necessary, but when predicting new observations we need to be acutely aware of the difference between these sets. In the following we develop predictors for the case where we want to extrapolate from the observed sample to the all possible OD-pairs, implying $\Gamma = \Gamma_{sample} \subset \Gamma_{pop} = \mathcal{F}$. Generalizations for the case where $\Gamma_{pop} \subseteq \mathcal{F}$ would not be much more complicated, though more tedious. (In this case we would have to introduce an additional population selector $S_{\Gamma_{pop}}$ that disappears under $\Gamma_{pop} = \mathcal{F}$, since $S_{\mathcal{F}} = I_N$).

The trend signal predictor depends on the observed values of y , meaning that it cannot be used for extrapolations, unless there is only a single unit to predict. The trend corrected predictor $\hat{y}^{*TC} = \hat{A}^{-1}Z\hat{\delta}$ should be based on the filter matrix for the full population. Even for in-sample units this leads to different predictions $\hat{y}^{*TCI} \neq S_{\Gamma}\hat{y}^{*TC}$. This inequality is due to the non-linearity of the inverse $\hat{A}^{*-1} = (S_{\Gamma}\hat{A}S_{\Gamma})^{-1} \neq S'_{\Gamma}\hat{A}^{-1}S_{\Gamma}$. For the same reason the impact measures should change when we consider the population to be larger than the sample. Indeed, one should also be aware that using \hat{A}^{*-1} entails the implicit assumption that the unobserved part of the population does not affect the sample. To derive a full population version of the best predictor we combine the in-, and out-of-sample versions of Goulard, Laurent, and Thomas-Agnan (2017) leading to

$$\hat{y}^{BP} = R_{\Gamma}(y + D_{Q^*}^{-1}QS_{\Gamma}(y^* - S'_{\Gamma}\hat{y}^{*TC}) + (I - R_{\Gamma})(\hat{y}^{*TC} + Q^{-1}R_{\Gamma}QS_{\Gamma}(y^* - S'_{\Gamma}\hat{y}^{*TC})). \tag{28}$$

The first term associated with R_Γ is based on the formula of \hat{y}^{*BPI} in (27), where \hat{y}^{*TCI} is replaced by its population version \hat{y}^{TC} . The second term associated with $(I - R_\Gamma)$ corresponds to the prediction for the unobserved part of the population. Its main computational challenge is the inversion of the precision matrix $Q = \frac{1}{\sigma^2}(A'A)$. To overcome this challenge we present an approximate version \hat{y}^{BPA} which only uses the inversion of the main-diagonal D_Q as in the exact version of the in-sample best predictor formula:

$$\begin{aligned}\hat{y}^{BPA} &= \hat{y}^{TC} - D_Q^{-1}(Q - D_Q)S_\Gamma(y^* - S'_\Gamma\hat{y}^{TC}) \\ &= yR_\Gamma + \hat{y}^{TC}(I_N - R_\Gamma) - D_Q^{-1}QS_\Gamma(y^* - S'_\Gamma\hat{y}^{TC}).\end{aligned}\tag{29}$$

Both predictors in (28) and (29) can be understood as a correction computed from the residuals added to a reference value. This reference is the response variable for in sample units and the \hat{y}^{TC} predictor for out of sample ones. Due to the replacement of Q^{-1} by D_Q^{-1} in (29), the correction only applies to units which are direct neighbors to in-sample ones, while (28) adds a correction to all observations.

4 Conclusion

This article develops a new framework for estimating interaction models of spatially correlated origin-destination flows. We extend the approach of LeSage and Pace (2008) to allow for missing values in the OD matrix and to account for situations where the list of origins may differ from the list of destinations. Our methodology allows to estimate the generalized model efficiently from a matrix representation of the flows, which we demonstrate for the MLE. With these generalizations, it is much easier to estimate the spatial econometric interaction model for increasingly common, high spatial resolution flow data. A limitation of the model is that the absence of a flow is not modeled explicitly, which means that, in general, the results apply only to the sub-sample of OD pairs with observed values for the flow. We leave extensions that simultaneously account for the selection mechanism and spatial autocorrelation for future research.

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Appendix A Some properties of Kronecker products

Consider the following four rectangular, four square matrices and four column vectors

$$\begin{array}{lll}
U(n_d \times n_o) & A(n_o \times n_o) & a(n_o \times 1) \\
V(n_d \times n_o) & C(n_o \times n_o) & c(n_o \times 1) \\
X(n_d \times k_x) & B(n_d \times n_d) & e(n_o \times 1) \\
Y(n_o \times k_y) & D(n_d \times n_d) & b(n_d \times 1) \\
Z(n_o \times k_z) & & d(n_d \times 1),
\end{array}$$

Most of the properties listed below are either well-known (see for example Harville 1998) or follow trivially from the linearity of the operators. Some of them have already been used by to increase the efficiency of estimators for the cartesian spatial interaction model (see for example LeSage and Pace 2008; LeSage and Pace 2009). Here we use $A_{[ij]}$ to access one element, $A_{[i\bullet]}$ to access one row, $A_{[\bullet j]}$ to access one column of the matrix A and $a_{[j]}$ for one element of the vector a .

$$\begin{array}{l}
\text{k1 : } (Y' \otimes X') \text{Vec}(V) = \text{Vec}(X'VY). \\
\text{k2 : } \text{Vec}(V)' \text{Vec}(U) = \iota'_{n_d}(V \odot U)\iota_{n_o} = \text{tr}(V'U) \\
\text{k3 : } \text{Vec}(V) \odot \text{Vec}(U) = \text{Vec}(V \odot U) \\
\text{k4 : } \text{Diag}(a)c = \text{Diag}(c)a = a \odot c \\
\text{k5 : } V \odot [\text{Diag}(b)U \text{Diag}(a)] = \text{Diag}(b)(V \odot U) \text{Diag}(a) \\
\text{k6 : } a' \text{Diag}(c)e = (a' \odot c')e = \sum_{j=1}^{n_o} a_{[j]}c_{[j]}e_{[j]} \\
\text{k7 : } Y' \text{Diag}(c)Z = \sum_{j=1}^{n_o} c_{[j]}Y'_{[j\bullet]}Z_{[j\bullet]} \\
\text{k8 : } \text{diag}(A' \text{Diag}(a)C) = (A' \odot C')a
\end{array}$$

Given these basic properties we derive some additional properties that can be directly applied to simplify the computations required for estimation and prediction of the spatial econometric interaction model.

$$\begin{array}{l}
\text{K1 : } (a' \otimes b') \text{Diag Vec}(V)(c \otimes d) = (b' \odot d')V(a \odot c) \\
\text{K2 : } (\iota'_{n_o} \otimes X') \text{Diag Vec}(V)(\iota_{n_o} \otimes X) = X' \text{Diag}(V\iota_{n_o})X \\
\text{K3 : } (\iota'_{n_o} \otimes X') \text{Diag Vec}(V)(Y \otimes \iota_{n_d}) = X'VY \\
\text{K4 : } (Y' \otimes \iota'_{n_d}) \text{Diag Vec}(V)(Y \otimes \iota_{n_d}) = Y' \text{Diag}(\iota_{n_d}V)Y \\
\text{K5 : } (I_{n_o} \otimes b') \text{Diag Vec}(V)(I_{n_o} \otimes d) = \text{Diag}[(b' \odot d')V] \\
\text{K6 : } (a' \otimes I_{n_d}) \text{Diag Vec}(V)(c \otimes I_{n_d}) = \text{Diag}[V(a \odot c)] \\
\text{K7 : } \text{diag}\{(A' \otimes B') \text{Diag Vec}(V)(C \otimes E)\} = \text{Vec}[(C' \otimes E')D(A \odot B)] \\
\text{K8 : } \text{tr}[(A \otimes B) \text{Diag Vec}(V)(C \otimes E) \text{Diag Vec}(U)] = \iota'_{n_d}\{V \odot [(B \odot E')U(A' \odot C)]\}\iota_{n_o}
\end{array}$$

A.1 Proof of K1

$$\begin{aligned}
(a' \otimes b') \text{Diag Vec}(V)(c \otimes d) &= (a' \otimes b') \text{Diag}(c \otimes d) \text{Vec}(V) \\
&= (a' \otimes b')(\text{Diag}(c) \otimes \text{Diag}(d)) \text{Vec}(V) \\
&= (a' \otimes b') \text{Vec}(\text{Diag}(d)V \text{Diag}(c)) \\
&= \text{Vec}(b' \text{Diag}(d)V \text{Diag}(c)a) \\
&= (b' \odot d')V(a \odot c) \quad \square
\end{aligned}$$

A.2 Proof of K2

For the proof of this property we can directly exploit the block structure that follows from the Kronecker product.

$$\begin{aligned}
(\iota'_{n_o} \otimes X') \text{Diag Vec}(V)(\iota_{n_o} \otimes X) &= (X'X' \dots X') \text{Diag Vec}(V)(X'X' \dots X')' \\
&= \sum_{j=1}^{n_o} X' \text{Diag}(V_{[\bullet, j]})X \\
&= X' \text{Diag}(\sum_{j=1}^{n_o} V_{[\bullet, j]})X \\
&= X' \text{Diag}(V \iota_{n_o})X \quad \square
\end{aligned}$$

A.3 Proof of K3

The proof of this property proceeds similarly to the previous one with the slight inconvenience that the blocks related to the second Kronecker product cannot be factored out of the sum. Note that in the line before the last we recover the inner product of two matrices.

$$\begin{aligned}
(\iota'_{n_o} \otimes X') \text{Diag Vec}(V)(Y \otimes \iota_{n_d}) &= (X' \dots X') \text{Diag Vec}(V)(Y'_{[1, \bullet]} \iota'_{n_d} \dots Y'_{[n_o, \bullet]} \iota'_{n_d})' \\
&= X' \sum_{j=1}^{n_o} \text{Diag}(V_{[\bullet, j]}) \iota_{n_d} Y_{[j, \bullet]} \\
&= X' \sum_{j=1}^{n_o} \text{Diag}(\iota_{n_d}) V_{[\bullet, j]} Y_{[j, \bullet]} \\
&= X' \sum_{j=1}^{n_o} V_{[\bullet, j]} Y_{[j, \bullet]} \\
&= X' V Y \quad \square
\end{aligned}$$

A.4 Proof of K4

We use the same procedure as for the previous two properties, noting that this time no factorization is possible.

$$\begin{aligned}
(Y' \otimes \iota'_{n_d}) \text{Diag Vec}(V)(Y \otimes \iota_{n_d}) &= (Y'_{[1, \bullet]} \iota'_{n_d} \dots Y'_{[n_o, \bullet]} \iota'_{n_d}) \text{Diag Vec}(V)(Y'_{[1, \bullet]} \iota'_{n_d} \dots Y'_{[n_o, \bullet]} \iota'_{n_d})' \\
&= \sum_{j=1}^{n_o} Y'_{[j, \bullet]} \iota'_{n_d} \text{Diag}(V_{[\bullet, j]}) \iota_{n_d} Y_{[j, \bullet]} \\
&= \sum_{j=1}^{n_o} Y'_{[j, \bullet]} \iota'_{n_d} V_{[\bullet, j]} Y_{[j, \bullet]} \\
&= \sum_{j=1}^{n_o} (\iota'_{n_d} V)_{[j]} Y'_{[j, \bullet]} Y_{[j, \bullet]} \\
&= Y' \text{Diag}(\iota'_{n_d} V) Y \quad \square
\end{aligned}$$

A.5 Proof of K5

To proof the statement $(I_{n_o} \otimes b') \text{Diag Vec}(V)(I_{n_o} \otimes d) = \text{Diag}[(b' \odot d')V]$, we may first observe that the result must be a diagonal matrix, where the diagonal elements are given by

$$b' \text{Diag}(V_{[\bullet, j]})d = b' \text{Diag}(d)V_{[\bullet, j]} = (b' \odot d')V_{[\bullet, j]},$$

for $j = 1, \dots, n_o$. Applying the same step to all diagonal elements directly yields the final result.

A.6 Proof of K6

To proof this property we rewrite the initial statement as a sum of n_o matrices of size $(n_d \times n_d)$.

$$\begin{aligned} (a' \otimes I_{n_d}) \text{Diag Vec}(V)(c \otimes I_{n_d}) &= \sum_{j=1}^{n_o} a[j] \text{Diag}(V_{[\bullet, j]})c[j] \\ &= \text{Diag}(\sum_{j=1}^{n_o} V_{[\bullet, j]}(a \odot c)_{[j]}) \\ &= \text{Diag}(V(a \odot c)) \quad \square \end{aligned}$$

for $j = 1, \dots, n_o$. The same applied to all diagonal elements leads directly to the result.

A.7 Proof of K7

$$\begin{aligned} \text{tr}[(A \otimes B) \text{Diag Vec}(V)(C \otimes D) \text{Diag Vec}(U)] & \\ &= \iota'_N \{(A \otimes B) \odot [\text{Diag Vec}(V)(C' \otimes D') \text{Diag Vec}(U)]\} \iota_N \\ &= \iota'_N \text{Diag Vec}(V)[(A \otimes B) \odot (C' \otimes D')] \text{Diag Vec}(U) \iota_N \\ &= \text{Vec}(V)'(A \odot C') \otimes (B \odot D') \text{Vec}(U) \\ &= \text{Vec}(V)' \text{Vec}[(B \odot D')U(A' \odot C)] \\ &= \iota'_{n_d} \{V \odot [(B \odot D')U(A' \odot C)]\} \iota_{n_o} \quad \square \end{aligned}$$

A.8 Proof of K8

We are interested in proving $\text{diag} \{(A' \otimes B') \text{Diag Vec}(V)(C \otimes E)\} = \text{Vec}[(C' \odot E')V(A \odot B)]$. The properties of Kronecker products allow to rewrite

$$\begin{aligned} (A' \otimes B') \text{Diag Vec}(V)(C \otimes E) &= (I_{n_o} \otimes B')(A' \otimes I_{n_d}) \text{Diag Vec}(V)(C \otimes I_{n_d})(I_{n_o} \otimes E) \\ &= (I_{n_o} \otimes B')(M)(I_{n_o} \otimes E) \\ &= (I_{n_o} \otimes B')(M^D + M^O)(I_{n_o} \otimes E) \end{aligned}$$

In the last equation the matrix $M = (A' \otimes I_{n_d}) \text{Diag Vec}(V)(C \otimes I_{n_d})$ is decomposed into a block diagonal matrix M^D with its diagonal blocks denoted by $M^{Dm}(n_d \times n_d)$, $m = 1, \dots, n_o$. The counterpart M^O contains all other blocks of M , with the diagonal ones set to zero. Since the other two Kronecker products lead to block diagonal matrices we find that

$$\text{diag} \{(I_{n_o} \otimes B')(M^D + M^O)(I_{n_o} \otimes E)\} = \text{diag} \{(I_{n_o} \otimes B')(M^D)(I_{n_o} \otimes E)\}.$$

The explicit expression of the first block if M^D is given by

$$\begin{aligned}
M^{D1} &= (A'[\cdot, 1] \otimes I_{n_d}) \text{Diag Vec}(V)(C[\cdot, 1] \otimes I_{n_d}) \\
&= (A[1, \cdot] \otimes I_{n_d})' \text{Diag Vec}(V)(C[\cdot, 1] \otimes I_{n_d}) \\
&= \text{Diag}(V(A[1, \cdot] \odot C[\cdot, 1])) \\
&= \text{Diag}(V(A \odot C)[\cdot, 1]).
\end{aligned}$$

With the same developments applied to all other diagonal blocks, we find that M^D is not only block diagonal but actually diagonal.

$$M^D = \text{Diag Vec}(V(A \odot C))$$

Denoting $V^* = V(A \odot C)$ allows to rewrite $(I_{n_o} \otimes B') \text{Diag Vec}(V^*)(I_{n_o} \otimes E) := M^*$, which is obviously a block-diagonal matrix. We may then find the diagonal of the first block $M^{*1}(n_d \times n_d)$.

$$\begin{aligned}
\text{diag}(M^{*1}) &= \text{diag}[B' \text{Diag}(V^*[\cdot, 1])D] \\
&= (B' \odot E')V^*[\cdot, 1]
\end{aligned}$$

Performing the above step for all the remaining blocks then allows to conclude the proof.

$$\begin{aligned}
\text{diag}(M^*) &= \text{Vec}[(B' \odot D')V^*] \\
&= \text{Vec}[(B' \odot D')V(A \odot C)]. \quad \square
\end{aligned}$$

Appendix B Log determinant for non-cartesian flows

We want to approximate the log determinant in the non-cartesian case based on the first four terms of its Taylor series expression.

In the following we first recall the intuition of the Martin (1992) approximation of the log-determinant term and then develop the terms required for the fourth-order approximation of the general spatial econometric interaction model. We start by expressing the determinant as the product of the eigenvalues denoted by $\lambda(A^*)$.

$$\log |A^*| = \log |I_{N^*} - W_F^*| = \log |\prod_{i=1}^{N^*} 1 - \lambda(W_F)_i|$$

For the next step we require that all eigenvalues of W_F are less than one in magnitude, which allows to remove the absolute value. We then write the log of a products as a sum of logs and replace the logarithm in each term by an infinite Taylor series.

$$\sum_{i=1}^{N^*} \log(1 - \lambda(W_F)_i) = - \sum_{i=1}^{N^*} \sum_{t=1}^{\infty} \frac{\lambda(W_F)_i^t}{t}$$

By interchanging the sums we express the above series in terms of the traces of W_F . With our constraint on the eigenvalues of W_F we are sure that the series converges and we can use the first m terms as an approximation.

$$\sum_{t=1}^{\infty} \sum_{i=1}^{N^*} \frac{\lambda(W_F)_i^t}{t} = \sum_{t=1}^{\infty} \frac{\text{tr}(W_F^t)}{t} \approx \sum_{t=1}^m \frac{\text{tr}(W_F^t)}{t}$$

In Section 3.2 we have seen that, when the model is cartesian, the traces $\text{tr}(W_F^t)$ may be calculated efficiently from those of $\text{tr}(OW^t)$ and $\text{tr}(DW^t)$. Unfortunately, this is not possible in the non-cartesian version, and we have to expand the terms of W_F^{*t} explicitly to compute the trace values.

$$\text{tr}(W_F^{*t}) = \text{tr}((\rho_d W_d^* + \rho_o W_o^* + \rho_w W_w^*)^t),$$

for each power $t = 1, \dots, m$. With a direct approach this would require 120 matrix products for the fourth order approximation, which is unpractical even for moderate sample sizes. We can do much better if we exploit the following properties:

- T1 : A well known property of the trace operator is that the trace of a product of matrices is invariant under cyclic permutations of the multiplication order.
- T2 : For any $t = 0, 1, 2, \dots$, we have $0 = \text{tr}(W_d^{*t} W_o^*) = \text{tr}(W_o^{*t} W_d^*) = \text{tr}(W_d^{*t} W_w^*) = \text{tr}(W_o^{*t} W_w^*)$. This property is demonstrated in the next subsection. It follows from the zero diagonal and the Kronecker product structure of the matrices W_o , W_d and W_w .
- T3 : For two square matrices A and B with the same size we have $\text{tr}(AB) = \iota(A \odot B')\iota$, which is a direct consequence of the definition of the trace and the matrix product.

The properties T1 and T2 can be used to avoid the computation of 92 out of 120 values as they are either zero or duplicated. In the following we show the 28 unique trace values that are required for the fourth order approximation:

For $t = 1$, we can use T2 to avoid any computation

$$\text{tr}(W_F^*) = \rho_d \underbrace{\text{tr}(W_d^*)}_0 + \rho_o \underbrace{\text{tr}(W_o^*)}_0 + \rho_w \underbrace{\text{tr}(W_w^*)}_0 = 0$$

For $t = 2$, we can use T2 to conclude that only 3 of the 9 required traces are different from zero.

$$\text{tr}(W_F^{*2}) = \rho_d^2 \text{tr}(W_d^{*2}) + \rho_o^2 \text{tr}(W_o^{*2}) + \rho_w^2 \text{tr}(W_w^{*2})$$

For $t = 3$, we can use T1 and T2 to infer that 12 out of 27 traces are zero and that among the remaining values only seven are unique.

$$\begin{aligned} \text{tr}(W_F^{*3}) &= \rho_d^3 \text{tr}(W_d^{*3}) + \rho_o^3 \text{tr}(W_o^{*3}) + \rho_w^3 \text{tr}(W_w^{*3}) \\ &\quad + 3\rho_d \rho_w^2 \text{tr}(W_d^* W_w^{*2}) + 3\rho_o \rho_w^2 \text{tr}(W_o^* W_w^{*2}) \\ &\quad + \rho_d \rho_o \rho_w [3 \text{tr}(W_d^* W_o^* W_w^*) + 3 \text{tr}(W_o^* W_d^* W_w^*)] \end{aligned}$$

For $t = 4$, we can use T1 and T2 to infer that 16 out of 81 traces are zero and that among the remaining 65 traces only 18 are unique.

$$\begin{aligned}
\text{tr}(W_F^4) &= \rho_d^4 \text{tr}(W_d^4) + \rho_o^4 \text{tr}(W_o^4) + \rho_w^4 \text{tr}(W_w^4) \\
&+ \rho_d^2 \rho_o^2 [2 \text{tr}(W_d^* W_o^* W_d^* W_o^*) + 4 \text{tr}(W_d^{*2} W_o^{*2})] \\
&+ \rho_d^2 \rho_w^2 [2 \text{tr}(W_d^* W_w^* W_d^* W_w^*) + 4 \text{tr}(W_d^{*2} W_w^{*2})] \\
&+ \rho_o^2 \rho_w^2 [2 \text{tr}(W_o^* W_w^* W_o^* W_w^*) + 4 \text{tr}(W_o^{*2} W_w^{*2})] \\
&+ \rho_d^2 \rho_o \rho_w [4 \text{tr}(W_d^* W_o^* W_d^* W_w^*) + 8 \text{tr}(W_d^{*2} W_o^* W_w^*)] \\
&+ \rho_d \rho_o^2 \rho_w [4 \text{tr}(W_d^* W_o^* W_w^* W_o^*) + 8 \text{tr}(W_d^* W_o^{*2} W_w^*)] \\
&+ \rho_d \rho_o \rho_w^2 [4 \text{tr}(W_d^* W_o^* W_w^{*2}) + 4 \text{tr}(W_o^* W_d^* W_w^{*2}) + 4 \text{tr}(W_d^* W_w^* W_o^* W_w^*)] \\
&+ \rho_d \rho_w^3 4 \text{tr}(W_d^* W_w^3) + \rho_o \rho_w^3 4 \text{tr}(W_o^* W_w^3)
\end{aligned}$$

Using T3 we can derive the 28 trace values from only ten matrix products that involve at most two of the weight matrices. An example of this calculation is $\text{tr}(W_d^4) = \ell'_{N^*} (W_d^{*2} \odot W_d^{*2}) \ell_{N^*}$. This makes clear that we avoid direct computation of matrix products of third and fourth order that become increasingly dense in comparison to the lower order products. Below are the ten matrices that need to be computed for the fourth-order approximation.

$$\begin{array}{ccccc}
W_d^* & W_o^* & W_w^* & W_d^* W_d^* & W_o^* W_o^* \\
W_w^* W_w^* & W_d^* W_o^* & W_o^* W_d^* & W_d^* W_w^* & W_o^* W_w^*
\end{array}$$

B.1 Proof of T2

We will demonstrate the four statements in T2: $0 = \text{tr}(W_d^{*t} W_o^*) = \text{tr}(W_o^{*t} W_d^*) = \text{tr}(W_d^{*t} W_w^*) = \text{tr}(W_o^{*t} W_w^*)$ in two steps. At first, we focus on the statements that involve powers of the destination weight matrix W_d^{*t} .

$$\begin{aligned}
0 &= \text{tr}(W_d^{*t} W_o^*) = \text{tr}((R_\Gamma W_d R_\Gamma)^t W_o R_\Gamma) \\
0 &= \text{tr}(W_d^{*t} W_w^*) = \text{tr}((R_\Gamma W_d R_\Gamma)^t W_w R_\Gamma)
\end{aligned} \tag{30}$$

The above development is possible because eliminating or replacing rows and columns by zero has the same effect on the trace value $\text{tr}(S_\Gamma^t W_d S_\Gamma) = \text{tr}(R_\Gamma^t W_d R_\Gamma)$. From the definition $W_d = I_{n_o} \otimes DW$ it is clear that the first term inside the two traces has the following block-diagonal structure

$$(R_1 W_d R_1)^t = \begin{bmatrix} (R_1 DW R_1)^t & 0 & \cdots & 0 \\ 0 & (R_2 DW R_2)^t & \cdots & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \cdots & (R_{n_o} DW R_{n_o})^t \end{bmatrix} \tag{31}$$

where $R_j (n_d \times n_d)$, for $j = 1, \dots, n_o$ are the diagonal blocs of the replacement matrix R_Γ . Equation (31) shows that we can concentrate on the diagonal blocks if we compute the traces given (30). If we then partition the matrices W_o and W_w into the same block structure we obtain zero matrices for the diagonal blocks, which makes clear that the traces in (30) are indeed zero.

To demonstrate the remaining two statements

$$\begin{aligned}
0 &= \text{tr}(W_o^{*t} W_d^*) = \text{tr}((R_\Gamma W_o R_\Gamma)^t W_d R_\Gamma) \\
0 &= \text{tr}(W_o^{*t} W_w^*) = \text{tr}((R_\Gamma W_o R_\Gamma)^t W_w R_\Gamma),
\end{aligned} \tag{32}$$

we again partition the matrix $(R_\Gamma W_o R_\Gamma)^t$ into n_o^2 blocks of size $n_d \times n_d$. This leads to a matrix, for which all blocks $D_{ij}(t)$ for $i, j = 1, \dots, n_o$ are diagonal matrices, whose entries vary with the powers $t = 1, \dots, m$.

$$(R_\Gamma W_o R_\Gamma)^t = \begin{bmatrix} D_{11}(t) & D_{12}(t) & \cdots & D_{1n_o}(t) \\ D_{21}(t) & D_{22}(t) & \cdots & \cdots \\ \cdots & \cdots & \ddots & \cdots \\ D_{n_o1}(t) & \cdots & \cdots & D_{n_on_o}(t) \end{bmatrix}, \quad (33)$$

Hence, if we compute the trace of a matrix product that involves $(R_\Gamma W_o R_\Gamma)^t$ we know that values off the main diagonal of the blocks will not play a role. For the matrices W_d and W_w the same partition leads to blocks that have zero diagonal, which confirms the statements in (32).

Appendix C Parameter space

In the following we derive the two results that were used to handle the issue of the feasible parameter space presented in Section 3.3. The first one is formulated as a general theorem and the second one is derived in the specific context of model (7).

C.1 Eigenvalues of a sum of Kronecker products

Proposition: Let $A(n_a \times n_a)$ and $B(n_b \times n_b)$ be two square matrices and denote $M = a(A \otimes I_{n_b}) + b(I_{n_a} \otimes B) + c(A \otimes B)$, where a, b and c are scalar values. The eigenvalue vector $\lambda_M(n_a \cdot n_b \times 1)$ of M and those of the matrices A and B denoted by λ_A and λ_B are linked by the relation

$$\lambda_M = a(\lambda_A \otimes \iota_{n_b}) + b(\iota_{n_a} \otimes \lambda_B) + c(\lambda_A \otimes \lambda_B). \quad (34)$$

Proof: By Schurs Lemma we know that for any square matrix X there exists a factorization $X = Q_X U_X Q_X^{-1}$ such that U_X is upper triangular with the main diagonal equal to the eigenvalues vector λ_X of X . Additionally, we may infer the Schur decomposition of a Kronecker product of two matrices $(A \otimes B)$ from the Schur decompositions of A and B .

$$\begin{aligned} (A \otimes B) &= Q_{(A \otimes B)} U_{(A \otimes B)} Q_{(A \otimes B)}^{-1} \\ &= (Q_A \otimes Q_B) (U_A \otimes U_B) (Q_A \otimes Q_B)^{-1} \\ &= (Q_A U_A Q_A^{-1} \otimes Q_B U_B Q_B^{-1}) \end{aligned}$$

Next, we have the following equivalence $M = Q_M U_M Q_M^{-1} \Leftrightarrow U_M = Q_M^{-1} M Q_M$. If we replace Q_M by $(Q_A \otimes Q_B)$ for $M = a(A \otimes I_{n_b}) + b(I_{n_a} \otimes B) + c(A \otimes B)$ and develop the resulting expression we obtain the following result:

$$\begin{aligned} U_M &= (Q_A \otimes Q_B)^{-1} [a(A \otimes I_{n_b}) + b(I_{n_a} \otimes B) + c(A \otimes B)] (Q_A \otimes Q_B) \\ &= a(Q_A^{-1} A Q_A \otimes Q_B^{-1} I_{n_b} Q_B) + b(Q_A^{-1} I_{n_a} Q_A \otimes Q_B^{-1} B Q_B) + c(Q_A^{-1} A Q_A \otimes Q_B^{-1} B Q_B) \\ &= a(U_A \otimes I_{n_b}) + b(I_{n_a} \otimes U_B) + c(U_A \otimes U_B) \end{aligned}$$

Since U_A and U_B are upper triangular matrices we conclude that U_M is upper triangular too, which confirms that we have indeed found a Schur decomposition of M . This triangular structure also allows to conclude that the eigenvalues of U_M are given by equation (34). Since M and U_M have the same spectrum the proof is finished.

C.2 Similarity and the selection operator

In Section 3.3 we rely on the fact that all eigenvalues of W_F^* are contained in the interval $[\lambda_{min}(W_F), \lambda_{max}(W_F)]$. When W_F is symmetric this follows directly from Cauchy's interlacing theorem. Here we show that this argument also holds for the more general form of W_F we have considered in this article.

The properties of $W_F = \rho_d(I_{no} \otimes DW) + \rho_o(OW \otimes I_{nd}) + \rho_w(OW \otimes DW)$ depend on the characteristics of the two node-level neighborhood matrices DW and OW . If these are symmetric, so is W_F and Cauchy's theorem applies. When they are row-normalized they are no longer symmetric, but we may still apply Cauchy's theorem if they were symmetric before the row-normalization. Let \overline{OW} and \overline{DW} to symmetric neighborhood matrices. Their row-normalized counterparts are given by

$$DW = D_d \overline{DW} \quad OW = D_o \overline{OW},$$

where D_d and D_o are diagonal matrices whose entries correspond to the inverse of the row-sums of DW and OW . It is clear that DW is similar to the symmetric matrix $D_d^{1/2} \overline{DW} D_d^{1/2}$ and that OW is similar to $D_o^{1/2} \overline{OW} D_o^{1/2}$. We may use the same argument to show that W_F is similar a symmetric matrix

$$W_F = D_F \overline{W_F} = D_F^{1/2} (D_F^{1/2} \overline{W_F} D_F^{1/2}) D_F^{-1/2},$$

where $D_F = D_o \otimes D_d$ and $\overline{W_F} = \rho_d(I_{no} \otimes \overline{DW}) + \rho_o(\overline{OW} \otimes I_{nd}) + \rho_w(\overline{OW} \otimes \overline{DW})$. The next step is to show that the same holds in the non-cartesian version, where we use the selection operator to obtain $W_F^* = S'_\Gamma D_F \overline{W_F} S_\Gamma$. Since replacing rows with zero before dropping them does not change the result we may write $S'_\Gamma D_F = S'_\Gamma D_F^{1/2} R_\Gamma D_F^{1/2}$. Using this argument and the link $R_\Gamma = S_\Gamma S'_\Gamma$ we obtain

$$W_F^* = (S'_\Gamma D_F^{1/2} S_\Gamma) (S'_\Gamma D_F^{1/2} \overline{W_F} D_F^{1/2} S_\Gamma) (S'_\Gamma D_F^{1/2} S_\Gamma)^{-1}.$$

The above equation clearly shows the similarity of W_F^* to the symmetric matrix $S'_\Gamma D_F^{1/2} \overline{W_F} D_F^{1/2} S_\Gamma$. Since this result does not depend on the specific subset selected by the operator S_Γ we are sure that the row-normalization of OW and DW does not compromise the applicability of Cauchy's interlacing theorem. Hence, we may conclude that the extreme eigenvalues of W_F^* are bounded by those of W_F .

Appendix D Matrix form of predictors

Computing \mathcal{Z} , such that $\text{Vec}(\mathcal{Z}) = Z\delta$ is not difficult and was explained by LeSage and Pace (2008).

$$\begin{aligned} \hat{y}^{*TS} &= \hat{\rho}_d W_d^* y^* + \hat{\rho}_d W_d^* y^* + \hat{\rho}_d W_d^* y^* + Z^* \hat{\delta} \\ &= S_\Gamma [\hat{\rho}_d (I_{no} \otimes DW) R_\Gamma y] + \hat{\rho}_o (OW \otimes I_{nd}) R_\Gamma y + \hat{\rho}_w (OW \otimes DW) R_\Gamma y + Z \hat{\delta} \\ &= S_\Gamma \{ [\hat{\rho}_d (I_{no} \otimes DW) + \hat{\rho}_o (OW \otimes I_{nd}) + \hat{\rho}_w (OW \otimes DW)] \text{Vec}(\mathcal{I}_\Gamma \odot Y) + \text{Vec}(\mathcal{Z}) \} \\ &= S_\Gamma \{ \text{Vec}(\hat{\rho}_d DW (\mathcal{I}_\Gamma \odot Y)) + \hat{\rho}_o (\mathcal{I}_\Gamma \odot Y) OW' + \hat{\rho}_w DW (\mathcal{I}_\Gamma \odot Y) OW' + \text{Vec}(\mathcal{Z}) \} \end{aligned}$$

Their formula for the best predictor can be further developed to appear as a correction on the true value of y instead of its expectation. Goulard, Laurent, and Thomas-Agnan (2017)

take an inspiration from Goldenberger's formula to derive their best predictors for the spatial econometric model:

$$\begin{aligned}
\hat{y}^{*BPI} &= \hat{A}^{*-1} Z^* \hat{\delta} - D_{\hat{Q}^*}^{-1} (\hat{Q}^* - D_{\hat{Q}^*}) (y^* - \hat{A}^{*-1} Z^* \hat{\delta}) \\
&= \hat{A}^{*-1} Z^* \hat{\delta} - (D_{\hat{Q}^*}^{-1} \hat{Q}^* - I_{N^*}) (y^* - \hat{A}^{*-1} Z^* \hat{\delta}) \\
&= y^* - D_{\hat{Q}^*}^{-1} \hat{Q}^* (y^* - \hat{A}^{*-1} Z^* \hat{\delta}) \\
&= y^* - D_{\hat{A}^*{}' \hat{A}^*}^{-1} \hat{A}^*{}' (\hat{A}^* y^* - Z^* \hat{\delta}) \\
&= y^* - D_{\hat{A}^*{}' \hat{A}^*}^{-1} \hat{A}^*{}' (y^* - \hat{y}^{*TS}).
\end{aligned}$$

An immediate advantage of this formulation is the removal of the inverse. The main diagonal of $D_{\hat{A}^*{}' \hat{A}^*}$, can be found explicitly using property K8.

$$\begin{aligned}
&\text{diag}(A^{*'} A^*) \\
&= S_\Gamma' \text{diag}(A' R_\Gamma A) \\
&= S_\Gamma' \{ \text{diag}(I_N R_\Gamma I_N) + \rho_d^2 \text{diag}(W_d' R_\Gamma W_d') + \rho_o^2 \text{diag}(W_o' R_\Gamma W_o') + \rho_w^2 \text{diag}(W_w' R_\Gamma W_w') \} \\
&= S_\Gamma' \text{Vec} \{ I_\Gamma + \rho_d^2 (DW \odot DW) I_\Gamma + \rho_o^2 I_\Gamma (OW \odot OW) + \rho_w^2 (DW \odot DW) I_\Gamma (OW \odot OW) \}
\end{aligned}$$

For the filtered residual term $\hat{\varepsilon}^{*TS} = \hat{A}^*{}' (y^* - \hat{y}^{*TS})$ we may apply the same techniques as previously to compute the spatial lag. The final form would then be

$$\hat{y}^{*BPI} = S_\Gamma (\text{Vec}(Y + D_{(A' R_\Gamma A)^{-1}} \odot \hat{\varepsilon}^{*TS}))$$

To use their formula to predict the full population we need to invert the precision matrix (using the original formula of the authors only the part of it linked to to unobserved units). This quickly becomes infeasible if we have many units to predict. Solution 1 is to solve a linear system instead of computing an inversion, solution 2 is an approximation in the same style as for the expected value, solution 3 is an alternative formulation of the predictor that is inspired by the in sample units.

$$\hat{y}^{BP} = \hat{A}^{-1} Z \hat{\delta} - \hat{Q}^{-1} \hat{Q} S_\Gamma S_\Gamma' (y - \hat{A}^{-1} Z \hat{\delta})$$

Approximation of the above

$$\hat{y}^{BPA} = y R_\Gamma + \hat{y}^{TC} (I_N - R_\Gamma) - D_{\hat{A}' \hat{A}}^{-1} \hat{A}' \hat{A} R_\Gamma (y - \hat{y}^{TC})$$