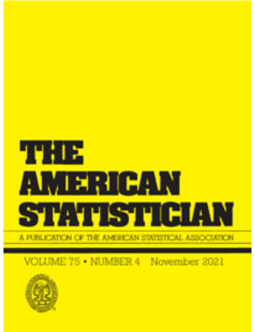

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On Deconfounding Spatial Confounding in Linear Models

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ABSTRACT
Spatial confounding, that is, collinearity between fixed effects and random effects in a spatial generalized linear mixed model, can adversely affect estimates of the fixed effects. Restricted spatial regression methods have been proposed as a remedy for spatial confounding. Such methods replace inference for the fixed effects of the original model with inference for those effects under a model in which the random effects are restricted to a subspace orthogonal to the column space of the fixed effects model matrix; thus, they "deconfound" the two types of effects. We prove, however, that frequentist inference for the fixed effects of a deconfounded linear model is generally inferior to that for the fixed effects of the original spatial linear model; in fact, it is even inferior to inference for the corresponding nonspatial model. We show further that deconfounding also leads to inferior predictive inferences, though its impact on prediction appears to be relatively small in practice. Based on these results, we argue that deconfounding a spatial linear model is bad statistical practice and should be avoided.

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Generalized least squares; Linear mixed model; Restricted spatial regression; Spatial model; Spatial prediction

1. Introduction

Spatial confounding refers to (approximate) collinearity between fixed effects and random effects in a spatial generalized linear mixed model. Although the concept was first described by Clayton, Bernardinelli, and Montomoli (1993), who called it a "confounding effect due to location," it was Reich, Hodges, and Zadnik (2006), henceforth RHZ2006, and Hodges and Reich (2010), henceforth HR2010, who coined the snappier term "spatial confounding" and described it in detail. For a study of socioeconomic status on stomach cancer incidence in Slovenian municipalities, RHZ2006 found that the estimate of the effect of that status from a fit of a fixed effects Poisson regression model was very different from the estimate of the same effect from a fit of the corresponding spatial mixed model; in fact the estimate went from being substantially negative in the fixed effects model (which made scientific sense) to being indistinguishable from zero (which did not). Troubled by this state of affairs, which they attributed to spatial confounding, RHZ2006 proposed as a possible remedy a method they called "restricted spatial regression" (RSR). This method replaces fitting the spatial mixed model with fitting a model in which the random effects are restricted to a subspace orthogonal to the column space of the fixed effects model matrix; thus, it "deconfounds" the two types of effects. The hope was that deconfounding the model in this manner would reduce variance inflation and thereby improve inferences about the fixed effects.

Considerable discussion about the merits of restricted spatial regression has ensued since it was first proposed, and several variations have been suggested (Hughes and Haran 2013; Hanks et al. 2015; Hefley et al. 2017; Hughes 2017; Prates, Assuncao, and Rodrigues 2019; Dupont, Wood, and Augustin 2020). However, only recently (Khan and Calder 2020) was a thorough analytical investigation of the statistical properties of restricted spatial regression undertaken. Like most of the literature on spatial confounding in general and restricted spatial regression in particular, however, the inferential context for Khan and Calder's investigation was Bayesian rather than frequentist, with a prior for the random effects (namely the intrinsic conditional autoregressive, or ICAR, model) that has a singular precision matrix and is thereby improper (Lavine and Hodges 2012). Within that inferential context, proofs of the properties of restricted spatial regression are rather complicated, and the methodology itself is rather less familiar to many actual and potential users of spatial regression methods. The purpose of this article is to derive exact, finite-sample inferential properties of restricted spatial regression using classical (frequentist) linear model theory. One key result is that the generalized residual mean squares corresponding to the spatial linear model and its restricted counterpart coincide, which (together with other results) establishes mathematically that confidence intervals for fixed effects based on the restricted regression model are too narrow. Another finding is that the best linear unbiased predictor of an as-yet-unobserved response based on the restricted spatial regression model is identical to the best linear unbiased predictor of that quantity under the original spatial model, but the corresponding prediction interval based on restricted spatial regression is likewise too narrow. An example with simulated data demonstrates how serious the problems with undercoverage may be, and also suggests that our conclusions may be extended to the less tractable setting in which the regressors are stochastic and possibly correlated with the random effects. Based on these results, we argue that the use of restricted spatial

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regression methods is bad statistical practice and should be avoided.

2. Background

Throughout this article it is assumed that the true model for a vector of spatially indexed observations $\mathbf{y}$ is the classical *spatial linear mixed model* (SLMM) given by

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{b} + \mathbf{d}, \tag{1}$$

where $\mathbf{X}$ is a specified nonrandom $n \times p$ matrix of full column rank, $\boldsymbol{\beta}$ is a nonrandom p-vector of unknown parameters (fixed effects), and $\mathbf{b}$ (the random effects) and $\mathbf{d}$ are independent random n-vectors whose distributions are multivariate normal with zero mean vectors and covariance matrices $\sigma^2\mathbf{G}$ and $\sigma^2\mathbf{I}$, respectively. Thus, the marginal covariance matrix of $\mathbf{y}$ is $\boldsymbol{\Sigma}_{\mathrm{SLMM}} \equiv \sigma^2(\mathbf{G} + \mathbf{I})$. The elements of $\mathbf{G}$ are known functions of an m-vector $\boldsymbol{\theta}$ of unknown parameters, and σ^2 is an unknown parameter. The parameter space for the model is $\{\boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta} : \boldsymbol{\beta} \in \mathbb{R}^p, \sigma^2 > 0, \boldsymbol{\theta} \in \Theta\}$ where Θ is the set of $\boldsymbol{\theta}$-values for which $\mathbf{G}$ is positive definite. The parameters are commonly estimated by likelihood-based methods, in particular maximum likelihood or residual maximum likelihood (REML). For the fixed effects, this coincides with a version of generalized least-squares (GLS) estimation, called empirical GLS, in which the unknown value of $\boldsymbol{\theta}$ is replaced by its maximum likelihood or REML estimate. That is, the empirical GLS estimator of $\boldsymbol{\beta}$ is defined as

$$\tilde{\boldsymbol{\beta}} = (\mathbf{X}^T\hat{\boldsymbol{\Sigma}}_{\mathrm{SLMM}}^{-1}\mathbf{X})^{-1}\mathbf{X}^T\hat{\boldsymbol{\Sigma}}_{\mathrm{SLMM}}^{-1}\mathbf{y},$$

where $\hat{\boldsymbol{\Sigma}}_{\mathrm{SLMM}} = \hat{\sigma}^2(\hat{\mathbf{G}}+\mathbf{I})$, $\hat{\sigma}^2$ is the likelihood-based estimator of σ^2, and $\hat{\mathbf{G}}$ is $\mathbf{G}$ evaluated at the likelihood-based estimate of $\boldsymbol{\theta}$. Important subclasses of SLMMs include Gaussian geostatistical models for point-referenced data, and (after suitable manipulation/marginalization) Gaussian simultaneous and conditional autoregressive (SAR and CAR) models for areal data.

Upon decomposing $\mathbf{b}$ in Equation (1) as $\mathbf{P_X}\mathbf{b} + (\mathbf{I} - \mathbf{P_X})\mathbf{b}$ where $\mathbf{P_X} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$, it may be seen that the fixed effects $\mathbf{X}\boldsymbol{\beta}$ and the portion $\mathbf{P_X}\mathbf{b}$ of the random effects lie within the same subspace of $\mathbb{R}^n$. Called spatial confounding by RHZ2006, this has consequences similar to those of ordinary confounding in fixed effects models; in particular, it tends to inflate the variances of fixed effect estimators. This led RHZ2006 and HR2010 to suggest that instead of fitting the SLMM, it might be advantageous to fit (by the same methods) the so-called restricted spatial regression model (RSRM) given by

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + (\mathbf{I} - \mathbf{P_X})\mathbf{b} + \mathbf{d},$$

where the distributions of $\mathbf{b}$ and $\mathbf{d}$ are the same as in the SLMM. (RHZ2006 actually made this suggestion in the more general context of a Bayesian spatial generalized linear mixed model, for which the present linear model is a special case.) In the RSRM, there is no confounding between the fixed effects and random effects, which, it was hoped, would lead to improved estimation of the fixed effects. It may be verified easily that the marginal covariance matrix of $\mathbf{y}$ in the RSRM is $\boldsymbol{\Sigma}_{\mathrm{RSRM}} \equiv \sigma^2[(\mathbf{I} - \mathbf{P_X})\mathbf{G}(\mathbf{I} - \mathbf{P_X}) + \mathbf{I}]$. Thus, the estimator of $\boldsymbol{\beta}$ obtained by applying empirical GLS to the RSRM is

$$\breve{\boldsymbol{\beta}}_{\mathrm{RSR}} = (\mathbf{X}^T\hat{\boldsymbol{\Sigma}}_{\mathrm{RSRM}}^{-1}\mathbf{X})^{-1}\mathbf{X}^T\hat{\boldsymbol{\Sigma}}_{\mathrm{RSRM}}^{-1}\mathbf{y},$$

where $\hat{\boldsymbol{\Sigma}}_{\mathrm{RSRM}}$ is $\boldsymbol{\Sigma}_{\mathrm{RSRM}}$ evaluated at likelihood-based estimates of σ^2 and $\boldsymbol{\theta}$.

It could be said that $(\mathbf{I} - \mathbf{P_X})\mathbf{b}$ in the RSRM has p superfluous dimensions, in the sense that it is n-dimensional but lies within a subspace of dimension $n - p$. However, as noted by RHZ2006, the RSRM may be reformulated in terms of a vector of random effects that has no superfluous dimensions, as follows:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{L}\mathbf{b}^* + \mathbf{d}. \tag{2}$$

Here, $\mathbf{L}$ is an $n \times (n - p)$ matrix whose columns are the $n - p$ eigenvectors of $\mathbf{I} - \mathbf{P_X}$ corresponding to its nonzero (hence unity) eigenvalues, and $\mathbf{b}^*$ has an $(n - p)$-dimensional normal distribution with mean $\mathbf{0}$ and positive definite covariance matrix $\sigma^2\mathbf{L}^T\mathbf{G}\mathbf{L}$. Under this reformulation, $\mathrm{var}(\mathbf{y}) = \sigma^2\mathbf{L}\mathbf{L}^T\mathbf{G}\mathbf{L}\mathbf{L}^T + \sigma^2\mathbf{I} = \sigma^2[(\mathbf{I} - \mathbf{P_X})\mathbf{G}(\mathbf{I} - \mathbf{P_X}) + \mathbf{I}]$. Thus, this is merely another way to write the RSRM.

Hughes and Haran (2013), henceforth HH2013, proposed a modification of restricted spatial regression that involves the adjacency matrix used in Moran's I, a well-known measure of spatial autocorrelation (Moran 1950). Their model, like that of RHZ2006, was a Bayesian generalized linear mixed model, but when specialized to a frequentist linear setting the model is

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{M}\mathbf{b}^* + \mathbf{d}, \tag{3}$$

where $\mathbf{M}$ is an $n \times q$ matrix whose columns are the first $q << n$ eigenvectors (non-normalized) of the so-called Moran operator $(\mathbf{I} - \mathbf{P_X})\mathbf{A}(\mathbf{I} - \mathbf{P_X})$, $\mathbf{A}$ is the $n \times n$ adjacency matrix whose (i, j)th element equals 1 if sites i and j are neighbors, and equals 0 otherwise, and $\mathbf{b}^*$ has a q-dimensional normal distribution with mean $\mathbf{0}$ and positive definite covariance matrix $\sigma^2\mathbf{M}^T\mathbf{G}\mathbf{M}$. HH2013 suggested that only those eigenvectors corresponding to positive spatial dependence (for which the corresponding eigenvalues are positive) should be included in $\mathbf{M}$; however, their general formulation does not require this. The covariance matrix of $\mathbf{y}$ under the modified restricted spatial regression model given by Equation (3) is $\boldsymbol{\Sigma}_{\mathrm{Moran}} \equiv \sigma^2(\mathbf{M}\mathbf{M}^T\mathbf{G}\mathbf{M}\mathbf{M}^T + \mathbf{I})$, and the corresponding empirical GLS estimator of $\boldsymbol{\beta}$ is

$$\breve{\boldsymbol{\beta}}_{\mathrm{Moran}} = (\mathbf{X}^T\hat{\boldsymbol{\Sigma}}_{\mathrm{Moran}}^{-1}\mathbf{X})^{-1}\mathbf{X}^T\hat{\boldsymbol{\Sigma}}_{\mathrm{Moran}}^{-1}\mathbf{y}$$

where $\hat{\boldsymbol{\Sigma}}_{\mathrm{Moran}}$ is defined analogously to $\hat{\boldsymbol{\Sigma}}_{\mathrm{RSRM}}$.

Actually, in addition to the Bayesian/frequentist and generalized linear model/linear model differences already mentioned, RHZ2006 and HH2013 formulated their models in a manner slightly different than that just described. RHZ2006 took $\mathbf{b}^*$ in (2) to have *precision* matrix $(1/\sigma^2)\mathbf{L}^T\mathbf{G}^{-1}\mathbf{L}$, which is not equal to the inverse of $\sigma^2\mathbf{L}^T\mathbf{G}\mathbf{L}$. Similarly, HH2013 took $\mathbf{b}^*$ in (3) to have precision matrix $(1/\sigma^2)\mathbf{M}^T\mathbf{G}^{-1}\mathbf{M}$, which is not equal to the inverse of $\sigma^2\mathbf{M}^T\mathbf{G}\mathbf{M}$. The explanation for the different formulations is not important here; we consider both in what follows and find that the corresponding inferential properties are very similar.

Also associated with each deconfounded model is an estimator of σ^2 given by the generalized residual mean square for that model. These estimators are

$$\begin{aligned}\breve{\sigma}^2_{\mathrm{RSR}} &= (\mathbf{y} - \mathbf{X}\breve{\boldsymbol{\beta}}_{\mathrm{RSR}})^T[(\mathbf{I} - \mathbf{P_X})\hat{\mathbf{G}}(\mathbf{I} - \mathbf{P_X}) + \mathbf{I}]^{-1} \\ &\quad \times (\mathbf{y} - \mathbf{X}\breve{\boldsymbol{\beta}}_{\mathrm{RSR}})/(n - p), \\ \breve{\sigma}^2_{\mathrm{Moran}} &= (\mathbf{y} - \mathbf{X}\breve{\boldsymbol{\beta}}_{\mathrm{Moran}})^T[(\mathbf{M}\mathbf{M}^T\hat{\mathbf{G}}\mathbf{M}\mathbf{M}^T + \mathbf{I})]^{-1} \\ &\quad \times (\mathbf{y} - \mathbf{X}\breve{\boldsymbol{\beta}}_{\mathrm{Moran}})/(n - p).\end{aligned}$$

For future reference, also define

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \quad \text{and} \quad \hat{\sigma}^2 = \mathbf{y}^T(\mathbf{I} - \mathbf{P}_\mathbf{X})\mathbf{y}/(n-p),$$

which are the ordinary least-squares (OLS) estimator of $\boldsymbol{\beta}$ and the residual mean square from an OLS fit of the Gauss-Markov model with the same fixed effects model matrix as the SLMM, and

$$\tilde{\sigma}^2 = (\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}})^T(\hat{\mathbf{G}} + \mathbf{I})^{-1}(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}})/(n-p),$$

which is the generalized residual mean square from the empirical GLS fit of the SLMM; it is also the REML estimator of σ^2.

Deconfounded estimators other than $\breve{\boldsymbol{\beta}}_{\mathrm{RSR}}$ and $\breve{\boldsymbol{\beta}}_{\mathrm{Moran}}$ (and their RHZ2006 and HH2013 variants) are possible. We define a deconfounded estimator of $\boldsymbol{\beta}$ more generally as the estimator obtained by applying empirical GLS to a model of the form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{H}\mathbf{b}^* + \mathbf{d}, \tag{4}$$

where $\mathbf{H}$ is any $n \times h$ matrix whose column space is an h-dimensional subspace of the column space of $\mathbf{I} - \mathbf{P}_\mathbf{X}$, $\mathbf{b}^*$ and $\mathbf{d}$ are independent, $\mathbf{b}^*$ has an h-variate normal distribution with mean $\mathbf{0}$ and positive definite covariance matrix $\sigma^2\mathbf{H}^T\mathbf{G}\mathbf{H}$, and $\mathbf{d}$ is distributed as in the SLMM. Such an estimator is represented henceforth by $\breve{\boldsymbol{\beta}}_D$, and the corresponding generalized residual mean square is denoted by $\breve{\sigma}^2_D$. The covariance matrix of $\mathbf{y}$ under this model is $\boldsymbol{\Sigma}_D \equiv \sigma^2(\mathbf{H}\mathbf{H}^T\mathbf{G}\mathbf{H}\mathbf{H}^T + \mathbf{I})$.

3. Inferential Properties of Deconfounded Estimation

In this section, we consider various inferential properties of deconfounded estimation and compare them to properties of OLS and empirical GLS estimation. For simplicity, in the first four subsections we assume that $\boldsymbol{\theta}$ is known, so that $\boldsymbol{\beta}$ may be estimated by GLS rather than empirical GLS. In the fifth subsection we indicate how, if at all, these results change when $\boldsymbol{\theta}$ is unknown.

3.1. Equivalences Among Fixed Effect Estimators

Although $\boldsymbol{\Sigma}_{\mathrm{RSRM}}$ does not generally coincide with either $\boldsymbol{\Sigma}_{\mathrm{SLMM}}$ or $\sigma^2\mathbf{I}$, it turns out that $\breve{\boldsymbol{\beta}}_{\mathrm{RSR}}$ coincides with $\hat{\boldsymbol{\beta}}$. The argument for this has two parts. First, $\boldsymbol{\Sigma}_{\mathrm{RSRM}}$ has "Rao's structure" (Rao 1967), that is, it is a special case of a matrix having form $\boldsymbol{\Sigma} = a\mathbf{I} + \mathbf{P}_\mathbf{X}\mathbf{B}\mathbf{P}_\mathbf{X} + (\mathbf{I} - \mathbf{P}_\mathbf{X})\mathbf{C}(\mathbf{I} - \mathbf{P}_\mathbf{X})$ for some scalar a and $n \times n$ symmetric matrices $\mathbf{B}$ and $\mathbf{C}$ for which $\boldsymbol{\Sigma}$ is nonnegative definite. (For $\boldsymbol{\Sigma}_{\mathrm{RSRM}}$, we may take $a = \sigma^2$, $\mathbf{B} = \mathbf{0}$ and $\mathbf{C} = \sigma^2\mathbf{G}$.) For models with covariance matrices having Rao's structure, the GLS and OLS estimators coincide (Rao 1967). Second, the estimators obtained by applying OLS to the RSR and Gauss-Markov models are identical because they have the same fixed effects model matrix. This argument is vastly more simple than the proof of an analogous Bayesian result provided by Khan and Calder (2020).

Moreover, *every* spatially deconfounded estimator coincides with $\hat{\boldsymbol{\beta}}$, and thus all deconfounded estimators are identical to each other. That this is so follows from the fact that the column space of $\mathbf{H}$ is by definition a subspace of the column space of $\mathbf{I} - \mathbf{P}_\mathbf{X}$, which implies that $\mathbf{H} = (\mathbf{I} - \mathbf{P}_\mathbf{X})\mathbf{K}$ for some $n \times h$ matrix $\mathbf{K}$, implying still further that $\boldsymbol{\Sigma}_D$ has Rao's structure (with $a = \sigma^2$, $\mathbf{B} = \mathbf{0}$, and $\mathbf{C} = \sigma^2\mathbf{K}\mathbf{H}^T\mathbf{G}\mathbf{H}\mathbf{K}^T$). Of the estimators being considered herein, only $\tilde{\boldsymbol{\beta}}$ is distinct from the others (except in those rare circumstances in which $\boldsymbol{\Sigma}_{\mathrm{SLMM}}$ itself has Rao's structure). However, the expectations of $\tilde{\boldsymbol{\beta}}$ and every deconfounded estimator under the SLMM are equal, as they are all unbiased for $\boldsymbol{\beta}$. This unbiasedness further implies that the estimators' mean square error matrices are equal to their covariance matrices, so that it suffices (under squared error loss) to compare the estimators on the basis of the latter.

3.2. Equivalences and Relationships Among Covariance Matrices of Fixed Effect Estimators

The equivalence of the spatially deconfounded point estimators and OLS estimator of $\boldsymbol{\beta}$ described in the previous subsection does not necessarily imply that the covariance matrices of those estimators computed under their corresponding models (subsequently called "nominal" covariance matrices) are equal. However, routine calculations yield

$$\begin{aligned}\mathrm{var}_{\mathrm{RSRM}}(\breve{\boldsymbol{\beta}}_{\mathrm{RSR}}) &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{\Sigma}_{\mathrm{RSRM}}\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1} \\ &= \sigma^2(\mathbf{X}^T\mathbf{X})^{-1},\end{aligned} \tag{5}$$

revealing, as first noted by Hanks et al. (2015), that the nominal covariance matrices of the RSR and OLS estimators of $\boldsymbol{\beta}$ do indeed coincide. In the same way, it may be shown that the nominal covariance matrices of *every* deconfounded estimator and $\hat{\boldsymbol{\beta}}$ coincide. Of course, these are not the estimators' "true" covariance matrices, that is, they are not the covariance matrices under the SLMM. The covariance matrix of an arbitrary deconfounded estimator under the SLMM is (by the equivalence among estimators established in the previous subsection) the same as that of $\hat{\boldsymbol{\beta}}$ under the SLMM, implying that

$$\begin{aligned}\mathrm{var}_{\mathrm{SLMM}}(\breve{\boldsymbol{\beta}}_D) &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{\Sigma}_{\mathrm{SLMM}}\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1} \\ &= \sigma^2[(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{G}\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1} + (\mathbf{X}^T\mathbf{X})^{-1}].\end{aligned}$$

The nominal and true covariance matrices just described are of interest because the advocates of restricted spatial regression have suggested that confidence intervals for the elements of $\boldsymbol{\beta}$ may be obtained by applying standard GLS methods to the deconfounded models (for which the mathematical expressions include nominal variances of the estimators). This leads to the question of how the nominal covariance matrix compares to the corresponding true covariance matrix and to the covariance matrix of $\tilde{\boldsymbol{\beta}}$. The well-known Gauss–Markov theorem tells us that

$$\mathrm{var}_{\mathrm{SLMM}}(\tilde{\boldsymbol{\beta}}) \le \mathrm{var}_{\mathrm{SLMM}}(\breve{\boldsymbol{\beta}}_D) \tag{6}$$

(in the sense that the matrix on the right minus that on the left is a nonnegative-definite matrix). Furthermore,

$$\mathrm{var}_D(\breve{\boldsymbol{\beta}}_D) \le \mathrm{var}_{\mathrm{SLMM}}(\tilde{\boldsymbol{\beta}}). \tag{7}$$

To see why Equation (7) holds, note first that $(\mathbf{I} + \mathbf{G})^{-1} = \mathbf{I} - (\mathbf{G}^{-1} + \mathbf{I})^{-1}$ by the Sherman-Woodbury-Morrison (SWM) formula. Then

$$\begin{aligned}\mathbf{X}^T(\mathbf{I} + \mathbf{G})^{-1}\mathbf{X} &= \mathbf{X}^T[\mathbf{I} - (\mathbf{G}^{-1} + \mathbf{I})^{-1}]\mathbf{X} \\ &= \mathbf{X}^T\mathbf{X} - \mathbf{X}^T(\mathbf{G}^{-1} + \mathbf{I})^{-1}\mathbf{X} \le \mathbf{X}^T\mathbf{X},\end{aligned}$$

yielding

$$(\mathbf{X}^T\mathbf{X})^{-1} \leq [\mathbf{X}^T(\mathbf{I}+\mathbf{G})^{-1}\mathbf{X}]^{-1} \tag{8}$$

and the claimed relation between covariance matrices. Thus, the nominal variance of any deconfounded estimator of an element of $\boldsymbol{\beta}$ coincides with that of the corresponding element of $\hat{\boldsymbol{\beta}}$ and is less than or equal to the variance of the corresponding element of $\tilde{\boldsymbol{\beta}}$, which in turn is less than or equal to the true variance of the deconfounded estimator. This suggests that if σ^2 was known, then using the nominal variance of a deconfounded estimator in a confidence interval for an element of $\boldsymbol{\beta}$ or any other linear combination of the elements of $\boldsymbol{\beta}$ (such as any that correspond to spatial smoothing) would result in an anticonservative (too narrow) interval. Before we can make or modify this conclusion for the practical case of unknown σ^2, however, we must consider how the generalized residual mean squares compare across the different models.

3.3. Equivalences and Relationships Among Residual Mean Squares

By the SWM formula once more,

$$\begin{aligned}&[\mathbf{I}+(\mathbf{I}-\mathbf{P}_\mathbf{X})\mathbf{G}(\mathbf{I}-\mathbf{P}_\mathbf{X})]^{-1}\\ &\quad=\mathbf{I}-(\mathbf{I}-\mathbf{P}_\mathbf{X})(\mathbf{G}^{-1}+\mathbf{I}-\mathbf{P}_\mathbf{X})^{-1}(\mathbf{I}-\mathbf{P}_\mathbf{X}).\end{aligned}$$

Using this result, we find that

$$\begin{aligned}\breve{\sigma}^2_{\mathrm{RSR}} &= \mathbf{y}^T(\mathbf{I}-\mathbf{P}_\mathbf{X})[\mathbf{I}-(\mathbf{I}-\mathbf{P}_\mathbf{X})(\mathbf{G}^{-1}+\mathbf{I}-\mathbf{P}_\mathbf{X})^{-1}\\ &\quad\times(\mathbf{I}-\mathbf{P}_\mathbf{X})](\mathbf{I}-\mathbf{P}_\mathbf{X})\mathbf{y}/(n-p)\\ &= \hat{\sigma}^2 - \mathbf{y}^T(\mathbf{I}-\mathbf{P}_\mathbf{X})(\mathbf{G}^{-1}+\mathbf{I}-\mathbf{P}_\mathbf{X})^{-1}\\ &\quad\times(\mathbf{I}-\mathbf{P}_\mathbf{X})\mathbf{y}/(n-p).\end{aligned} \tag{9}$$

This shows that the generalized residual mean square from the GLS fit of the RSRM is numerically smaller (with probability one) than the ordinary residual mean square from the Gauss–Markov model—a fact that was also noted by Hanks et al. (2015, p. 246), but without explanation. Remarkably, it can further be shown that

$$\breve{\sigma}^2_{\mathrm{RSR}} = \tilde{\sigma}^2. \tag{10}$$

This equality is all the more surprising in light of the fact that $\breve{\boldsymbol{\beta}}_{\mathrm{RSR}} \neq \tilde{\boldsymbol{\beta}}$ in general. And, it has tremendously important consequences for confidence intervals of linear functions of $\boldsymbol{\beta}$ based on deconfounded models, as shown in the next subsection. To prove Equation (10), we first present the following lemma, which is of some interest in its own right. Because the lemma and its proof are quite elementary, it is plausible that they have already appeared somewhere in the literature on linear model theory, but if so, we have not found them. A proof of the lemma is given in Appendix 1.

Lemma 1. Consider two normal linear models, both given by the model equation $\mathbf{y}=\mathbf{X}\boldsymbol{\beta}+\mathbf{e}$, where the error vector $\mathbf{e}$ is normally distributed with expectation $\mathbf{0}$ (under both models) but different positive definite covariance matrices: $\sigma^2\mathbf{W}_1$ or $\sigma^2\mathbf{W}_2$. Let S_1^2 and S_2^2 denote the generalized residual mean squares obtained by fitting the two models by generalized least squares. Then $S_1^2 = S_2^2$ for all $\mathbf{y}$ if and only if $\mathbf{W}_2 = \mathbf{W}_1 + \mathbf{X}\mathbf{C} + \mathbf{C}^T\mathbf{X}^T$ for some matrix $\mathbf{C}$.

Since

$$\begin{aligned}(1/\sigma^2)\boldsymbol{\Sigma}_{\mathrm{RSRM}} &= (\mathbf{I}-\mathbf{P}_\mathbf{X})\mathbf{G}(\mathbf{I}-\mathbf{P}_\mathbf{X})+\mathbf{I}\\ &= \mathbf{G}+\mathbf{I}-\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{G}\\ &\quad-\mathbf{G}\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T+\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{G}\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T,\end{aligned}$$

it becomes apparent that $(1/\sigma^2)\boldsymbol{\Sigma}_{\mathrm{RSRM}}$ has the form specified in Lemma 1 with $\mathbf{W}_1 = \mathbf{G}+\mathbf{I}$ and $\mathbf{C} = -(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{G} + \frac{1}{2}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{G}\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$. This establishes Equation (10).

The same argument that was used to establish Equation (9) may also be used to show that $\breve{\sigma}^2_{\mathrm{Moran}}$ is also less than $\hat{\sigma}^2$. In general, however, $\boldsymbol{\Sigma}_{\mathrm{Moran}}$ does not have the structure specified by Lemma 1, so $\breve{\sigma}^2_{\mathrm{Moran}}$ is not equal to $\breve{\sigma}^2_{\mathrm{RSR}}$; furthermore, numerical examples reveal that neither is almost surely greater than or equal to the other. The question then arises as to whether one of the corresponding expectations under the SLMM is greater than the other. A standard result for the expectation of a quadratic form, for example, Schott (2005, theor. 10.18), may be used to show that

$$\begin{aligned}&E_{\mathrm{SLMM}}(\breve{\sigma}^2_{\mathrm{Moran}}) - E_{\mathrm{SLMM}}(\breve{\sigma}^2_{\mathrm{RSR}})\\ &\quad= [\sigma^2/(n-p)]\mathrm{trace}[(\boldsymbol{\Sigma}^{-1}_{\mathrm{Moran}} - \boldsymbol{\Sigma}^{-1}_{\mathrm{RSRM}})\boldsymbol{\Sigma}_{\mathrm{SLMM}}].\end{aligned}$$

The matrix $\boldsymbol{\Sigma}^{-1}_{\mathrm{Moran}} - \boldsymbol{\Sigma}^{-1}_{\mathrm{RSRM}}$ is generally not nonnegative definite, so determining which estimator has the larger expectation does not appear to be straightforward. However, for all models considered in the simulation study of Section 4, the expectation of $\breve{\sigma}^2_{\mathrm{Moran}}$ exceeded that of $\breve{\sigma}^2_{\mathrm{RSR}}$.

3.4. Comparisons of Confidence Intervals

Associated with each deconfounded estimation procedure is a confidence interval for any linear function $\mathbf{c}^T\boldsymbol{\beta}$ having arbitrary nominal coverage probability $1-\alpha$, where $0 < \alpha < 1$. This confidence interval is of the form

$$\mathbf{c}^T\breve{\boldsymbol{\beta}}_D \pm t_{\alpha/2,n-p}[(\breve{\sigma}^2_D/\sigma^2)\mathbf{c}^T\mathrm{var}_D(\breve{\boldsymbol{\beta}}_D)\mathbf{c}]^{1/2},$$

where $t_{\alpha/2,n-p}$ is the $100(1-\alpha/2)$th percentile of the central t distribution with $n-p$ degrees of freedom. Using results from previous subsections, we can compare the widths of these confidence intervals to each other and to the width of the standard confidence interval based on the SLMM. Specifically, by Equations (7) and (10), the nominal $100(1-\alpha)\%$ confidence interval for $\mathbf{c}^T\boldsymbol{\beta}$ based on the RSRM is narrower than the standard SLMM-based confidence interval, with the consequence that the RSRM-based interval is invalid (it undercovers). Moreover, by Equation (6), the $100(1-\alpha)\%$ RSRM-based interval would need to be even wider than the SLMM-based $100(1-\alpha)\%$ confidence interval to be valid.

The results of the previous subsection also reveal that neither of the nominal $100(1-\alpha)\%$ confidence intervals for $\mathbf{c}^T\boldsymbol{\beta}$ based on the RSR and HH2013 models is almost surely wider than the other. It remains an open question whether the expected width of one of these intervals is larger than the other; however, the empirical average width of the latter was larger than that of the former for all models considered in the simulation study of Section 4.

3.5. Accounting for the Estimation of Covariance Parameters

Now suppose that $\boldsymbol{\theta}$ is unknown, and that a likelihood-based estimate $\hat{\boldsymbol{\theta}}$ is used in place of $\boldsymbol{\theta}$ to evaluate the covariance matrix in the expression for a deconfounded estimator. Such a covariance matrix still has Rao's structure, hence the deconfounded estimators continue to equal each other and $\hat{\boldsymbol{\beta}}$. Moreover, the simple argument that led to expression (5) for the nominal covariance matrix of the RSR estimator continues to apply, so the nominal covariance matrices of all deconfounded estimators continue to coincide with that of the OLS estimator. Their true covariance matrices likewise are unaffected by the lack of knowledge of $\boldsymbol{\theta}$ and thus are still at least as large as their nominal counterparts. Khan and Calder (2020, theor. 2) established an analogous result in a Bayesian context; however, the argument presented here is much more straightforward.

Although the sampling properties of deconfounded estimators are not affected by the estimation of $\boldsymbol{\theta}$, those of $\tilde{\boldsymbol{\beta}}$ are. However, it is known that the empirical GLS estimator of $\boldsymbol{\beta}$ is unbiased (under the SLMM) and has variance at least as large as the GLS estimator, provided that these moments exist (Kackar and Harville 1984). Thus, Equation (7) still holds for the empirical GLS estimator (subject to the existence-of-moments proviso). Whether Equation (6) also holds for the empirical GLS estimator is not known; in any case, knowledge of the relationship between the true covariance matrices of the empirical GLS estimator and a deconfounded estimator is unimportant insofar as the merits of proposed restricted spatial regression methods are concerned. Furthermore, the proofs of Equations (9) and (10) apply equally well whether $\mathbf{G}$ is evaluated at $\boldsymbol{\theta}$ or $\hat{\boldsymbol{\theta}}$. Thus, while the nominal $100(1-\alpha)\%$ confidence interval based on the empirical GLS estimator may undercover to some extent, its coverage probability remains larger than that of the nominal $100(1-\alpha)\%$ confidence interval corresponding to any deconfounded estimator. Incidentally, methods exist for modifying confidence intervals based on the empirical GLS estimator so that they achieve near-nominal coverage; see Jeske and Harville (1988) and Kenward and Roger (1997).

4. Effects of Deconfounding on Prediction

RHZ2006 and HR2010 originally proposed restricted spatial regression for the purpose of improving estimation of fixed effects. Their setting was one in which the support of the data was areal, and in that setting spatial prediction is usually not relevant. However, for geostatistical data, spatial prediction is extremely relevant. Page et al. (2017) studied the effects of spatial confounding on prediction, and Hanks et al. (2015) considered how the restrictions of RSR might be modified for the purpose of prediction in a geostatistical setting, but neither group of authors actually investigated the effects of RSR on prediction. In this section we summarize what we have discovered about those effects. For simplicity, we assume that $\boldsymbol{\theta}$ is known; extensions to the case where $\boldsymbol{\theta}$ is unknown are analogous to those described for estimation in Section 3.5.

Let $\mathbf{y}_u$ represent a vector of unobserved responses at n_u arbitrary spatial locations. Augmented for the purpose of prediction of $\mathbf{y}_u$, the SLMM becomes

$$\begin{pmatrix} \mathbf{y}_o \\ \mathbf{y}_u \end{pmatrix} = \begin{pmatrix} \mathbf{X}_o \\ \mathbf{X}_u \end{pmatrix} \boldsymbol{\beta} + \begin{pmatrix} \mathbf{b}_o \\ \mathbf{b}_u \end{pmatrix} + \begin{pmatrix} \mathbf{d}_o \\ \mathbf{d}_u \end{pmatrix}, \tag{11}$$

where the quantities subscripted by "o" (for "observed") are identical to the quantities defined formerly without a subscript and the quantities subscripted by "u" (for "unobserved") are defined analogously but for the unobserved responses. The same model may be written more succinctly as

$$\mathbf{y}_+ = \mathbf{X}_+\boldsymbol{\beta} + \mathbf{b}_+ + \mathbf{d}_+.$$

The joint distribution of the observed and unobserved responses under this augmented SLMM is multivariate normal with mean vector $\mathbf{X}_+\boldsymbol{\beta}$ and covariance matrix

$$\boldsymbol{\Sigma}_{\text{SLMM}+} \equiv \sigma^2 \begin{pmatrix} \mathbf{G}_{oo} + \mathbf{I}_n & \mathbf{G}_{ou} \\ \mathbf{G}_{ou}^T & \mathbf{G}_{uu} + \mathbf{I}_{n_u} \end{pmatrix} \equiv \sigma^2(\mathbf{G}_+ + \mathbf{I}),$$

where the upper left block, $\sigma^2(\mathbf{G}_{oo} + \mathbf{I}_n)$, was written previously as $\boldsymbol{\Sigma}_{\text{SLMM}}$. The vector of best linear unbiased predictors (BLUPs) of $\mathbf{y}_u$ under this model is

$$\tilde{\mathbf{y}}_u = \mathbf{X}_u\tilde{\boldsymbol{\beta}} + \mathbf{G}_{ou}^T(\mathbf{G}_{oo} + \mathbf{I})^{-1}(\mathbf{y}_o - \mathbf{X}_o\tilde{\boldsymbol{\beta}}),$$

for which the covariance matrix of prediction errors is

$$\begin{aligned}
&\text{var}_{\text{SLMM}+}(\tilde{\mathbf{y}}_u - \mathbf{y}_u) = \sigma^2\{(\mathbf{G}_{uu} + \mathbf{I}_{n_u}) \\
&\quad - \mathbf{G}_{ou}^T(\mathbf{G}_{oo} + \mathbf{I})^{-1}\mathbf{G}_{ou} + [\mathbf{X}_u^T - \mathbf{X}_o^T(\mathbf{G}_{oo} + \mathbf{I})^{-1}\mathbf{G}_{ou}]^T \\
&\quad \times [\mathbf{X}_o^T(\mathbf{G}_{oo} + \mathbf{I})^{-1}\mathbf{X}_o]^{-1}[\mathbf{X}_u^T - \mathbf{X}_o^T(\mathbf{G}_{oo} + \mathbf{I})^{-1}\mathbf{G}_{ou}]\}.
\end{aligned}$$

How might one deconfound the augmented SLMM for the purpose of prediction, and how is prediction affected by the deconfounding? Hanks et al. (2015) argued that the most natural way to extend the restrictions of RSR to model (11) is to restrict the augmented random effects vector $\mathbf{b}_+$ to be orthogonal to the augmented model matrix $\mathbf{X}_+$. Using this restriction, best linear unbiased prediction under the augmented SLMM is replaced with best linear unbiased prediction under the augmented RSRM

$$\mathbf{y}_+ = \mathbf{X}_+\boldsymbol{\beta} + (\mathbf{I}_{n+n_u} - \mathbf{P}_{\mathbf{X}_+})\mathbf{b}_+ + \mathbf{d}_+, \tag{12}$$

where $\mathbf{P}_{\mathbf{X}_+} = \mathbf{X}_+(\mathbf{X}_+^T\mathbf{X}_+)^{-1}\mathbf{X}_+^T$. The marginal covariance matrix of $\mathbf{y}_+$ under this model is

$$\begin{aligned}
\text{var}(\mathbf{y}_+) &\equiv \boldsymbol{\Sigma}_{\text{RSRM}+} \\
&= \sigma^2\left[(\mathbf{I}_{n+n_u} - \mathbf{P}_{\mathbf{X}_+})\begin{pmatrix} \mathbf{G}_{oo} & \mathbf{G}_{ou} \\ \mathbf{G}_{ou}^T & \mathbf{G}_{uu} \end{pmatrix}(\mathbf{I}_{n+n_u} - \mathbf{P}_{\mathbf{X}_+}) + \mathbf{I}_{n+n_u}\right] \\
&= \sigma^2\begin{pmatrix} \mathbf{V}_{oo} & \mathbf{V}_{ou} \\ \mathbf{V}_{ou}^T & \mathbf{V}_{uu} \end{pmatrix},
\end{aligned}$$

say, where $\mathbf{V}_{oo}$ is $n \times n$. The BLUP of $\mathbf{y}_u$ under this model is

$$\breve{\mathbf{y}}_u = \mathbf{X}_u\breve{\boldsymbol{\beta}}_{\text{RSR}+} + \mathbf{V}_{ou}^T\mathbf{V}_{oo}^{-1}(\mathbf{y}_o - \mathbf{X}_o\breve{\boldsymbol{\beta}}_{\text{RSR}+}),$$

where $\breve{\boldsymbol{\beta}}_{\text{RSR}+}$ is the GLS estimator of $\boldsymbol{\beta}$ under this model (which generally differs from $\tilde{\boldsymbol{\beta}}$, and also from $\breve{\boldsymbol{\beta}}_{\text{RSR}}$). The nominal covariance matrix of prediction errors of $\breve{\mathbf{y}}_u$ is

$$\begin{aligned}
&\text{var}_{\text{RSRM}+}(\breve{\mathbf{y}}_u - \mathbf{y}_u) = \sigma^2[(\mathbf{V}_{uu} - \mathbf{V}_{ou}^T\mathbf{V}_{oo}^{-1}\mathbf{V}_{ou} \\
&\quad + (\mathbf{X}_u^T - \mathbf{X}_o^T\mathbf{V}_{oo}^{-1}\mathbf{V}_{ou})^T(\mathbf{X}_o^T\mathbf{V}_{oo}^{-1}\mathbf{X}_o)^{-1} \\
&\quad \times (\mathbf{X}_u^T - \mathbf{X}_o^T\mathbf{V}_{oo}^{-1}\mathbf{V}_{ou})].
\end{aligned}$$

After tedious calculations (see Appendix 2), it can be shown that $\boldsymbol{\Sigma}_{\mathrm{RSRM}+}$ satisfies the conditions of Corollary 2.1 of Haslett and Puntanen (2010), implying, remarkably, that $\check{\mathbf{y}}_u$ and $\tilde{\mathbf{y}}_u$ coincide! However, it also turns out that, analogous to (7),

$$\mathrm{var}_{\mathrm{RSRM}+}(\check{\mathbf{y}}_u - \mathbf{y}_u) \leq \mathrm{var}_{\mathrm{SLMM}+}(\tilde{\mathbf{y}}_u - \mathbf{y}_u), \tag{13}$$

and that the generalized residual mean squares under the augmented RSRM and SLMM coincide. These additional results also are proved in Appendix 2. Thus, prediction intervals for $\mathbf{y}_u$ based on the augmented RSRM will tend to undercover, just as their confidence interval counterparts do.

5. Illustrative Example

To illustrate the undercoverage of confidence and prediction intervals proved analytically in this article, and to better understand the magnitude of the undercoverage, let us consider an example of data simulated from a spatial linear mixed model on a $k \times k$ square grid with $k = 5$ or 10 and unit spacing. Let $\sigma^2 = 1$ and take the elements of $\mathbf{G}$ to be determined by the isotropic correlation function $\rho(r) = \rho^r$ where $\rho = 0.2$, 0.5, or 0.8 and r is the Euclidean distance between sites. Furthermore, consider four cases of the model matrix $\mathbf{X}$. Each case has two columns, of which the first is a column of ones (corresponding to an overall intercept) and the second is either:

(i) a fixed vector with elements equal to the mean-corrected sum of the row and column grid indices of the corresponding observations, so that $\mathbf{X}\boldsymbol{\beta}$ is a linear trend from the lower left to upper right corners of the grid;
(ii) a fixed vector with elements equal to the same values as in Case i, but rearranged so that $\mathbf{X}\boldsymbol{\beta}$ is a parabolic cylinder (approximately) with its ridge of relative maxima extending from the upper left to the lower right grid corners;
(iii) a stochastic vector drawn, independently of $\mathbf{b}$ and $\mathbf{e}$, from a N(0,25/6) distribution (for the 5×5 grid) or a N(0,97/6) distribution (for the 10×10 grid); the means and variances of these normal distributions are identical to the sample means and variances of the fixed regressors in Cases i and ii; and
(iv) a stochastic vector drawn jointly with $\mathbf{b}$ from a $2k^2$-dimensional normal distribution with mean vector $\mathbf{0}$ and covariance matrix $\begin{pmatrix} \tau^2\mathbf{G} & \gamma\tau\mathbf{G} \\ \gamma\tau\mathbf{G} & \mathbf{G} \end{pmatrix}$ (but still independently of $\mathbf{e}$), where $\tau^2 = 25/6$ or $97/6$, and $\gamma = 0.5$ or 0.2, for the 5×5 and 10×10 grids, respectively. The means and variances of the regressors are identical to those in Case iii, but the correlation between each element of $\mathbf{b}$ and the corresponding element of the second column of $\mathbf{X}$ is either 0.5 (when $k = 5$) or 0.2 (when $k = 10$), which causes these two vectors to be moderately or slightly collinear.

For all cases, the true value of $\boldsymbol{\beta} = (\beta_0, \beta_1)^T$ is taken to be $(1, 1)^T$. We estimate $\boldsymbol{\beta}$ (and σ^2) as if ρ was known, so that GLS rather than more computationally demanding empirical GLS methods may be used. It is the (interval) estimation of β_1 that is of particular interest.

Table 1 gives the empirical coverage probability of the nominal 95% confidence interval for β_1 based on 10,000 pseudo-random samples, for each of four estimation methods: GLS, OLS, RSR, and Moran. Results for the RSR and Moran variants were very similar to those for the versions introduced in Section 2, hence not shown. (Following HH2013's suggestion, for their method only the eigenvectors corresponding to positive eigenvalues were included in $\mathbf{M}$). As expected, the coverage probability of the confidence interval corresponding to GLS estimation is very close to 95% except in Case iv; its drop in that case occurs primarily because the interval is not centered properly, due to the well-known bias incurred in estimating spatial regression coefficients by standard methods when regressors are stochastic and correlated with model errors (Paciorek 2010). Correlations larger than those used for Case iv resulted in even worse bias and very poor coverage; of course, if there is concern that it may be more realistic to regard the regressors as stochastic and correlated with model errors, other interval estimation methods, such as those based on measurement-error models, may have better unconditional coverage. Also as expected, the OLS-based confidence interval's coverage probability is uniformly less than that of the GLS-based interval; its relative performance, though not terrible when the spatial correlation is relatively weak, deteriorates rapidly as the spatial correlation gets stronger. But most importantly insofar as the main thrust of this article is concerned, coverage probabilities of intervals corresponding to all of the restricted spatial regression methods are uniformly less than those of the GLS-based and OLS-based intervals, regardless of grid size, strength of spatial correlation, whether the regressors are fixed or stochastic, or how collinear the regressor is with the random effect. The Moran-based confidence interval performs somewhat better overall than its RSR counterpart, but is still badly anticonservative.

Hanks et al. (2015) performed a simulation study comparing GLS and RSR to each other in a scenario similar to our Case iv, obtaining results broadly equivalent to ours for that case.

The deleterious effects of deconfounding on interval estimation of fixed effects carry over to smoothing. To illustrate,

Table 1. Empirical coverage probability of the nominal 95% confidence interval for the slope parameter based on OLS, GLS, and two restricted spatial regression methods.

		Empirical coverage probability (under SLMM)					
		$k = 5$			$k = 10$		
Case	Estimator	$\rho = 0.2$	$\rho = 0.5$	$\rho = 0.8$	$\rho = 0.2$	$\rho = 0.5$	$\rho = 0.8$
i	GLS	0.951	0.951	0.946	0.952	0.948	0.951
	OLS	0.912	0.829	0.797	0.884	0.692	0.518
	RSR	0.791	0.705	0.730	0.734	0.552	0.433
	Moran	0.866	0.759	0.751	0.813	0.596	0.445
ii	GLS	0.954	0.950	0.947	0.945	0.954	0.951
	OLS	0.932	0.911	0.922	0.887	0.779	0.724
	RSR	0.815	0.807	0.872	0.745	0.627	0.609
	Moran	0.884	0.851	0.886	0.824	0.676	0.629
iii	GLS	0.951	0.951	0.950	0.951	0.951	0.952
	OLS	0.944	0.915	0.887	0.942	0.869	0.721
	RSR	0.837	0.815	0.829	0.821	0.726	0.611
	Moran	0.901	0.856	0.848	0.889	0.774	0.631
iv	GLS	0.600	0.669	0.788	0.715	0.763	0.844
	OLS	0.588	0.617	0.695	0.694	0.667	0.622
	RSR	0.380	0.447	0.611	0.481	0.501	0.520
	Moran	0.480	0.515	0.639	0.582	0.548	0.539

NOTE: Probabilities for a given grid size ($k \times k$) and correlation strength (ρ) are estimated from the same 10,000 pseudo-random samples; hence their standard errors are bounded above by 0.005.

consider the 95% confidence interval for $E(y|x = 5)$ in Case i with $k = 5$ and $\rho = 0.5$. Using the same simulated realizations that yielded the entries in Table 1 for this case, empirical coverage probabilities of the intervals obtained using the GLS, OLS, RSR, and Moran approaches were 0.948, 0.703, 0.579, and 0.633, respectively. These coverage probabilities, except for that corresponding to GLS, are substantially lower than the confidence intervals for the slope coefficient itself.

Finally, we also considered the effect of deconfounding on prediction intervals. For all of the same cases for which empirical coverage probabilities of confidence intervals for the slope were reported in Table 1, we obtained empirical coverage probabilities of the 95% prediction intervals for a single predictand using the augmented SLMM and RSRM approaches. We took the predictand to be the value of the response at one of the four corner sites of the grid, which was predicted using the observations at the remaining sites (which numbered 24 or 99, according to whether $k = 5$ or $k = 10$). As expected, the coverage probability of the augmented SLMM-based interval was very close to 0.95 and larger than the coverage probability of the augmented RSRM-based interval, but in no case was the difference in coverage probabilities larger than 0.011. Thus, while deconfounding results in inferior predictive inferences, the harm it inflicts on them appears to be small in practice.

6. Discussion

We have shown analytically, in a frequentist linear model context with fixed regressors, that spatial deconfounding methodologies, a.k.a. restricted spatial regression methods, produce inferences for the fixed effects that are inferior to those obtained by applying standard GLS methods to the original spatial linear mixed model. In fact, spatial deconfounding-based inferences for fixed effects are not even as good as those obtained by applying OLS methods to the corresponding nonspatial Gauss-Markov model (for which there is likewise no spatial confounding). Our simulation-based results indicate that the adverse effects of deconfounding on fixed effects estimation and smoothing can be quite serious in practice and also demonstrate that deconfounding-based inferences are inferior when the regressors are stochastic, whether or not they are correlated with the random effects. We have also shown analytically that deconfounding adversely affects predictive inference, although the best linear unbiased predictors under versions of the RSR and spatial linear models augmented for prediction are identical and deconfounding's effects on prediction in practice are much smaller than its effects on estimation. Thus, insofar as prediction is concerned, deconfounding might best be described as superfluous rather than harmful.

Based on these facts, it is our view that restricted spatial regression methods should never be used when the classical spatial linear mixed model is the true or intended model, regardless of any spatial confounding. Instead, we recommend sticking with standard empirical GLS methods. The latter yield valid confidence and prediction intervals (in the fixed regressors setting) whether or not the estimated fixed effects are appreciably affected by spatial confounding. If a data analyst were to insist that spatial confounding had, to paraphrase a portion of the title of HR2010, "messed up the fixed effect that they love" by causing its estimate to stray too far from its true value (which is what RHZ2006 imply happened to the effect of socioeconomic status on stomach cancer, as described in Section 1), then we would recommend that they proceed with either of two alternatives. One is to revert to inference based on the Gauss–Markov model, which though also invalid, is not as bad as inference based on restricted spatial regression; furthermore, it could be made less anticonservative (perhaps too much so, however!) by replacing the nominal variance of the OLS estimator in the confidence interval's expression with its true variance under the spatial model. A second option—this one yielding valid inferences—is to constrain the parameter space of the cherished fixed effect to an interval within which the analyst believes that it lies, and then estimate it subject to this constraint. In a likelihood-based framework, this would require maximizing the likelihood over the constrained parameter space; in a Bayesian framework it could be accomplished by placing a highly informative prior on the effect.

Finally, lest it be thought that deconfounding, despite its inferential shortcomings, might have computational advantages over GLS estimation of the SLMM, we offer the following counterargument. It is certainly true that the HH2013 version of deconfounding presents an opportunity to reduce the computational burden of estimation for large spatial datasets. As HH2013 demonstrated, this opportunity arises because (i) the eigenvectors of the Moran operator $(\mathbf{I} - \mathbf{P_X})\mathbf{A}(\mathbf{I} - \mathbf{P_X})$ are strongly spatially structured, (ii) the eigenvalues of that operator take on many distinct values, including many that are close to 0 or negative, and (iii) the eigenvectors corresponding to larger positive eigenvalues have the larger scale structure. The precision matrix for the HH2013 model may therefore be approximated using a truncated spectral decomposition of the Moran operator that includes a relatively small proportion (they recommend 10%) of the eigenvectors. A similar opportunity does not arise with the ordinary RSRM because $\mathbf{I} - \mathbf{P_X}$ is not strongly spatially structured and its eigenvalues are mostly equal to 1 (with a few zeros). However, a similar potential for computational gains does exist for the SLMM because its covariance matrix can also be well-approximated by a truncated spectral decomposition with relatively few eigenvectors. In fact, fixed-rank kriging (Cressie and Johannesson 2008) is tantamount to such an approach, and of course there are many other methods for reducing the computational burden of (maximum likelihood) estimation in spatial linear models, for example, Gaussian predictive process models (Banerjee et al. 2008), covariance tapering (Kaufman, Schervish, and Nychka 2008), and data partitioning (Vecchia 1988; Stein, Chi, and Welty 2004). Thus, neither RSR nor its HH2013 variant have an inherent computational advantage over GLS applied to the SLMM.

Appendix 1. Proof of Lemma 1

Define $\mathbf{E}_1 = \mathbf{W}_1^{-1} - \mathbf{W}_1^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{X})^{-}\mathbf{X}^T\mathbf{W}_1^{-1}$ and $\mathbf{E}_2 = \mathbf{W}_2^{-1} - \mathbf{W}_2^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_2^{-1}\mathbf{X})^{-}\mathbf{X}^T\mathbf{W}_2^{-1}$, where $\mathbf{Q}^{-}$ denotes an arbitrary generalized inverse of any matrix $\mathbf{Q}$. Then $S_1^2 = \mathbf{y}^T\mathbf{E}_1\mathbf{y}/[n - \text{rank}(\mathbf{X})]$ and $S_2^2 = \mathbf{y}^T\mathbf{E}_2\mathbf{y}/[n - \text{rank}(\mathbf{X})]$ where n denotes the number of rows of $\mathbf{X}$. It may be verified easily that $\mathbf{E}_1\mathbf{X} = \mathbf{E}_2\mathbf{X} = \mathbf{0}$, $\mathbf{E}_1\mathbf{W}_1\mathbf{E}_1 = \mathbf{E}_1$, and

$\mathbf{E}_2\mathbf{W}_2\mathbf{E}_2 = \mathbf{E}_2$. Furthermore,

$$\begin{aligned}\mathbf{E}_1\mathbf{W}_1\mathbf{E}_2 &= [\mathbf{W}_1^{-1} - \mathbf{W}_1^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_1^{-1}]\mathbf{W}_1 \\ &\quad \times [\mathbf{W}_2^{-1} - \mathbf{W}_2^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_2^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_2^{-1}] \\ &= \mathbf{W}_2^{-1} - \mathbf{W}_1^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_2^{-1} \\ &\quad - \mathbf{W}_2^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_2^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_2^{-1} \\ &\quad + \mathbf{W}_1^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_2^{-1} \\ &= \mathbf{E}_2\end{aligned}$$

and similarly $\mathbf{E}_1\mathbf{W}_2\mathbf{E}_2 = \mathbf{E}_1$. Still further, it is easily verified that $\mathbf{W}_1\mathbf{E}_1\mathbf{W}_2 = \mathbf{W}_2 - \mathbf{X}(\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{W}_2$ and $\mathbf{W}_1\mathbf{E}_2\mathbf{W}_2 = \mathbf{W}_1 - \mathbf{W}_1\mathbf{W}_2^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_2^{-1}\mathbf{X})^-\mathbf{X}^T$.

Now suppose that $\mathbf{W}_2 = \mathbf{W}_1 + \mathbf{X}\mathbf{C} + \mathbf{C}^T\mathbf{X}^T$ for some matrix $\mathbf{C}$. Then using some of the preceding results,

$$\begin{aligned}\mathbf{E}_1 &= \mathbf{E}_1\mathbf{W}_2\mathbf{E}_2 \\ &= \mathbf{E}_1\mathbf{W}_1\mathbf{E}_2 + \mathbf{E}_1\mathbf{X}\mathbf{C}\mathbf{E}_2 + \mathbf{E}_1\mathbf{C}^T\mathbf{X}^T\mathbf{E}_2 \\ &= \mathbf{E}_2,\end{aligned}$$

implying that $S_1^2 = S_2^2$ for all $\mathbf{y}$. Conversely, suppose that $S_1^2 = S_2^2$ for all $\mathbf{y}$. Then $\mathbf{E}_1 = \mathbf{E}_2$, implying that $\mathbf{W}_1\mathbf{E}_1\mathbf{W}_2 = \mathbf{W}_1\mathbf{E}_2\mathbf{W}_2$, that is,

$$\begin{aligned}&\mathbf{W}_2 - \mathbf{X}(\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{W}_2 \\ &\quad = \mathbf{W}_1 - \mathbf{W}_1\mathbf{W}_2^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_2^{-1}\mathbf{X})^-\mathbf{X}^T\end{aligned}$$

or equivalently, $\mathbf{W}_2 = \mathbf{W}_1 + \mathbf{X}\mathbf{A} + \mathbf{B}\mathbf{X}^T$ for $\mathbf{A} = (\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{W}_1^{-1}\mathbf{W}_2$ and $\mathbf{B} = -\mathbf{W}_1\mathbf{W}_2^{-1}\mathbf{X}(\mathbf{X}^T\mathbf{W}_2^{-1}\mathbf{X})^-$. Now because $\mathbf{W}_2 - \mathbf{W}_1$ is symmetric, so is $\mathbf{X}\mathbf{A} + \mathbf{B}\mathbf{X}^T$, implying that it is possible to express $\mathbf{W}_2$ equivalently as $\mathbf{W}_1 + \frac{1}{2}(\mathbf{X}\mathbf{A} + \mathbf{B}\mathbf{X}^T) + \frac{1}{2}(\mathbf{A}^T\mathbf{X}^T + \mathbf{X}\mathbf{B}^T) = \mathbf{W}_1 + \mathbf{X}\mathbf{C} + \mathbf{C}^T\mathbf{X}^T$, say, where $\mathbf{C} = \frac{1}{2}(\mathbf{A} + \mathbf{B}^T)$. This completes the proof.

Appendix 2. Derivation of the Effects of Restricted Spatial Regression on Prediction

Observe that

$$\mathbf{X}_+^T\mathbf{X}_+ = (\mathbf{X}_o^T, \mathbf{X}_u^T)\begin{pmatrix}\mathbf{X}_o \\ \mathbf{X}_u\end{pmatrix} = \mathbf{X}_o^T\mathbf{X}_o + \mathbf{X}_u^T\mathbf{X}_u,$$

so by the Sherman–Woodbury–Morrison formula,

$$\begin{aligned}(\mathbf{X}_+^T\mathbf{X}_+)^{-1} &= (\mathbf{X}_o^T\mathbf{X}_o)^{-1} - (\mathbf{X}_o^T\mathbf{X}_o)^{-1}\mathbf{X}_u^T \\ &\quad \times (\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{X}_u(\mathbf{X}_o^T\mathbf{X}_o)^{-1}\end{aligned}$$

where $\mathbf{W}_{uu} = \mathbf{X}_u(\mathbf{X}_o^T\mathbf{X}_o)^{-1}\mathbf{X}_u^T$. Define $\mathbf{W}_{oo} = \mathbf{X}_o(\mathbf{X}_o^T\mathbf{X}_o)^{-1}\mathbf{X}_o^T$ and $\mathbf{W}_{ou} = \mathbf{X}_o(\mathbf{X}_o^T\mathbf{X}_o)^{-1}\mathbf{X}_u^T$. Then routine calculations yield

$$\begin{aligned}&\mathbf{I} - \mathbf{P}_{\mathbf{X}_+} \\ &= \begin{pmatrix}\mathbf{I} - \mathbf{P}_{\mathbf{X}_o} + \mathbf{W}_{ou}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{ou}^T & -\mathbf{W}_{ou} + \mathbf{W}_{ou}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{uu} \\ -\mathbf{W}_{ou}^T + \mathbf{W}_{uu}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{ou}^T & \mathbf{I} - \mathbf{W}_{uu} + \mathbf{W}_{uu}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{uu}\end{pmatrix}.\end{aligned}$$

Substituting this expression into Equation (12) yields, after tedious calculations, a block matrix expression for $(1/\sigma^2)\mathrm{var}(\mathbf{y}_+)$ whose upper left $n \times n$ block is

$$\begin{aligned}\mathbf{V}_{oo} &\equiv (\mathbf{I} - \mathbf{P}_{\mathbf{X}_o})\mathbf{G}_{oo}(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) + \mathbf{W}_{ou}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{ou}^T\mathbf{G}_{oo} \\ &\quad \times (\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) - \mathbf{W}_{ou}\mathbf{G}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) \\ &\quad + \mathbf{W}_{ou}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{uu}\mathbf{G}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) + \mathbf{T}_o\mathbf{X}_o^T + \mathbf{I} \qquad (14)\end{aligned}$$

and lower left $n_u \times n$ block is

$$\begin{aligned}\mathbf{V}_{ou}^T &\equiv -\mathbf{W}_{ou}^T\mathbf{G}_{oo}(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) + \mathbf{W}_{uu}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{ou}^T\mathbf{G}_{oo} \\ &\quad \times (\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) + (\mathbf{I} - \mathbf{W}_{uu})\mathbf{G}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) \\ &\quad + \mathbf{W}_{uu}(\mathbf{I} + \mathbf{W}_{uu})^{-1}\mathbf{W}_{uu}\mathbf{G}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) + \mathbf{T}_u\mathbf{X}_o^T\end{aligned}$$

for some matrices $\mathbf{T}_o$ and $\mathbf{T}_u$ whose exact forms are unimportant for the present purpose. Then

$$\begin{pmatrix}\mathbf{V}_{oo}(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) \\ \mathbf{V}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o})\end{pmatrix} = \begin{pmatrix}(\mathbf{G}_{oo} + \mathbf{I})(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) \\ \mathbf{G}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o})\end{pmatrix} + \begin{pmatrix}\mathbf{X}_o \\ \mathbf{X}_u\end{pmatrix}\mathbf{Q}$$

where again the exact form of $\mathbf{Q}$ is unimportant. Thus,

$$\mathcal{C}\begin{pmatrix}\mathbf{V}_{oo}(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) \\ \mathbf{V}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o})\end{pmatrix} \subset \mathcal{C}\begin{pmatrix}\mathbf{X}_o & (\mathbf{G}_{oo} + \mathbf{I})(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o}) \\ \mathbf{X}_u & \mathbf{G}_{ou}^T(\mathbf{I} - \mathbf{P}_{\mathbf{X}_o})\end{pmatrix},$$

which, by Haslett and Puntanen (2010, corol. 2.1), is sufficient for the BLUP of $\mathbf{y}_u$ under the augmented RSRM to coincide with the BLUP of $\mathbf{y}_u$ under the augmented SLLM.

Next we establish Equation (13). By the coincidence of the BLUPs just established, $\check{\mathbf{y}}_u - \mathbf{y}_u$ and $\tilde{\mathbf{y}}_u - \mathbf{y}_u$ may both be represented as $\mathbf{R}^T\mathbf{y}_+$ for some matrix $\mathbf{R}$. Then exactly the same argument that was used to obtain Equation (8) yields, when applied to the augmented SLMM,

$$(\mathbf{X}_+^T\mathbf{X}_+)^{-1} \le [\mathbf{X}_+^T(\mathbf{I} + \mathbf{G}_+)^{-1}\mathbf{X}_+]^{-1}.$$

Thus,

$$\begin{aligned}&\mathrm{var}_{\mathrm{RSRM}+}(\check{\mathbf{y}}_u - \mathbf{y}_u) = \sigma^2\mathbf{R}^T(\mathbf{X}_+^T\mathbf{X}_+)^{-1}\mathbf{R} \\ &\quad \le \sigma^2\mathbf{R}^T[\mathbf{X}_+^T(\mathbf{I} + \mathbf{G}_+)^{-1}\mathbf{X}_+]^{-1}\mathbf{R} = \mathrm{var}_{\mathrm{SLMM}+}(\tilde{\mathbf{y}}_u - \mathbf{y}_u), \quad (15)\end{aligned}$$

proving (13).

Finally, observe that $\mathbf{V}_{oo}$ as given by Equation (14) may be written as $\mathbf{I} + \mathbf{G}_{oo} + \mathbf{X}\mathbf{A} + \mathbf{B}\mathbf{X}^T$ for some matrices $\mathbf{A}$ and $\mathbf{B}$ and hence as $\mathbf{I} + \mathbf{G}_{oo} + \mathbf{X}\mathbf{C} + \mathbf{C}^T\mathbf{X}^T$ for some matrix $\mathbf{C}$. It follows immediately from Lemma 1 that the generalized residual variances from GLS fits of the augmented RSRM and SLMM coincide. This and Equation (15) imply that the nominal $100(1-\alpha)\%$ prediction interval for $\mathbf{y}_u$ obtained using the augmented RSRM is too narrow.

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