

Can Conventional Measures Identify Geographically Varying Mixed Regression Relationships? A Simulation-based Analysis of Locally Weighted Regression

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1 Background

Imagine a simple linear model,

$$Y = \beta_0 + \beta_1 * X_1 + \beta_2 * X_2 + \epsilon. \quad (1)$$

In addition to the three variables listed above (Y , X_1 , and X_2), assume we know the geographical location for each of our N observations. Thus, our data consists of an $N \times 5$ matrix, where Y may be house prices, X_1 and X_2 could be the living space and lot size associated with each house, and the final two columns determine the location of the observations (for instance, latitude and longitude, or distances north and east from a prescribed point).

The simple model in (1) exemplifies spatial stationarity in the parameters: the β coefficients are constant over space. Alternatively, the coefficients could exhibit spatial non-stationarity, in which case one, two, or all three of the β coefficients are a function of location. This has a natural interpretation in the current real estate example: location matters. However, location can matter in different ways. For instance, if the value of land varies over space, then we would expect the coefficient on lot size to vary over space, while it is also possible that the intercept varies over space to reflect variation in prices of similar houses in different locations.

It is possible to parameterize the variation in coefficients, for instance by including a variable measuring the distance from an observation to an important amenity such as the Central Business District and then this distance variable could be interacted with variables whose value are predicted to vary over space. However, it is not implausible to believe that the variation in coefficients might not be easily parameterized (for instance, if land values are a non-monotonic function of distance). Researchers may instead interact variables with fixed effects for cities or census tracts. However, such strategies require the analyst to make assumptions that severely limit the type and degree of variation in the parameters. For instance, interaction terms with geographic boundaries assume discrete differences

in the value of parameters across the boundaries, while instead the parameters may instead be a continuous function of location. Additionally, numerous interaction terms may unduly reduce the degrees of freedom.

1.1 Geographically Weighted Regression to the Rescue?

Locally Weighted Regression (also referred to as Geographically Weighted Regression) is one possible solution to the challenge presented by spatially non-stationary regression coefficients. Locally Weighted Regression (LWR) techniques (also known as Geographically Weighted Regression) are described in detail by Cleveland and Devlin (1988), Brunsdon et al. (1998), Fotheringham et al. (2002), and others. It is a weighted least squares methodology in which regression coefficients are estimated over space as a function of the local data as described in Equation (2),

$$\hat{\beta}(\text{location}_i) = (X'W(\text{location}_i)X)^{-1}X'W(\text{location}_i)Y, \quad (2)$$

where X is a $N \times 2$ matrix of independent variables, W_i is the $N \times N$ weights matrix, and Y is the $N \times 1$ vector of dependent variable values. The weights matrix, W_i is a diagonal matrix where element w_{jj} denotes the weight that the j^{th} data point will receive in the regression coefficients estimated at location i in the dataset. We employ a bi-square weights function and a k -nearest neighbor bandwidth approach as described in equation (3),

$$w_{jj} = \left[1 - \left(\frac{d_{ij}}{d_k} \right)^2 \right]^2 \text{ if } d_{ij} < d_{ik}, \text{ otherwise } = 0, \quad (3)$$

where d_{ij} denotes the distance between observations i and j , and d_{ik} is the distance from observation i to the k^{th} nearest observation. This function assigns weights close to 1 for data points near observation i , weights positive but closer to zero for observations farther away, and zero for all $n - k$ observations farther away than the k^{th} nearest observation.

A key decision in estimating LWR models is choosing the number of observations to include in the bandwidth. Bandwidths that are too large in the presence of spatial non-stationarity create bias in the regression estimates (the large bandwidth creates weights matrices that are similar over space and therefore the regression coefficients are forced to be similar when they should vary over space). Bandwidths that are too small add unnecessary error in our estimates by excluding informative observations. Often, researchers choose a bandwidth by minimizing a cross validation metric.

This choice is further complicated in the context of mixed models where only some coefficients exhibit spatial stationarity (in contrast to standard models in which all coefficients are treated as spatially stationary or LWR models in which no coefficients are treated as stationary). Little is known about model performance when models are selected across multiple mixed models and among multiple different potential bandwidth sizes. This paper uses simulated data generated under multiple conditions to begin to answer some of the outstanding questions in the area of geographically mixed models.

1.2 Model Selection Metrics

We compare four important cross-validation/information criteria: Leave One Out Cross Validation (LOOCV), Generalized Cross Validation (GCV), Standardized Cross Validation (SCV), and the Akaike Information Criterion (AIC). How frequently can researchers utilizing these metrics identify the correct model among the various possible combinations? Are certain metrics more/less prone to false positive/negatives? Do they suggest no spatial variation when in fact it exists? Do they suggest spatial variation when in fact there is not?

1.2.1 Leave One Out Cross Validation

Perhaps the most common cross validation metric used in the literature is the Leave One Out Cross Validation score (LOOCV), which is calculated as follows,

$$LOOCV = \frac{1}{N} \sqrt{\sum_{i=1}^N (y - \hat{y}_{\neq i})^2}, \quad (4)$$

where $\hat{y}_{\neq i}$ represents the dependent variable estimate for observation i while excluding observation i from the regression. This prevents the observation from having undue influence in the regression with small bandwidths and overfitting the model. Such a model, while intuitively appealing, can be computationally expensive, as regressions must be estimated first while excluding individual observations to calculate the LOOCV and then again while including the observation to obtain the regression coefficients.

1.2.2 Generalized Cross Validation

An alternative cross validation metric is known as the Generalized Cross Validation (GCV) score, which only requires calculating the regressions once per location and explicitly calculates the leverage each observation has over the regression coefficients. The GCV score calculation is detailed in equation (5),

$$n * \sum_{i=1}^n \frac{(y_i - \hat{y}_i)^2}{(n - v_1)^2}, \quad (5)$$

where \hat{y}_i is the predicted dependent variable value for observation i , and v_1 can be interpreted as the “effective number of model parameters,” and calculated as $v_1 = \text{tr}(\mathbf{S})$, where the matrix \mathbf{S} is the “hat matrix” which maps y onto \hat{y} ,

$$\hat{y} = \mathbf{S}y, \quad (6)$$

and each row of \mathbf{S} , r_i is given by:

$$r_i = X_i(X'W_iX)^{-1}X'W_i. \quad (7)$$

The GCV score is a convenient model selection metric that rewards models that provide a good fit to the data, while penalizing models with a greater number of model parameters (Loader, 1999; McMillen and Redfearn, 2010). (Paez et al., 2011; McMillen and Redfearn, 2010; McMillen, 2012).

1.2.3 Standardized Cross Validation

The Standardized Cross Validation Score was suggested by (Farber and Páez, 2007) and elaborated on in (Paez et al., 2011) as an alternative to conventional metrics. This metric is designed to limit the influence of outliers which may disproportionately impact the choice of bandwidth. The Standardized Cross Validation score for a given observation i and bandwidth k is,

$$SCV_i(k) = \frac{\sum (y_i - \hat{y}_{-i}(k))^2}{\sum_k (y_i - \hat{y}_{-i})^2}, \quad (8)$$

and the total score for bandwidth k is then,

$$SCV(k) = \sum_i SCV_i(k). \quad (9)$$

Equation (8) calculates a partial score for each observation as a proportion of the total squared deviance at that observation across the different bandwidths, while (9) then calculates the sum across all observations for a given bandwidth. Note that, contrary to the other metrics described here, the SCV score has to be calculated after all possible bandwidths have been implemented.

1.2.4 Akaike Information Criterion

As noted in (Fotheringham et al., 2002), the well-known Akaike Information Criterion is calculated in the geographically weighted regression framework as follows,

$$2 * n * \ln(\hat{\sigma}) + n * \ln(2 * \pi) + n * \frac{n + v_1}{n - 2 - v_1} \quad (10)$$

where $\hat{\sigma}$ is the estimated standard error of the regression, n is the sample size, and v_1 remains the “effective number of parameters” estimated by the model as described above.

1.3 Experimental Design

For a given sample size, $n \in \{50, 100, 200, 800\}$ we generate an $n \times 4$ matrix of independently uniformly distributed values between 0 and 1. Let the first two of these columns be called *East* and *North* and denote the location of each of our observations within a two-dimensional unit grid (East, North), while the remaining two columns be X_1 and X_2 and serve as the independent variables in our regression equation.

Our goal is to generate data according to the following process:

$$Y_i = \beta_0(East_i, North_i) + \beta_1(East_i, North_i) * X_{1i} + \beta_2(East_i, North_i) * X_{2i} + \epsilon_i, \quad (11)$$

where $\epsilon_i \sim N(0, \sigma^2)$. Equation 11 states that the dependent variable value for a given observation depends on the values of X_1 , X_2 , a normally distributed error term, and the values of three β coefficients, each of which is a function of the location within our dataset.

The relationship between location and β_1 is given by,

$$\beta_1 = 2 + \eta_1 \times (East - .5), \quad (12)$$

where the η_1 parameter changes the degree to which the β_1 coefficient varies over space. When $\eta_1 = 0$, equation (12) simplifies to $\beta_1 = 2$ and there is no spatial variation in the coefficient. When $\eta_1 \in \{1, 2\}$, there is a linear relationship between β_1 and the *East* location of the data point. Note that the expected value of $\beta_1 = 2$ for all three cases of $\eta_1 \in \{0, 1, 2\}$ because of the uniform distribution of $East \in [0, 1]$. A visual representation of the relationship is presented in the first row of Figure 1.

Similar to β_1 , the relationship between location and β_2 is given by,

$$\beta_2 = 2 + \eta_2 \times (North - .5), \quad (13)$$

where the η_2 parameter changes the degree to which the β_2 coefficient varies over space. When $\eta_2 = 0$, equation (13) simplifies to $\beta_2 = 2$ and there is no spatial variation in the coefficient. When $\eta_2 \in \{1, 2\}$, there is a linear relationship between β_2 and the *North* location of the data point. Note that the expected value of $\beta_2 = 2$ for all three cases of $\eta_2 \in \{0, 1, 2\}$ because of the uniform distribution of $North \in [0, 1]$. A visual representation of the relationship is presented in the second row of Figure 1.

The β_1 and β_2 coefficients are orthogonal to one another (β_1 is a function of the *East* locational variable, while β_2 is a function of *North*.) In order to introduce spatial non-stationarity in the β_0 coefficient without also creating high and/or perfect multicollinearity among the coefficients, we generated the β_0 coefficient by the following,

$$\beta_0 = 2 + \eta_0 \times \left[.387452 + \cos \left(2\pi \times \sqrt{\frac{(East - .5)^2 + (North - .5)^2}{.5}} \right) \right], \quad (14)$$

which is presented visually in the third row of Figure 1.

Here are the parameters for the simulation.

```
sampleSizes <- c(50, 100, 200, 400, 800)
B0.SpVar <- c(0, 2, 4)
B1.SpVar <- c(0, 2, 4)
B2.SpVar <- c(0, 2, 4)
errors <- c(0.25, .5, 1, 2, 3)
numRepeats <- 100
```

which we use as follows:

```
n = sampleSize # number of observations in our simulation
east = runif(n) # create a location variable
north = runif(n) # create another location variable
x0 = rep(1, n) # create a vector of 1's to serve as the intercept column
x1 = runif(n) # create a vector for x1 values
```

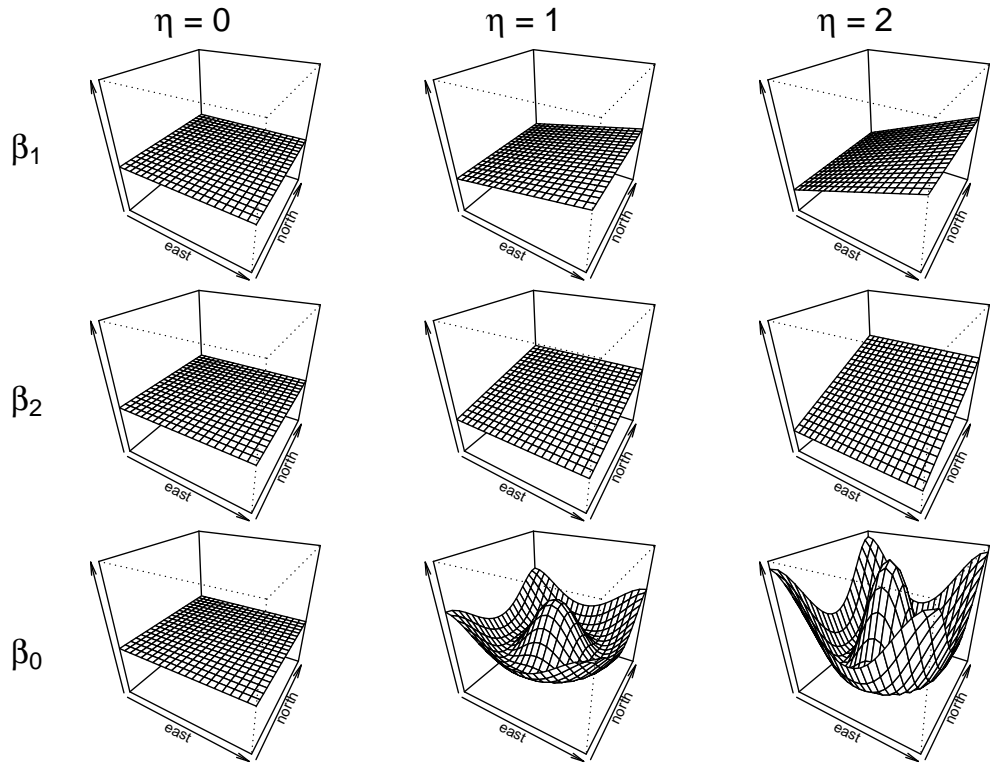


Figure 1: Visual Representation of the Spatial Variation for the Three Coefficients as Described in Equations (12) - (14)

```

x2 = runif(n) # create a vector for x2 values
error = rnorm(n, 0, errorSD) # create an error term

# now generating the betas...
# they will ALWAYS have an expectation of 2 and have an expected correlation of 0
# (except for corner cases in LLL)
B1 <- 2 - .5*B1.SpVar + east*B1.SpVar
B2 <- 2 - .5*B2.SpVar + north*B2.SpVar
B0 <- 2 + B0.SpVar*(.387452 + cos(2*pi*sqrt((east - .5)^2 + (north- .5)^2)/sqrt(.5)))

```

2 Simulation Results

2.1 Starting Simple: All Coefficients are Spatially Stationary

We begin by examining the simulation results for the spatially stationary data generation process. With no spatial variation for any of the coefficients, these data are consistent with standard OLS regression. We label this model ‘GGG’ to denote that all three coefficients are ‘Global’ rather than ‘Local’.¹ Table 1 displays the percentage of simulation iterations that each of the eight different mixed GWR models was ‘selected’ by each of the four different metrics: LOOCV, GCV, SCV, and AIC. Correspondingly, each column sums to 100 (subject to rounding error).

		Metric				
		LOOCV	GCV	SCV	AIC	
Model Selected	GGG	72	0	8	0	3/3 Correct
	LGG	7	28	29	28	2/3 Correct
	GLG	8	36	22	37	
	GGL	8	33	22	34	
	LLG	1	1	5	0	1/3 Correct
	LGL	2	1	5	1	
	GLL	1	1	8	0	
	LLL	0	0	1	0	0/3 Correct
		100	100	100	100	

Table 1: Distribution of Model Selected by Metric when True Model = GGG (All Coefficients are Non-Stationary).

Cell values denote the percentage of simulations in which each model yielded the best metric value. For instance, the GGG model had the smallest LOOCV value for 72 percent of our simulations. Each column sums to 100 subject to rounding error. Cell shading denotes the number of coefficients that are correctly identified as stationary or not.

Table 1 shows a distinct difference between LOOCV and the three other metrics. Almost three-fourths of the time the LOOCV was minimized using the model that

¹The eight GWR models representing the unique mixture/combinations of (non-)stationarity across the three coefficients are labeled: GGG, LGG, GLG, GGL, LLG, LGL, GLL, and LLL.

was “correct” across all three coefficients. Conversely, the SCV metric selected the correct (‘GGG’) model in less than 10 percent of the simulations and both the GCV and AIC metrics selected the correct model less than 1 percent of the time. Interestingly, while the GCV, SCV, and AIC metrics did not choose the correct model nearly as frequently as the LOOCV metric, they tend to make a correctly identify the spatial (non-)stationarity for two out of three coefficients. The GCV and AIC metric almost exclusively selected one of the ‘LGG’, ‘GLG’, and ‘GGL’ models. Almost 20 percent of the time the SCV metric selected a model that was incorrect about two (‘LLG’, ‘LGL’, ‘GLL’) or all (‘LLL’) of the coefficients stationarity.

At first glance, the high frequency of type one error displayed in Table 1 is frustrating. However, the goal of regression analyses tends to be the efficient, consistent, and unbiased estimation of a particular variable coefficient rather than identifying the exact model specification. We therefore also calculated the Root Mean Square Error for each regression coefficient across all of our model specifications as,

$$\text{RMSE } \hat{\beta}_m = \sqrt{\frac{1}{N} \sum_{i=1}^N (\hat{\beta}_{mi} - \beta_{mi})^2}, \quad (15)$$

where i denotes the observation, N is the sample size, and $m \in \{0, 1, 2\}$ specifies the model coefficient in question. Unlike the metrics in Table 1, these model performance metrics are not available to researchers with observational data. These measures of estimated coefficient accuracy can only be calculated because we know the true underlying data generating process. Table 2 shows the distribution of models selected by having the smallest RMSE for each coefficient.

		Coefficient RMSE		
		\widehat{B}_0	\widehat{B}_1	\widehat{B}_2
Model Selected	GGG	6	6	7
	LGG	3	23	24
	GLG	22	4	24
	GGL	23	23	3
	LLG	5	3	33
	LGL	5	36	2
	GLL	32	4	4
	LLL	4	2	3
		100	100	100

Table 2: Distribution of Model Selected by RMSE when True Model = GGG (All Coefficients are Non-Stationary).

Cell values denote the percentage of simulations in which each model yielded the lowest RMSE value for each coefficient. For instance, the GGG model had the smallest RMSE \widehat{B}_0 value for 6 percent of our simulations. Each column sums to 100 subject to rounding error. Shaded cells denote model for which the spatial non-stationarity of the column coefficient is correct.

An interesting pattern emerges upon examination of Table 2. The largest value in each column represents approximately one-third of the simulations, but is not

the perfect model. The ‘GGG’ row of Table 2 shows that the correct model yielded the smallest RMSE for a given \hat{B} in only 6 to 7 percent of simulations. Instead, the model most frequently minimizing the RMSE for \hat{B} correctly identifies the spatial stationarity of the coefficient in question, but incorrectly treats both of the other coefficients as non-stationary. For instance, in 32 percent of these simulations with a true ‘GGG’ model, the smallest RMSE for \hat{B}_0 was obtained using the ‘GGL’ model. In each column the four respective models that correctly identify the spatial non-stationarity of the respective coefficient yield the most accurate estimates of the coefficient in question for approximately 85 percent of our simulations. It is relatively rare for the most accurate stationary regression coefficient estimates to be obtained from a model that incorrectly identifies it as spatially non-stationary. Approximately half of our simulations yielded minimum RMSEs using models that were correct about the coefficient in question, but were incorrect about one of the two remaining coefficients.

2.1.1 Model and Bandwidth

The previous section explored the model selected by different metrics in the presence of an underlying globally stationary data generation process. The results showed that the correct model, ‘GGG’, was only selected relatively frequently by the LOOCV metric. However, we have also seen that some of the most accurate estimates of the individual regression coefficients come from incorrect models. We have not yet quantified how wrong these incorrect model are. For instance, a model may incorrectly identify a coefficient as spatially non-stationary, but might estimate a very small degree of variation in the coefficient by using a large bandwidth relative to our sample size. That is, it is potentially very different to select the ‘GGL’ model instead of the ‘GGG’ with a large vs. small bandwidth. A small bandwidth can yield more variation in coefficient estimates across our sample, while a large bandwidth will restrict the non-stationary coefficients to be more similar.

In each of our simulations we estimated the seven models allowing non-stationarity in at least coefficient for seven different bandwidths, ranging from using all of the data to just under 10 percent of the observations in the mixed models with the smallest bandwidth. Figure 2 shows the distribution of model selected and bandwidth size for each of the seven metrics we’ve discussed.

2.2 All Local Coefficients

The previous section investigated the simulation results when the true model was stationary across all three coefficients. In this section we examine the opposite extreme: all non-stationary coefficients. To begin, we construct a figure similar to Figure 2 but with a true model of ‘LLL.’

Figure 3 reveals a stark pattern. Although the true underlying model is non-stationary, none of the four metrics choose the ‘LLL’ model in more than 10 percent of our simulations. Instead, the ‘LGG’ model is selected over 50 percent of the time by each metric. The LOOCV, GCV, and AIC metrics all select the ‘LGG’ model with the smallest bandwidth much more frequently than any other

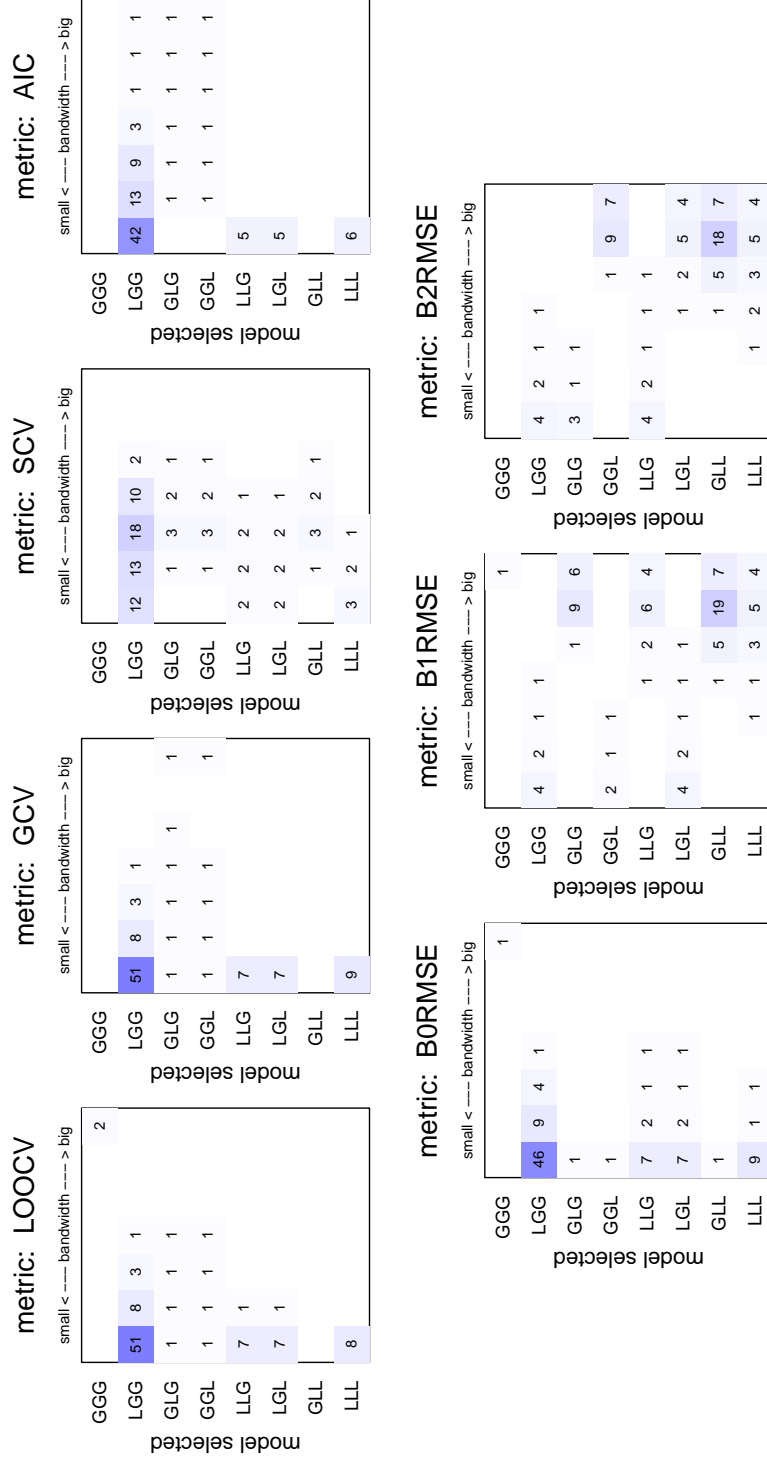


Figure 3: Model and Bandwidth Selected by Metric when the True Model = 'LLL' (All coefficients are non-stationary) Each subfigure shows the percentage of simulations a given model and bandwidth combination was selected among the 50 possible combinations (7 bandwidths for each of the seven mixed models plus the GGG model) for a given metric. The sum of all values in a given subfigure sum to 100 subject to rounding error. For convenience, cell values less than 0.5 percent are omitted. The color saturation of the cells helps denote the magnitude of the values.

model/bandwidth combination. For instance, LOOCV and GCV select the ‘LGG’ model with the smallest bandwidth over 50 percent of the time.

The second row of results in Figure 3 displays the model and bandwidth combinations that yield the smallest RMSE for the coefficients in our model. The pattern for the smallest RMSE associated with the intercept term, β_0 closely resembles the pattern of models and bandwidths for LOOCV, GCC, and AIC. Roughly 10 percent of simulations have the smallest RMSE using the ‘LLL’ model, while roughly half of the simulations selected the ‘LGG’ model with the smallest bandwidth. However, we see a different pattern for β_1 and β_2 . In both instances, no single model and bandwidth combination yielded the smallest RMSE more than 20 percent of the time (the ‘GLL’ model with the second largest bandwidth). That is, the intercept was fixed while the other two coefficients were treated as non-stationary and the bandwidth was comprised of approximately two-thirds of the observations.

The simulations contained in Figure 3 actually contain a lot of variation in the amount of coefficient non-stationarity. Recalling that we implemented two amounts of spatial variation in each coefficient (think of it as ‘some’ and ‘more’) there are actually eight combinations of ‘LLL’ models ranging from “some, some, some,” to “more, more, more.” We therefore present a comparison of the following three models, the ‘GGG’ model we’ve already discussed, the ‘LLL’ model containing the smallest amount of overall spatial non-stationarity in all coefficients (the “some, some, some” model), and the largest amount of overall spatial non-stationarity (the “more, more, more” model).

2.3 One Local Coefficient

What have we learned in the previous sections?

1. LOOCV does the best identifying the non-stationary models
2. most accurate $\hat{\beta}$ estimates do not necessarily come from the correct model
3. SCV sucks
4. something else.

Now we explore the mixed model cases in which some of the coefficients are stationary and some are non-stationary. We begin with the case of a single non-stationary coefficient.

Figure 5 shows that most metrics can correctly identify the proper mixed model when only one coefficient is non-stationary.

2.4 Two Local Coefficients

Now we explore the mixed model cases in which two of the coefficients are non-stationary.

Figure 6 shows that most metrics can.

Spatial Variation in All Three Coefficients:

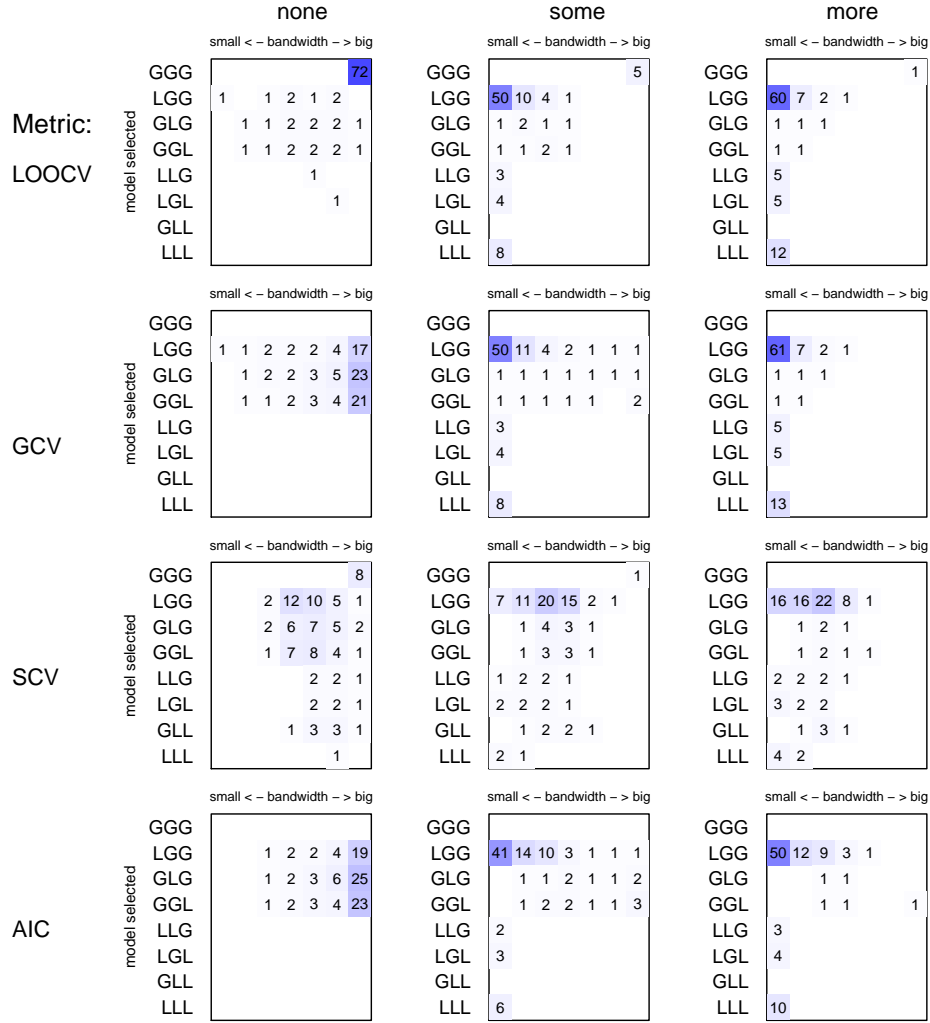


Figure 4: Model and Bandwidth Selected by Metric for ‘None’, ‘Some’, and ‘More’ Spatial Variation in the Three Regression Coefficients

Each subfigure shows the percentage of simulations a given model and bandwidth combination was selected among the 50 possible combinations (7 bandwidths for each of the seven mixed models plus the GGG model) for a given metric. The sum of all values in a given subfigure sum to 100 subject to rounding error. For convenience, cell values less than 0.5 percent are omitted. The color saturation of the cells helps denote the magnitude of the values.

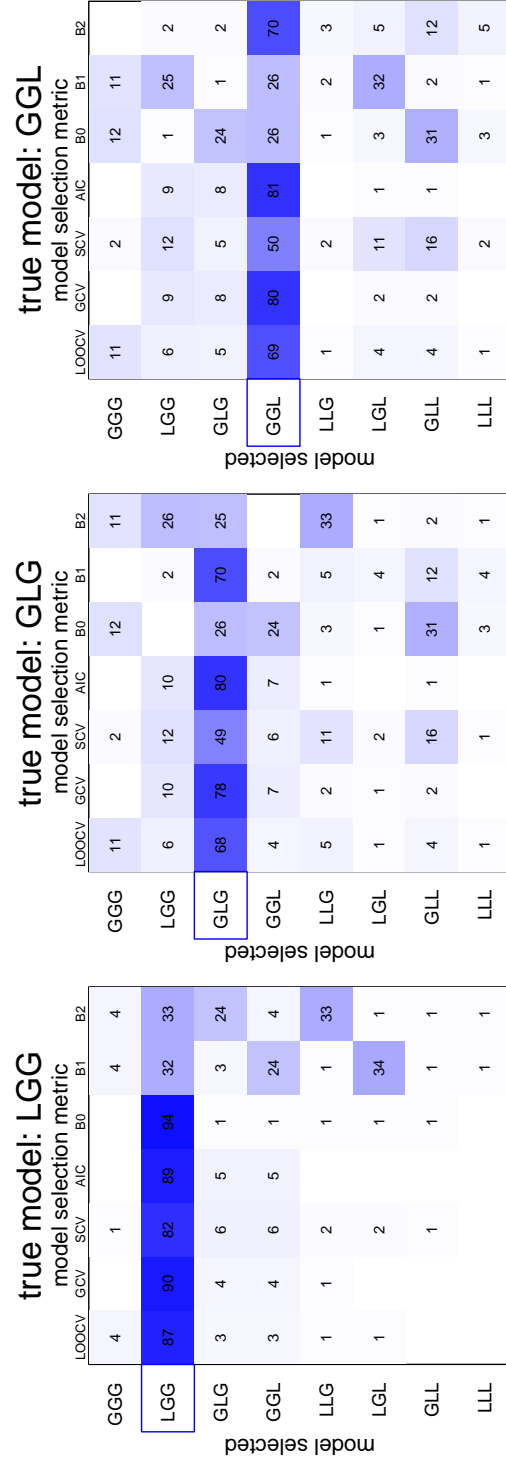


Figure 5: This figure shows

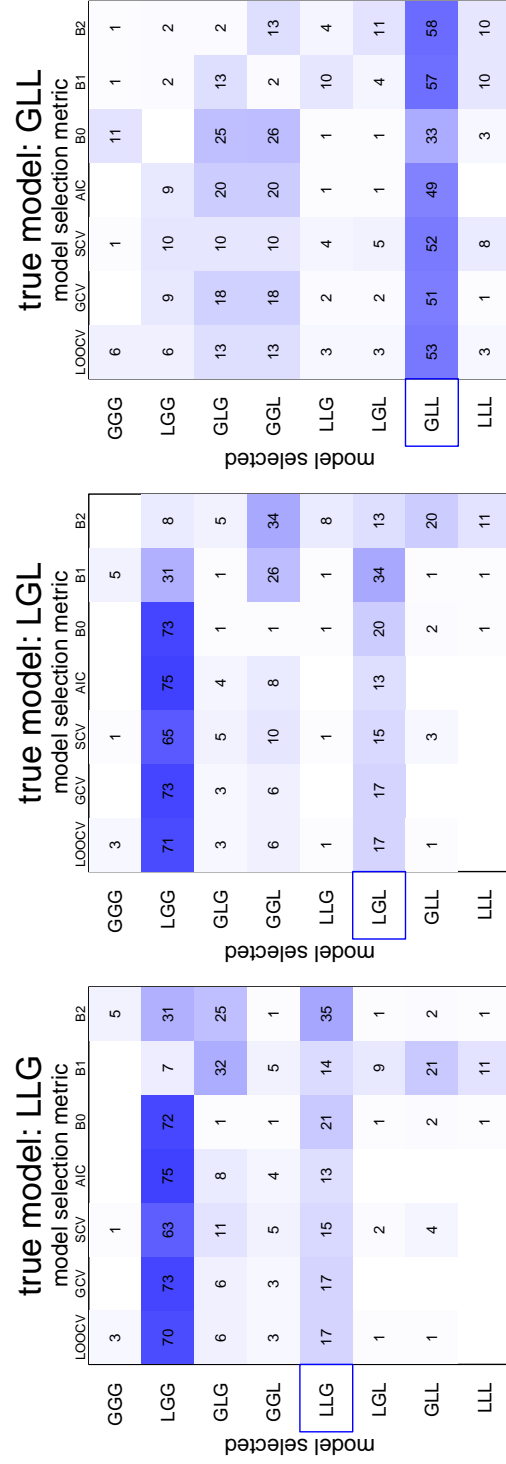


Figure 6: This figure shows

3 Discussion

Let's show the model selection by metric across our 8 different models.

The left (right) column in Figure 7 contains the four models in which the intercept coefficient is (non-)stationary over the study area. In the top row of the figure both β_1 and β_2 are stationary, the middle two rows contain one stationary and one non-stationary coefficient, and in the bottom row both β_1 and β_2 are non-stationary. An interesting pattern is visible. The models on the left tend to be more accurately identified by the metrics than the models on the right. That is, if the intercept term is stationary, our information metrics do a pretty good job identifying whether or not the other coefficients are stationary or not. However, when the intercept term is stationary, our metrics commonly choose the 'LGG' model even when one or both of the other coefficients is non-stationary.

Figure 8 shows

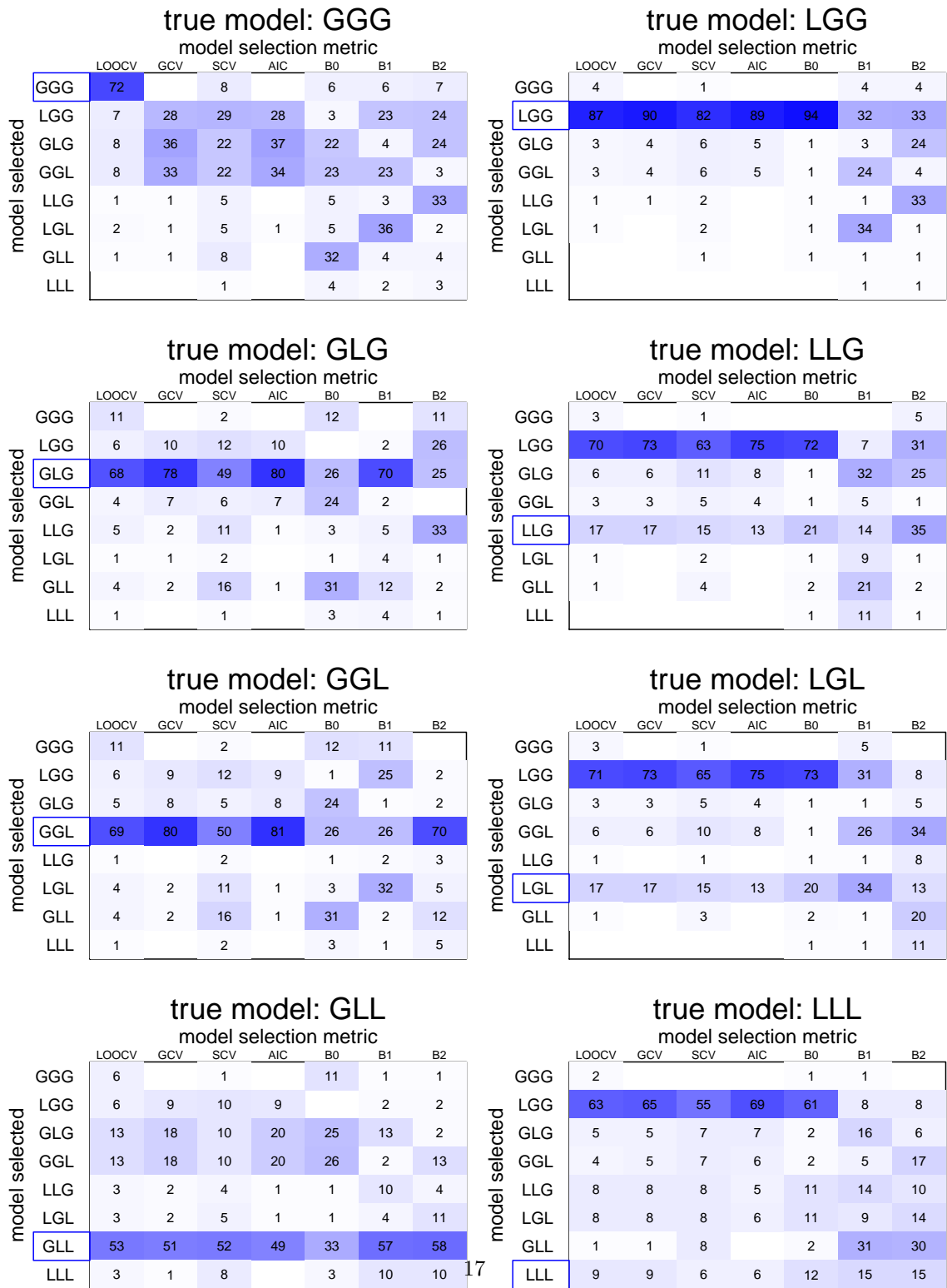


Figure 7: This figure shows

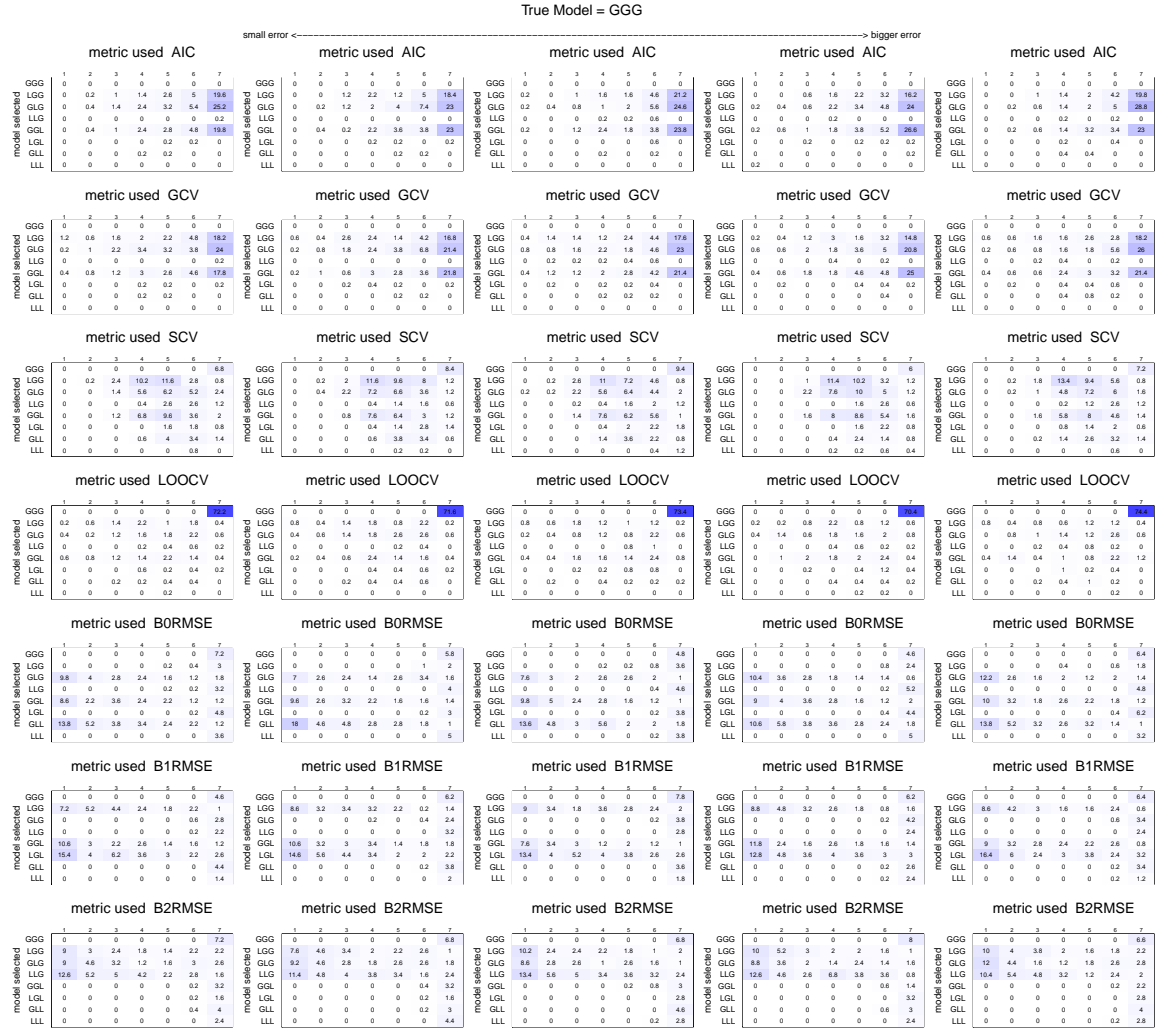


Figure 8: This figure shows the GLG model...

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