# SPMODEL: SPATIAL STATISTICAL MODELING AND PREDICTION IN R

#### A Preprint

## Michael Dumelle \*

United States Environmental Protection Agency 200 SW 35th St, Corvallis, OR, 97333 Dumelle.Michael@epa.gov

## Matt Higham

Department of Math, Computer Science, and Statistics St. Lawrence University 23 Romoda Drive, Canton, NY, 13617 mhigham@stlawu.edu

## Jay M. Ver Hoef

National Oceanic and Atmospheric Administration Alaska Fisheries Science Center Marine Mammal Laboratory, Seattle, WA, 98115 jay.verhoef@noaa.gov

July 22, 2022

#### Abstract

Fit, summarize, and predict for a variety spatial statistical models. Parameters are estimated using various methods. Additional modeling features include anisotropy, random effects, partition factors, big data approaches, and more. Model-fit statistics are used to summarize, visualize, and compare models. Predictions at unobserved locations are readily obtainable. This manuscript corresponds to spmodel version 0.1.0.

Keywords Spatial linear model  $\cdot$  Spatial autoregressive model  $\cdot$  Covariance  $\cdot$  Estimation  $\cdot$  Prediction (Kriging)  $\cdot$  Big Data

# 1 Introduction

spmodel is an **R** package used to fit, summarize, and predict for a variety of spatial statistical models. In Section 2, we give a brief theoretical introduction to spatial linear models. In Section 3, we outline the variety of methods used to estimate the parameters of spatial linear models. In Section 4, we explain how to obtain predictions at unobserved locations. In Section 5, we detail some advanced modeling features, including random effects, partition factors, anisotropy, and big data approaches. In Section 6, we end with a short discussion. Before proceeding, we load spmodel by running

R> library(spmodel)

We will create visualizations using ggplot2 (Wickham 2016), which we load by running

R> library(ggplot2)

# 2 The Spatial Linear Model

Statistical linear models are often parameterized as

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

<sup>\*</sup>Corresponding Author

where for a sample size n,  $\mathbf{y}$  is an  $n \times 1$  vector of response variables,  $\mathbf{X}$  is an  $n \times p$  design (model) matrix of explanatory variables,  $\boldsymbol{\beta}$  is an  $p \times 1$  vector of fixed effects controlling the impact of  $\mathbf{X}$  on  $\mathbf{y}$ , and  $\boldsymbol{\epsilon}$  is an  $n \times 1$  vector of random errors. Typically, it is assumed that  $\mathbf{E}(\boldsymbol{\epsilon}) = \mathbf{0}$  and  $\mathbf{Cov}(\boldsymbol{\epsilon}) = \sigma_{\epsilon}^2 \mathbf{I}$ , where  $\mathbf{E}(\cdot)$  denotes expectation,  $\mathbf{Cov}(\cdot)$  denotes covariance,  $\sigma_{\epsilon}^2$  denotes a variance parameter, and  $\mathbf{I}$  denotes the identity matrix.

The model in Equation 1 assumes the elements of  $\mathbf{y}$  are uncorrelated. Typically for spatial data, elements of  $\mathbf{y}$  are correlated, as observations close together in space tend to be more similar than observations far apart (Tobler 1970). Failing to properly accommodate the spatial dependence in  $\mathbf{y}$  can cause researchers to draw incorrect conclusions about their data. To accommodate spatial dependence in  $\mathbf{y}$ , an  $n \times 1$  spatial random effect,  $\boldsymbol{\tau}$ , is added to Equation 1, yielding the model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\tau} + \boldsymbol{\epsilon},\tag{2}$$

where  $E(\tau) = \mathbf{0}$ ,  $Cov(\tau) = \sigma_{\tau}^2 \mathbf{R}$ , and  $\mathbf{R}$  is a matrix that determines the spatial dependence structure in  $\mathbf{y}$  and depends on a range parameter,  $\phi$ . The parameter  $\sigma_{\tau}^2$  is called the spatially dependent random error variance or partial sill. The parameter  $\sigma_{\epsilon}^2$  is called the spatially independent random error variance or nugget. These two variance parameters are henceforth more intuitively written as  $\sigma_{de}^2$  and  $\sigma_{ie}^2$ , respectively. The covariance of  $\mathbf{y}$  is denoted  $\mathbf{\Sigma}$  and given by  $\sigma_{de}^2 \mathbf{R} + \sigma_{ie}^2 \mathbf{I}$ . The parameters that compose this covariance are typically referenced by the vector  $\boldsymbol{\theta}$ , which is called the covariance parameter vector.

Equation 2 is called the spatial linear model. The spatial linear model applies to both point-referenced and areal data. Data are point-referenced when the elements in  $\mathbf{y}$  are observed at point-locations indexed by x-coordinates and y-coordinates on a spatially continuous surface with an infinite number of locations. The  $\mathtt{splm}()$  function is used to fit spatial linear models for point-referenced data (these are often called geostatistical models). One spatial covariance function available in  $\mathtt{splm}()$  is the exponential spatial covariance function, which has an  $\mathbf{R}$  matrix given by

$$\mathbf{R} = \exp(-\mathbf{h}/\phi),$$

where  $\mathbf{h}$  is a matrix of Euclidean distances among observations. Recall  $\phi$  is the range parameter, controlling the behavior of  $\mathbf{R}$  as a function of distance. Parameterizations for  $\mathrm{splm}$ () spatial covariance types and their  $\mathbf{R}$  matrices can be seen by running  $\mathrm{help}("\mathrm{splm}", "\mathrm{spmodel}")$  or  $\mathrm{vignette}("\mathrm{technical}", "\mathrm{spmodel}")$ .

Data are areal when the elements in  $\mathbf{y}$  are observed as part of a finite network of polygons whose connections are indexed by a neighborhood structure. For example, the polygons may represent counties in a state who are neighbors if they share at least one boundary. The  $\mathtt{spautor}()$  function is used to fit spatial linear models for areal data (these are often called spatial autoregressive models). One spatial autoregressive covariance function available in  $\mathtt{spautor}()$  is the simultaneous autoregressive spatial covariance function, which has an  $\mathbf{R}$  matrix given by

$$\mathbf{R} = [(\mathbf{I} - \phi \mathbf{W})(\mathbf{I} - \phi \mathbf{W})^{\top}]^{-1},$$

where W is a weight matrix describing the neighborhood structure in y. Paremertizations for spattal covariance types and their R matrices can be seen by running help("spattor", "spmodel") or vignette("technical", "spmodel").

## 3 Model Fitting

In this section, we show how to use the splm() and spautor() functions to estimate parameters of the spatial linear model. We also explore diagnostic tools in spmodel that evaluate model fit. The splm() and spautor() functions share similar syntactic structure with the lm() function used to fit non-spatial linear models (linear models without spatial dependence) from Equation 1. splm() and spautor() generally require at least three arguments:

- formula: a formula that describes the relationship between the response variable (y) and explanatory variables (X)
  - formula in splm() is the same as formula in lm()
- data: a data.frame or sf object that contains the response variable, explanatory variables, and spatial information
- spcov\_type: the spatial covariance type ("exponential", "matern", "car", etc)

If data is an sf (Pebesma 2018) object, spatial information is stored in the object's geometry. If data is a data.frame, then for point-referenced data the x-coordinates and y-coordinates must be provided via the

xcoord and ycoord arguments, and for areal data, the weight matrix must be provided via the W argument. Appendix A uses the caribou data, a tibble (a special data.frame), to show how to explicitly provide spatial information via xcoord and ycoord (in splm()) or W (in spautor()).

In the following subsections, we use the point-referenced moss data, an sf object that contains data on heavy metals in mosses near a mining road in Alaska. We view the first few rows of moss by running

#### R> moss

```
Simple feature collection with 365 features and 7 fields
Geometry type: POINT
Dimension:
              XY
Bounding box:
              xmin: -445884.1 ymin: 1929616 xmax: -383656.8 ymax: 2061414
Projected CRS: NAD83 / Alaska Albers
# A tibble: 365 x 8
   sample field_dup lab_rep year sideroad log_dist2road log_Zn
                                                                           geometry
                            <fct> <fct>
                                                                        <POINT [m]>
   <fct> <fct>
                    <fct>
                                                   <dbl>
                                                          <dbl>
 1 001PR 1
                            2001 N
                                                           7.33 (-413585.3 1997623)
                    1
                                                    2.68
 2 001PR 1
                    2
                            2001 N
                                                           7.38 (-413585.3 1997623)
                                                    2.68
 3 002PR 1
                    1
                            2001 N
                                                    2.54
                                                           7.58 (-415367.2 1996769)
 4 003PR 1
                    1
                            2001 N
                                                    2.97
                                                           7.63
                                                                  (-417186 1995645)
 5 004PR 1
                    1
                            2001 N
                                                    2.72
                                                           7.26 (-411756.6 1999907)
 6 005PR 1
                    1
                            2001 N
                                                    2.76
                                                           7.65 (-419008.8 1994950)
7 006PR 1
                                                           7.59 (-420822.6 1994480)
                    1
                            2001 S
                                                    2.30
8 007PR 1
                    1
                            2001 N
                                                    2.78
                                                           7.16 (-404383.2 2007420)
9 008PR 1
                            2001 N
                                                    2.93
                                                           7.19 (-409964.1 2003323)
                    1
10 009PR 1
                    1
                            2001 N
                                                    2.79
                                                           8.07 (-424469.7 1992184)
# ... with 355 more rows
```

We can learn more about moss by running help("moss", "spmodel").

#### 3.1 Estimation

Generally the covariance parameters ( $\theta$ ) and fixed effects ( $\beta$ ) of the spatial linear model require estimation. The default estimation method in spmodel is restricted maximum likelihood (Patterson and Thompson 1971; Harville 1977; Wolfinger, Tobias, and Sall 1994). Maximum likelihood estimation is also available. For point-referenced data, semivariogram weighted least squares (Cressie 1985) and semivariogram composite likelihood (Curriero and Lele 1999) are additional estimation methods. The estimation method is controlled using the estmethod argument.

To visualize the distribution of log zinc concentration in the moss data (Figure 1), run

```
R> ggplot(moss, aes(color = log_Zn)) +
    geom_sf(size = 2) +
    scale_color_viridis_c() +
    theme_gray(base_size = 14)
```

We estimate parameters of a spatial linear model regressing log zinc concentration (log\_Zn) on log distance to a haul road (log\_dist2road) using an exponential spatial covariance function by running

```
R> spmod <- splm(log_Zn ~ log_dist2road, moss, spcov_type = "exponential")
```

We summarize the model fit by running

R> summary(spmod)

```
Call:
```

```
splm(formula = log_Zn ~ log_dist2road, data = moss, spcov_type = "exponential")
```

Residuals:

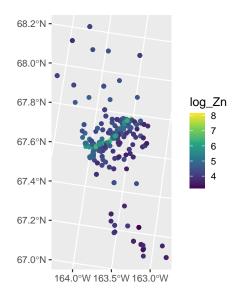


Figure 1: Distribution of log zinc concentration in the moss data.

```
Min
             1Q Median
                              3Q
                                    Max
-2.6801 -1.3606 -0.8103 -0.2485
Coefficients (fixed):
              Estimate Std. Error z value Pr(>|z|)
(Intercept)
               9.76825
                          0.25216
                                    38.74
                                             <2e-16 ***
                                   -27.96
log_dist2road -0.56287
                          0.02013
                                             <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Pseudo R-squared: 0.683
Coefficients (exponential spatial covariance):
       de
                 ie
                        range
3.595e-01 7.897e-02 8.237e+03
```

The fixed effects coefficient table contains estimates, standard errors, z-statistics, and asymptotic p-values for each fixed effect. From this table, we notice there is evidence that log zinc concentration significantly decreases with distance from the haul road (p-value < 2e-16). We see the fixed effect estimates by running

```
R> coef(spmod)
  (Intercept) log_dist2road
    9.7682525 -0.5628713
```

The model summary also contains the exponential spatial covariance parameter estimates, which we can view by running

The dependent random error variance  $(\sigma_{de}^2)$  is estimated to be approximately 0.36 and the independent random error variance  $(\sigma_{ie}^2)$  is estimated to be approximately 0.079. The range  $(\phi)$  is estimated to be

# Fitted spatial covariance function

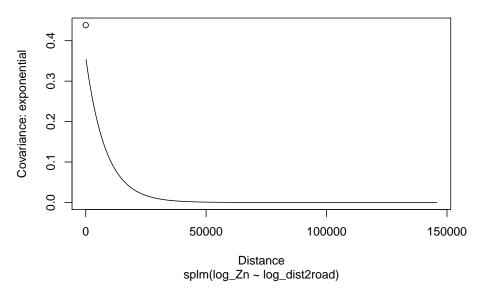


Figure 2: Empirical spatial covariance of fitted model.

approximately 8,237. The effective range is the distance at which the spatial covariance is approximately zero. For the exponential covariance, the effective range is  $3\phi$ . This means that observations whose distance is greater than 24,711 meters are approximately uncorrelated. The rotate and scale parameters affect the modeling of anisotropy (Section 5.4). By default, they are assumed to be zero and one, respectively, which means that anisotropy is not modeled (i.e., the spatial covariance is assumed isotropic, or independent of direction). We plot the fitted spatial covariance function (Figure 2) by running

R> plot(spmod, which = 7)

We can learn more about the plots available for fitted models by running help("plot.spmod", "spmodel").

# 3.2 Model-Fit Statistics

The quality of model fit can be assessed using a variety of statistics readily available in spmodel. The first model-fit statistic we consider is the pseudo R-squared. The pseudo R-squared is a generalization of the classical R-squared from non-spatial linear models that quantifies the proportion of variability in the data explained by the fixed effects. The pseudo R-squared is defined as

$$PR2 = 1 - \frac{\mathcal{D}(\hat{\mathbf{\Theta}})}{\mathcal{D}(\hat{\mathbf{\Theta}}_0)},$$

where  $\mathcal{D}(\hat{\Theta})$  is the deviance of the fitted model indexed by parameter vector  $\hat{\Theta}$  and  $\mathcal{D}(\hat{\Theta}_0)$  is the deviance of an intercept-only model indexed by parameter vector  $\hat{\Theta}_0$ . We compute the pseudo R-squared by running

## R> pseudoR2(spmod)

## [1] 0.6829687

Roughly 68% of the variability in log zinc is explained by log distance from the road. The pseudo R-squared can be adjusted to account for the number of explanatory variables using the adjust argument. Pseudo R-squared (and the adjusted version) is most helpful for comparing models that have the same covariance structure.

The next two model-fit statistics we consider are the spatial AIC and AICc (Hoeting et al. 2006). The AIC and AICc evaluate the fit of a model with a penalty for the number of parameters estimated. This penalty

balances model fit and model parsimony. The AICc is a correction to AIC for small sample sizes. As the sample size increases, the AIC and AICc become closer to one another. The lower the AIC and AICc, the better the balance of model fit and parsimony.

The spatial AIC and AICc are given by

$$AIC = -2\ell(\hat{\mathbf{\Theta}}) + 2(|\hat{\mathbf{\Theta}}|)$$
  

$$AICc = -2\ell(\hat{\mathbf{\Theta}}) + 2n(|\hat{\mathbf{\Theta}}|)/(n - |\hat{\mathbf{\Theta}}| - 1),$$

where  $\ell(\hat{\Theta})$  is the log-likelihood of the data evaluated at the estimated parameter vector  $\hat{\Theta}$  maximizing  $\ell(\Theta)$ , and n is the sample size. For maximum likelihood,  $\hat{\Theta} = \{\hat{\theta}, \hat{\beta}\}$ . For restricted maximum likelihood  $\hat{\Theta} = \{\hat{\theta}\}$ . AIC comparisons between a model fit using restricted maximum likelihood and a model fit using maximum likelihood are meaningless, as the models are fit with different likelihoods. AIC comparisons between models fit using restricted maximum likelihood are only valid when the models have the same fixed effect structure. In contrast, AIC comparisons between models fit using maximum likelihood are valid when the models have different fixed effect structures.

Suppose we want to quantify the difference in model quality between the spatial model and a non-spatial model using the AIC and AICc criteria. We fit a non-spatial model (Equation 1) in spmodel by running

```
R> lmod <- splm(log_Zn ~ log_dist2road, moss, spcov_type = "none")
```

We compute the spatial AIC and AICc of the spatial model and non-spatial model by running

R> AIC(spmod, lmod)

df AIC spmod 3 373.2089 lmod 1 636.0635

R> AICc(spmod, lmod)

df AICc spmod 3 373.2754 lmod 1 636.0745

The noticeably lower AIC and AICc of of the spatial model indicate that it is a better fit to the data than the non-spatial model.

Another approach to comparing the model fits is to perform leave-one-out cross validation. In leave-one-out cross validation, a single observation is removed from the data, the model is re-fit, and a prediction is made for the held-out observation. Then a loss metric like mean-squared-prediction error is computed and used to evaluate model fit. The lower the mean-squared-prediction error, the better the model fit. For computational efficiency, leave-one-out cross validation in spmodel is performed by first estimating  $\theta$  using all the data and then re-estimating  $\beta$  for each observation. We perform leave-one-out cross validation for the spatial and non-spatial model by running

R> loocv(spmod)

[1] 0.1110895

R> loocv(lmod)

[1] 0.3237897

The noticeably lower mean-squared-prediction error of the spatial model indicates that it is a better fit to the data than the non-spatial model.

## 3.3 Diagnostics

An observation is said to have high leverage if its combination of explanatory variable values is far from the mean vector of the explanatory variables. For a non-spatial model, the leverage of the ith observation is the

ith diagonal element of the hat matrix given by

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}.$$

For a spatial model, the leverage of the ith observation is the ith diagonal element of the spatial hat matrix given by

$$\mathbf{H}^* = (\mathbf{X}^* (\mathbf{X}^{*\top} \mathbf{X})^{-1} \mathbf{X}^{*\top}),$$

where  $\mathbf{X}^* = \mathbf{\Sigma}^{-1/2}\mathbf{X}$  and  $\mathbf{\Sigma}^{-1/2}$  is the matrix square root of the covariance matrix,  $\mathbf{\Sigma}$  (Montgomery, Peck, and Vining 2021). The spatial hat matrix can be viewed as the non-spatial hat matrix applied to the "whitened"  $\mathbf{X}$  matrix,  $\mathbf{X}^*$ . We compute the hat values (leverage) by running

## R> hatvalues(spmod)

The larger the hat value, the larger the leverage.

The fitted value of an observation is the estimated mean response given the observation's explanatory variable values and the model fit:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}.$$

We compute the fitted values by running

#### R> fitted(spmod)

Fitted values for the spatially dependent random errors  $(\tau)$ , spatially independent random errors  $(\epsilon)$ , and random effects can also be obtained via fitted() by changing the type argument.

The residuals act as estimates of errors, measuring each response's deviation from its fitted value. The raw residuals are given by

$$\mathbf{e}_r = \mathbf{y} - \hat{\mathbf{y}}.$$

We compute the raw residuals of the spatial model by running

#### R> residuals(spmod)

The raw residuals are typically not directly checked for linear model assumptions, as they have covariance closely resembling the covariance of  $\mathbf{y}$ . These residuals can be "whitened" by pre-multiplying by  $\hat{\Sigma}^{-1/2}$ , yielding the Pearson residuals:

$$\mathbf{e}_p = \mathbf{\hat{\Sigma}}^{-1/2} \mathbf{e}_r.$$

When the model is correct, the Pearson residuals have mean zero, variance approximately one, and are uncorrelated. We compute the Pearson residuals of the spatial model by running

R> residuals(spmod, type = "pearson")

The covariance of  $\mathbf{e}_p$  is  $(\mathbf{I} - \mathbf{H}^*)$ , which is approximately  $\mathbf{I}$  for large sample sizes. Explicitly dividing  $\mathbf{e}_p$  by the respective diagonal element of  $(\mathbf{I} - \mathbf{H}^*)$  yields the standardized residuals:

$$\mathbf{e}_s = \frac{\mathbf{e}_p}{\sqrt{(1 - diag(\mathbf{H}^*))}},$$

where  $diag(\mathbf{H}^*)$  denotes the diagonal of  $\mathbf{H}^*$ .

We compute the standardized residuals of the spatial model by running

R> residuals(spmod, type = "standardized")

or

## R> rstandard(spmod)

When the model is correct, the standardized residuals have mean zero, variance one, and are uncorrelated. It is common to check linear model assumptions through visualizations. We can plot the standardized residuals vs fitted values by running

R> plot(spmod, which = 1) # figure omitted

When the model is correct, the standardized residuals should be evenly spread around zero with no discernible pattern. We can plot a normal QQ-plot of the standardized residuals by running

R> plot(spmod, which = 2) # figure omitted

When the standardized residuals are normally distributed, they should closely follow the normal QQ-line.

An observation is said to be influential if its omission has a large impact on model fit. Typically this is measured using Cook's distance (Cook and Weisberg 1982). For the non-spatial model, the Cook's distance of the ith observation is denoted  $\mathbf{D}$  and given by

$$\mathbf{D} = \mathbf{e}_s^2 \frac{diag(\mathbf{H})}{p(1 - diag(\mathbf{H}))}.$$

For a spatial model, the Cook's distance of the ith observation is denoted  $\mathbf{D}^*$  and given by

$$\mathbf{D}^* = \mathbf{e}_s^2 \frac{diag(\mathbf{H}^*)}{p(1 - diag(\mathbf{H}^*))}.$$

The larger the Cook's distance, the larger the influence. We compute Cook's distance by running

R> cooks.distance(spmod)

We visualize the Cook's distance versus leverage (hat values) by running

R> plot(spmod, which = 6) # figure omitted

## 3.4 The broom functions: tidy(), glance(), and augment()

The tidy(), glance(), and augment() functions from the broom **R** package (Robinson, Hayes, and Couch 2021) are defined for spmodel objects. The tidy() function returns a tidy tibble of the coefficient table from summary():

R> tidy(spmod)

#### # A tibble: 2 x 5

	term	estimate	std.error	statistic	p.value	
	<chr></chr>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	
1	(Intercept)	9.77	0.252	38.7	0	
2	log_dist2road	-0.563	0.0201	-28.0	0	

This tibble format makes it easy to pull out the coefficient names, estimates, standard errors, z-statistics, and p-values from the summary() output. The glance() function returns a tidy tibble of model-fit statistics:

R> glance(spmod)

## # A tibble: 1 x 9

```
n p npar value AIC AICc logLik deviance pseudo.r.squared <int> <dbl> <int> <dbl> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> 0.683
```

The glances() function can be used to look at many models simultaneously:

R> glances(spmod, lmod)

## # A tibble: 2 x 10

	model	n	р	npar	value	AIC	AICc	logLik	deviance	pseudo.r.squared
	<chr></chr>	<int></int>	<dbl></dbl>	<int></int>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>
1	spmod	365	2	3	367.	373.	373.	-184.	363	0.683
2	lmod	365	2	1	634.	636.	636.	-317.	363.	0.671

The augment() function augments the original data with model diagnostics:

#### R> augment(spmod)

```
Simple feature collection with 365 features and 7 fields
Geometry type: POINT
Dimension:
               XY
Bounding box: xmin: -445884.1 ymin: 1929616 xmax: -383656.8 ymax: 2061414
Projected CRS: NAD83 / Alaska Albers
# A tibble: 365 x 8
   log_Zn log_dist2road .fitted .resid
                                                 .cooksd .std.resid
                                           .hat
    <dbl>
                          <dbl> <dbl>
                                                   <dbl>
                  <dbl>
                                          <dbl>
                                                              <dbl>
 1
    7.33
                   2.68
                           8.26 -0.928 0.102
                                               0.112
                                                             -1.48
 2
    7.38
                   2.68
                           8.26 -0.880 0.0101 0.000507
                                                             -0.316
 3
    7.58
                   2.54
                           8.34 -0.755 0.0170 0.000475
                                                             -0.236
 4
    7.63
                   2.97
                           8.09 -0.464 0.0137 0.000219
                                                              0.178
 5
                           8.24 -0.977 0.0177 0.00515
    7.26
                   2.72
                                                             -0.762
                           8.21 -0.568 0.0147 0.000929
 6
    7.65
                   2.76
                                                             -0.355
 7
                   2.30
                           8.47 -0.886 0.0170 0.00802
                                                             -0.971
    7.59
 8
                   2.78
                           8.20 -1.05 0.0593 0.0492
    7.16
                                                             -1.29
9
    7.19
                   2.93
                           8.12 -0.926 0.00793 0.000451
                                                             -0.337
                   2.79
                           8.20 -0.123 0.0265 0.00396
10
    8.07
                                                              0.547
# ... with 355 more rows, and 1 more variable: geometry <POINT [m]>
```

By default, only the columns of data used to fit the model are returned alongside the diagnostics. All original columns of data are returned by setting drop to FALSE.

## 3.5 An Areal Data Example

Next we use the areal seal data, an sf object that contains the log of the estimated harbor-seal trends from abundance data across polygons in Alaska. We view the first few rows of seal by running

#### R> seal

```
Simple feature collection with 62 features and 1 field
Geometry type: POLYGON
Dimension:
                XY
Bounding box: xmin: 913618.8 ymin: 1007542 xmax: 1116002 ymax: 1145054
Projected CRS: NAD83 / Alaska Albers
# A tibble: 62 x 2
   log_trend
                                                                                        geometry
       <dbl>
                                                                                   <POLYGON [m]>
              ((1035002 1054710, 1035002 1054542, 1035002 1053542, 1035002 1052542, 103500~
 1
    NA
              ((1037002 1039492, 1037006 1039490, 1037017 1039492, 1037035 1039496, 103704~
   -0.00121 ((1070158 1030216, 1070185 1030207, 1070187 1030207, 1070211 1030207, 107027~
    0.0354 ((1054906 1034826, 1054931 1034821, 1054936 1034822, 1055001 1034828, 105500~
 4
              ((1025142 1056940, 1025184 1056889, 1025222 1056836, 1025256 1056780, 102527~
 5
    -0.0160
             ((1026035 1044623, 1026037 1044605, 1026072 1044610, 1026083 1044612, 102611~
     0.0872
 6
             ((1100345 1060709, 1100287 1060706, 1100228 1060706, 1100170 1060711, 110011~ ((1030247 1029637, 1030248 1029637, 1030265 1029642, 1030328 1029656, 103039~
 7
    -0.266
8
    0.0743
9
              ((1043093 1020553, 1043097 1020550, 1043101 1020550, 1043166 1020557, 104323~
10 -0.00961 ((1116002 1024542, 1116002 1023542, 1116002 1022542, 1116002 1021554, 111598~
# ... with 52 more rows
```

We can learn more about the data by running help("seal", "spmodel").

To visualize the distribution of log seal trends in the seal data (Figure 3), run

<sup>+</sup> geom\_sf(size = 0.75) +

<sup>+</sup> scale\_fill\_viridis\_c() +

<sup>+</sup> theme\_gray(base\_size = 14)

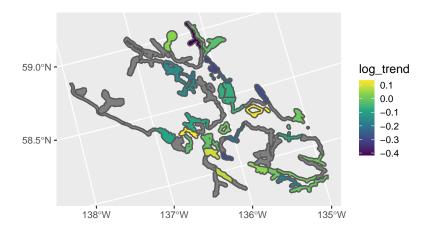


Figure 3: Distribution of log seal trends in the seal data. Polygons are gray where seal trends were not available.

Polygons are considered neighbors if they share at least one boundary. Polygons are gray if the log trend is missing. It is important to keep these missing observations in the data while fitting the model to preserve the neighborhood structure.

We estimate parameters of a spatial autoregressive model regressing log seal trends (log\_trend) on an intercept using a conditional autoregressive (CAR) spatial covariance by running

```
R> sealmod <- spautor(log_trend ~ 1, seal, spcov_type = "car")
```

By default, spautor() calculates the weight matrix internally by defining observations as neighbors if they share at least one border (observations are not neighbors with themselves), uses row standardization, and assumes ie equals zero.

We tidy and glance at the fitted model and augment the data by running

## R> tidy(sealmod)

```
# A tibble: 1 x 5
```

## R> glance(sealmod)

# A tibble: 1 x 9

#### R> augment(sealmod)

Simple feature collection with 34 features and 6 fields

Geometry type: POLYGON

Dimension: XY

Bounding box: xmin: 980001.5 ymin: 1010815 xmax: 1116002 ymax: 1145054

Projected CRS: NAD83 / Alaska Albers

# A tibble: 34 x 7

```
.hat .cooksd .std.resid
   log trend .fitted
                     .resid
                                                                                  geometry
                                      <dbl>
                                                <dbl>
                                                                             <POLYGON [m]>
 *
       <dbl>
               <dbl>
                       <dbl>
                             <dbl>
 1
   -0.282
            -0.0710 -0.211 0.0179 0.0233
                                               -1.14 ((1037002 1039492, 1037006 1039490~
2
   -0.00121 -0.0710 0.0698 0.0699 0.0412
                                                0.767 ((1070158 1030216, 1070185 1030207~
 3
                                                0.705 ((1054906 1034826, 1054931 1034821~
    0.0354 -0.0710 0.106 0.0218 0.0109
 4
   -0.0160 -0.0710 0.0550 0.0343 0.00633
                                                0.430 ((1025142 1056940, 1025184 1056889~
 5
    0.0872 -0.0710 0.158 0.0229 0.0299
                                                1.14 ((1026035 1044623, 1026037 1044605~
                                                      ((1100345 1060709, 1100287 1060706~
 6
   -0.266
            -0.0710 -0.195 0.0280 0.0493
                                               -1.33
 7
    0.0743 -0.0710 0.145 0.0480 0.0818
                                                1.30 ((1030247 1029637, 1030248 1029637~
   -0.00961 -0.0710 0.0614 0.0143 0.00123
                                                0.293 ((1116002 1024542, 1116002 1023542~
                                               -1.09 ((1079864 1025088, 1079895 1025084~
   -0.182
            -0.0710 -0.111 0.0131 0.0155
   0.00351 -0.0710 0.0745 0.0340 0.0107
                                                0.561 ((1110363 1037056, 1110346 1037040~
10
# ... with 24 more rows
```

## 4 Prediction

In this section, we show how to use predict() to perform spatial prediction (also called Kriging) in spmodel. We fit a model using the point-referenced sulfate data, an sf object that contains sulfate measurements in the conterminous United States. We make predictions for each location in the point-referenced sulfate\_preds data, an sf object that contains locations in the conterminous United States at which to predict sulfate. We visualize the distribution of the sulfate data (Figure 4, left) by running

```
R> ggplot(sulfate, aes(color = sulfate)) +
    geom_sf(size = 2.5) +
    scale_color_viridis_c(limits = c(0, 45)) +
    theme gray(base size = 18)
```

We fit a spatial linear model regressing sulfate on an intercept using a spherical spatial covariance function by running

```
R> sulfmod <- splm(sulfate ~ 1, sulfate, spcov_type = "spherical")
```

Then we obtain best linear unbiased predictions (Kriging predictions) using predict(), where the newdata argument contains the locations at which to predict:

```
R> predict(sulfmod, newdata = sulfate_preds)
```

We make and predictions at the locations in sulfate\_preds and store them as a new variable called preds in the sulfate\_preds data set and then visualize them (Figure 4, right) by running

```
R> sulfate_preds$preds <- predict(sulfmod, newdata = sulfate_preds)
R> ggplot(sulfate_preds, aes(color = preds)) +
      geom_sf(size = 2.5) +
      scale_color_viridis_c(limits = c(0, 45)) +
      theme_gray(base_size = 18)
```

If explanatory variables were used to fit the model, the same explanatory variables must be included in newdata with the same names they have in data. If data is a data.frame, coordinates must be included in newdata with the same names as they have in data. If data is an sf object, coordinates must be included in newdata with the same geometry name as they have in data. When using projected coordinates, the projection for newdata should be the same as the projection for data.

Prediction standard errors are returned by setting the se.fit argument to TRUE:

```
R> predict(sulfmod, newdata = sulfate_preds, se.fit = TRUE)
```

The interval argument determines the type of interval returned. If interval is "none" (the default), no interval is returned. If interval is "prediction", a 100 \* level% prediction interval is returned (the default is a 95% prediction interval):

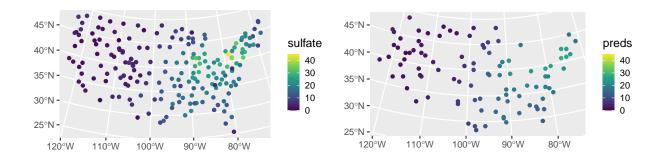


Figure 4: Distribution of observed sulfate (left) and sulfate predictions (right) in the conterminous United States.

R> predict(sulfmod, newdata = sulfate\_preds, interval = "prediction")

If interval is "confidence", the predictions are instead the estimated mean given each observation's explanatory variable values. The corresponding 100 \* level% confidence interval is returned:

R> predict(sulfmod, newdata = sulfate\_preds, interval = "confidence")

Previously we used the augment() function to augment data with model diagnostics. We can also use augment() to augment newdata with predictions, standard errors, and intervals. We remove the model predictions from sulfate\_preds before showing how augment() is used to obtain the same predictions by running

R> sulfate\_preds\$preds <- NULL

We then view the first few rows of sulfate\_preds augmented with a 90% prediction interval by running

R> augment(sulfmod, newdata = sulfate\_preds, interval = "prediction", level = 0.90)

Simple feature collection with 100 features and 3 fields

Geometry type: POINT Dimension: XY

Bounding box: xmin: -2283774 ymin: 582930.5 xmax: 1985906 ymax: 3037173

Projected CRS: NAD83 / Conus Albers

# A tibble: 100 x 4  $\,$ 

```
.fitted .lower .upper
                                      geometry
     <dbl>
            <dbl>
                   <dbl>
                                   <POINT [m]>
      1.40
            -5.33
                    8.14
                           (-1771413 1752976)
 1
 2
     24.5
                    30.8
            18.2
                             (1018112 1867127)
 3
      8.99
             2.36
                   15.6
                          (-291256.8 1553212)
 4
     16.4
             9.92
                    23.0
                             (1274293 1267835)
 5
            -1.56
                   11.4
                          (-547437.6 1638825)
      4.91
 6
     26.7
            20.4
                    33.0
                             (1445080 1981278)
 7
      3.00
            -3.65
                    9.66
                           (-1629090 3037173)
 8
             7.97
                             (1302757 1039534)
     14.3
                    20.6
9
            -5.08
                    8.06
                           (-1429838 2523494)
      1.49
     14.4
             7.97
                    20.8
                             (1131970 1096609)
10
```

# ... with 90 more rows

Here  $\tt.fitted$  represents the predictions.

Alternatively, we can include missing responses (NA values) in the data used for model fitting. The missing responses will be ignored for model fitting but stored in the fitted model object. We can add a column of missing responses to sulfate\_preds, bind it together with sulfate, and re-fit the model by running

```
R> sulfate_preds$sulfate <- NA
R> sulfate_with_NA <- rbind(sulfate, sulfate_preds)
R> sulfmod_with_NA <- splm(sulfate ~ 1, sulfate_with_NA, "spherical")</pre>
```

We can then make predictions at the observations with missing responses by running

```
R> predict(sulfmod with NA)
```

This call to predict() finds in sulfmod\_with\_NA the newdata object, which is a subset of data that contains only the observations with missing responses:

#### R> sulfmod\_with\_NA\$newdata

```
Simple feature collection with 100 features and 1 field
Geometry type: POINT
Dimension:
Bounding box:
              xmin: -2283774 ymin: 582930.5 xmax: 1985906 ymax: 3037173
Projected CRS: NAD83 / Conus Albers
First 10 features:
    sulfate
                             geometry
198
        NA POINT (-1771413 1752976)
199
        NA
             POINT (1018112 1867127)
200
        NA POINT (-291256.8 1553212)
201
        NA POINT (1274293 1267835)
        NA POINT (-547437.6 1638825)
202
203
        NA POINT (1445080 1981278)
204
        NA POINT (-1629090 3037173)
205
        NA
            POINT (1302757 1039534)
206
        NA POINT (-1429838 2523494)
             POINT (1131970 1096609)
207
        NA
```

We can also use augment() to make the predictions by running

R> augment(sulfmod\_with\_NA, newdata = sulfmod\_with\_NA\$newdata)

```
Simple feature collection with 100 features and 2 fields
Geometry type: POINT
Dimension:
               XΥ
Bounding box: xmin: -2283774 ymin: 582930.5 xmax: 1985906 ymax: 3037173
Projected CRS: NAD83 / Conus Albers
# A tibble: 100 x 3
   sulfate .fitted
                              geometry
     <dbl>
             <dbl>
                           <POINT [m]>
 1
       NA
              1.40 (-1771413 1752976)
 2
       NA
            24.5
                     (1018112 1867127)
 3
       NA
             8.99 (-291256.8 1553212)
            16.4
 4
       NA
                     (1274293 1267835)
 5
       NA
              4.91 (-547437.6 1638825)
 6
        NA
             26.7
                     (1445080 1981278)
 7
              3.00 (-1629090 3037173)
        NA
 8
       NA
             14.3
                     (1302757 1039534)
9
       NA
              1.49
                    (-1429838 2523494)
             14.4
                     (1131970 1096609)
10
       NA
# ... with 90 more rows
```

Recall that omitting the newdata argument and running augment(sulfmod\_with\_NA) returns model diagnostics, not predictions.

For areal data, predictions cannot be computed at locations that were not incorporated in the neighborhood structure used to fit the model. Thus predictions are only possible for observations in data whose response values are missing (NA), as their locations are incorporated into the neighborhood structure. For example, we make predictions of log seal trends at the missing polygons from Figure 3 by running

```
R> predict(sealmod)
```

We can also use augment() to make the predictions:

R> augment(sealmod, newdata = sealmod\$newdata)

```
Simple feature collection with 28 features and 2 fields
Geometry type: POLYGON
Dimension:
Bounding box: xmin: 913618.8 ymin: 1007542 xmax: 1115097 ymax: 1132682
Projected CRS: NAD83 / Alaska Albers
# A tibble: 28 x 3
   log_trend .fitted
                                                                                   geometry
                                                                              <POLYGON [m]>
       <dbl>
               <dbl>
          NA -0.113 ((1035002 1054710, 1035002 1054542, 1035002 1053542, 1035002 1052542~
 1
          NA -0.0108 ((1043093 1020553, 1043097 1020550, 1043101 1020550, 1043166 1020557~
 2
 3
          NA -0.0608 ((1099737 1054310, 1099752 1054262, 1099788 1054278, 1099849 1054301~
          NA -0.0383 ((1099002 1036542, 1099134 1036462, 1099139 1036431, 1099145 1036366~
 4
 5
          NA -0.0730 ((1076902 1053189, 1076912 1053179, 1076931 1053179, 1076996 1053177~
 6
          NA -0.0556 ((1070501 1046969, 1070317 1046598, 1070308 1046542, 1070306 1046534~
 7
          NA -0.0968 ((1072995 1054942, 1072996 1054910, 1072997 1054878, 1072997 1054847~
          NA -0.0716 ((960001.5 1127667, 960110.8 1127542, 960144.1 1127495, 960178.6 112~
 8
 9
          NA -0.0776 ((1031308 1079817, 1031293 1079754, 1031289 1079741, 1031257 1079627~
          NA -0.0647 ((998923.7 1053647, 998922.5 1053609, 998950 1053631, 999001.5 10536~
10
# ... with 18 more rows
```

## 5 Advanced Features

spmodel offers several advanced features for fitting spatial linear models. We briefly discuss each next using the moss data and simulated data, though technical details for each advanced feature can be seen by running vignette("technical", "spmodel").

## 5.1 Fixing Spatial Covariance Parameters

We may desire to fix specific spatial covariance parameters at a particular value. Perhaps some parameter value is known, for example. Or perhaps we want to compare nested models where a reduced model uses a fixed parameter value while the full model estimates the parameter. Fixing spatial covariance parameters while fitting a model is possible using the spcov\_initial argument to spmod() and spautor(). The spcov\_initial argument takes an spcov\_initial object (run help("spcov\_initial", "spmodel") for more). spcov\_initial objects can also be used to specify initial values used during optimization, even if they are not assumed to be fixed. By default, spmodel uses a grid search to find suitable initial values to use during optimization.

Suppose the goal is to compare the full model to a model that assumes the independent random error variance (nugget) is zero. First, the <code>spcov\_initial</code> object is specified:

```
R> init <- spcov_initial("exponential", ie = 0, known = "ie")
R> print(init)

$initial
ie
    0

$is_known
    ie
TRUE

attr(,"class")
[1] "exponential"
```

The init output shows that the ie parameter has an initial value of zero that is assumed to be known. Next the model is fit:

```
R> spmod_red <- splm(log_Zn ~ log_dist2road, moss, spcov_initial = init)</pre>
```

Notice that because the spcov\_initial object contains information about the spatial covariance type, the spcov\_type argument is not required when spcov\_initial is provided. We can use glances() to glance at both models:

R> glances(spmod, spmod\_red)

```
# A tibble: 2 x 10
  model
                       p npar value
                                        AIC AICc logLik deviance pseudo.r.squared
  <chr>
            <int> <dbl> <int> <dbl> <dbl> <dbl> <dbl>
                                                    <dbl>
                                                              <dbl>
                                                    -184.
                                                                                0.683
1 spmod
                       2
                                                               363
              365
                             3
                                367.
                                       373.
                                              373.
                                                    -189.
                       2
                              2
                                       382.
                                              382.
                                                               374.
                                                                                0.703
2 spmod_red
              365
                                 378.
```

The lower AIC and AICc of the full model compared to the reduced model indicates that the independent random error variance is important to the model. A likelihood ratio test comparing the full and reduced models is also possible using anova().

#### 5.2 Random Effects

Random effects incorporate additional sources of variability into model fitting. They are accommodated in spmodel using similar syntax as for random effects in the nlme (Pinheiro and Bates 2006) and lme4 (Bates et al. 2015) **R** packages. Random effects are specified via a formula passed to the random argument. Next we show two examples incorporating random effects into the spatial linear model using the moss data.

The first example explores random intercepts for the sample variable. The sample variable indexes each unique location, which can have replicate observations due to field duplicates (field\_dup) and lab replicates (lab\_rep). We create extra correlation for repeated observations from a sample by creating a random intercept for each level of sample. We incorporate the random intercepts for sample by running

```
R> rand1 <- splm(
+ log_Zn ~ log_dist2road,
+ moss,
+ spcov_type = "exponential",
+ random = ~ sample
+ )</pre>
```

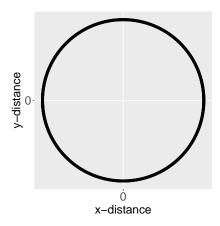
Note that sample is shorthand for (1 | sample), which is more explicit notation that indicates random intercepts for each level of sample.

The second example adds a random intercept for year, which creates extra correlation for observations within a year. It also adds a random slope for log\_dist2road within year, which lets the effect of log\_dist2road vary between years. We fit this model by running

```
R> rand2 <- splm(
+ log_Zn ~ log_dist2road,
+ moss,
+ spcov_type = "exponential",
+ random = ~ sample + (log_dist2road | year)
+ )</pre>
```

Note that sample + (log\_dist2road | year) is shorthand for (1 | sample) + (log\_dist2road | year). If only random slopes within year are desired (and no random intercepts), a - 1 is given to the relevant portion of the formula: (log\_dist2road - 1 | year). When there is more than one term in random, each term must be surrounded by parentheses (recall that the random intercept shorthand automatically includes relevant parentheses). More examples of random effect syntax are provided in Appendix B.

We glance at all three models by running



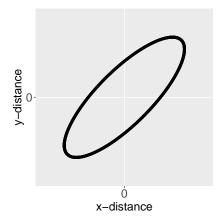


Figure 5: Ellipses for an isotropic (left) and anisotropic (right) covariance function centered at the origin. The black outline of each ellipse is a level curve of equal correlation.

R> glances(spmod, rand1, rand2)

```
# A tibble: 3 x 10
  model
                   p npar value
                                    AIC
                                        AICc logLik deviance pseudo.r.squared
            n
                                                          <dbl>
  <chr> <int> <dbl> <int> <dbl> <dbl> <dbl> <dbl>
                                                <dbl>
                                   202.
                                          202.
                                                                            0.215
1 rand2
          365
                   2
                         6
                            190.
                                                -94.9
                                                           363.
2 rand1
          365
                   2
                          4
                             335.
                                   343.
                                          343. -168.
                                                           363
                                                                             0.661
3 spmod
          365
                         3
                            367.
                                   373.
                                          373. -184.
                                                           363
                                                                             0.683
```

rand2 has the lowest AIC and AICc.

It is possible to fix random effect variances using the randcov\_initial argument. randcov\_initial can also be used to set initial values for optimization.

## 5.3 Partition Factors

A partition factor is a variable that assumes observations are uncorrelated when they are from different levels of the partition factor. Partition factors are specified in spmodel by providing a formula with a single variable to the partition\_factor argument. Suppose that for the moss data, it is appropriate to assume observations in different years (year) are uncorrelated. We fit a model that treats year as a partition factor by running

```
R> part <- splm(
+ log_Zn ~ log_dist2road,
+ moss,
+ spcov_type = "exponential",
+ partition_factor = ~ year
+ )</pre>
```

#### 5.4 Anisotropy

A spatial covariance function for point-referenced data is isotropic if it behaves similarly in all directions (i.e., is independent of direction) as a function of distance. An anisotropic covariance function does not behave similarly in all directions as a function of distance. Consider the spatial covariance imposed by an eastward-moving wind pattern. A one-unit distance in the x-direction likely means something different than a one-unit distance in the y-direction. Figure 5 shows ellipses for an isotropic and anisotropic covariance function centered at the origin (a distance of zero).

The black outline of each ellipse is a level curve of equal correlation. The left ellipse (a circle) represents an isotropic covariance function. The distance at which the correlation between two observations lays on the level curve is the same in all directions. The right ellipse represents an anisotropic covariance function. The

distance at which the correlation between two observations lays on the level curve is different in different directions.

Accounting for anisotropy involves a rotation and scaling of the x-coordinates and y-coordinates such that the spatial covariance function that uses these transformed distances is isotropic. We fit a model with anisotropy by running

```
R> spmod anis <- splm(
    log_Zn ~ log_dist2road,
    moss.
    spcov_type = "exponential",
    anisotropy = TRUE
R> summary(spmod anis)
Call:
splm(formula = log Zn ~ log dist2road, data = moss, spcov type = "exponential",
    anisotropy = TRUE)
Residuals:
    Min
             10 Median
                             3Q
                                    Max
-2.5279 -1.2239 -0.7202 -0.1921 1.1659
Coefficients (fixed):
              Estimate Std. Error z value Pr(>|z|)
                                            <2e-16 ***
(Intercept)
               9.54798
                          0.22291
                                    42.83
log_dist2road -0.54601
                          0.01855
                                   -29.44
                                             <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Pseudo R-squared: 0.7048
Coefficients (exponential spatial covariance):
                 ie
                        range
                                 rotate
                                             scale
3.561e-01 6.812e-02 8.732e+03 2.435e+00 4.753e-01
```

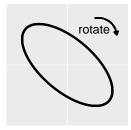
The rotate parameter is between zero and  $\pi$  radians and represents the angle of a clockwise rotation of the ellipse. The scale parameter is between zero and one and represents the ratio of the distance between the origin and the edge of the ellipse along the minor axis to the distance between the origin and the edge of the ellipse along the major axis. Figure 6 shows the transformation that turns an anisotropic ellipse into an isotropic one (i.e., a circle). This transformation requires rotating the the coordinates clockwise by rotate and then scaling them the reciprocal of scale. The transformed coordinates are then used instead of the original coordinates to compute distances and spatial covariances.

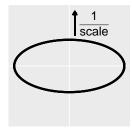
Note that specifying an initial value for rotate that is different from zero, specifying an initial value for scale that is different from one, or assuming either rotate or scale are unknown in spcov\_initial will cause splm() to fit a model with anisotropy (and will override anisotropy = FALSE). Estimating anisotropy parameters is only possible for maximum likelihood and restricted maximum likelihood estimation, but fixed anisotropy parameters can be accommodated for semivariogram weighted least squares or semivariogram composite likelihood estimation. Also note that anisotropy is not relevant for areal data because the spatial covariance function depends on a neighborhood structure instead of distances between points.

## 5.5 Simulating Spatial Data

The sprnorm() function is used to simulate normal (Gaussian) spatial data. To use sprnorm(), the spcov\_params() function is used to create an spcov\_params object. The spcov\_params() function requires the spatial covariance type and and parameter values. We create an spcov\_params object by running

```
R> sim_params <- spcov_params("exponential", de = 5, ie = 1, range = 0.5)
```





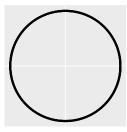


Figure 6: A visual representation of the anisotropy transformation. In the left figure, the first step is to rotate the anisotropic ellipse clockwise by the **rotate** parameter. In the middle figure, the second step is to scale the minor axis by the reciprocal of the **scale** parameter. In the right figure, the anisotropic ellipse has been transformed into an isotropic one (i.e., a circle). The transformed coordinates are then used instead of the original coordinates to compute distances and spatial covariances.

We set a reproducible seed and then simulate data at 3000 random locations in the unit square using the spatial covariance parameters in sim\_params by running

There is noticeable spatial patterning in the response variable (sim\_resp). The default mean in sprnorm() is zero for all observations, though a mean vector can be provided using the mean argument. The default number of samples generated in sprnorm() is one, though this is changed using the samples argument. Because dat is a tibble (data.frame) and not an sf object, the columns in dat representing the x-coordinates and y-coordinates must be provided to sprnorm().

Note that the output from coef(object, type = "spcov") is a spcov\_params object. This is useful if one wants to simulate data given the estimated spatial covariance parameters from a fitted model. Random effects are incorporated into simulation via the randcov\_params argument.

## 5.6 Big Data

The computational cost associated with model fitting is exponential in the sample size for all estimation methods. For maximum likelihood and restricted maximum likelihood, the computational cost of estimating  $\boldsymbol{\theta}$  is cubic. For semivariogram weighted least squares and semivariogram composite likelihood, the computational cost of estimating  $\boldsymbol{\theta}$  is quadratic. The computational cost associated with estimating  $\boldsymbol{\beta}$  and prediction is cubic in the model-fitting sample size, regardless of estimation method. Typically samples sizes approaching 10,000 make the computational cost of model fitting and prediction infeasible, which necessitates the use of big data methods. spmodel offers big data methods for model fitting of point-referenced data via the local argument to splm(), capable of fitting models with hundreds of thousands to millions of observations rather quickly. Because of the neighborhood structure of areal data, the big data methods used for point-referenced data do not apply to areal data. Thus there is no big data method for areal data or local argument to spautor() and model fitting sample sizes cannot be too large.

spmodel offers big data methods for prediction of point-referenced data or areal data via the local argument to predict(), capable of making predictions at hundreds of thousands to millions of locations rather quickly.

To show how to use spmodel for big data estimation and prediction, we use the sim\_data data from Section 5.5. Because sim\_data is a tibble (data.frame) and not an sf object, the column in data representing the x-coordinates and y-coordinates must be explicitly provided to splm(). Though the sample sizes used next for model fitting and prediction are relatively small, the purpose of the following examples is simply to illustrate the big data approaches.

## 5.6.1 Model-fitting

spmodel uses a "local indexing" approximation for big data model fitting of point-referenced data. Observations are first assigned an index. Then for the purposes of model fitting, observations with different indexes are assumed uncorrelated. This approach has some connections to composite likelihood and to the partition factors discussed earlier.

The local argument to splm() controls the big data options. local is a list with several arguments. The arguments to the local list control the method used to assign the indexes, the number of observations with the same index, the number of unique indexes, variance adjustments to the covariance matrix of  $\hat{\beta}$ , whether or not to use parallel processing, and if parallel processing is used, the number of cores.

The simplest way to accommodate big data is to set local to TRUE. This is shorthand for local = list(method = "random", size = 50, var\_adjust = "theoretical", parallel = FALSE), which creates groups with approximately 50 observations each using a random assignment of groups to indexes, uses the theoretically-correct variance adjustment, and does not use parallel processing.

```
R> local1 <- splm(sim_resp ~ 1, sim_data, spcov_type = "exponential",
                 xcoord = x, ycoord = y, local = TRUE)
R> summary(local1)
Call:
splm(formula = sim_resp ~ 1, data = sim_data, spcov_type = "exponential",
    xcoord = x, ycoord = y, local = TRUE)
Residuals:
    Min
             1Q Median
                             3Q
                                    Max
-5.0356 -1.3514 -0.1468 1.2842 6.5381
Coefficients (fixed):
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.021
                          0.699
                                  -1.46
                                           0.144
Coefficients (exponential spatial covariance):
    de
           ie range
2.8724 0.9735 0.2644
```

Instead of using local = TRUE, we can explicitly set local. For example, we fit a model using using k-means clustering (MacQueen and others 1967) on the x-coordinates and y-coordinates to create 60 groups (clusters), the pooled variance adjustment, and parallel processing with two cores by running

We can use loocv() to evaluate model fit. Note that loocv() has big data options that are passed to predict(), which we discuss in Section 5.6.2.

```
R> loocv(local1, local = list(method = "distance", parallel = TRUE, ncores = 2))
[1] 1.243062
R> loocv(local2, local = list(method = "distance", parallel = TRUE, ncores = 2))
[1] 1.242925
```

Likelihood-based statistics like AIC(), AICc(), logLik(), and deviance() should not be used to compare a model fit with a big data approximation to a model fit without a big data approximation, as the two approaches maximize different likelihoods.

#### 5.6.2 Prediction

For point-referenced data, **spmodel** uses a "local neighborhood" approximation for big data prediction. Each prediction is computed using a subset of the observed data instead of all the observed data. Before further discussing big data prediction, we simulate 1000 locations in the unit square requiring prediction:

```
R> n_pred <- 1000
R> x <- runif(n_pred)
R> y <- runif(n_pred)
R> sim_preds <- tibble::tibble(x = x, y = y)</pre>
```

The local argument to predict() controls the big data options. local is a list with several arguments. The arguments to the local list control the method used to subset the observed data, the number of observations in each subset, whether or not to use parallel processing, and if parallel processing is used, the number of cores.

The simplest way to accommodate big data prediction is to set local to TRUE. This is shorthand for local = list(method = "covariance", size = 50, parallel = FALSE), which implies that uniquely for each location requiring prediction, only the 50 observations in the data most correlated with it are used in the computation and parallel processing is not used. Using the local1 fitted model, we store these predictions as a variable called preds in the sim\_preds data by running

```
R> sim_preds$preds <- predict(local1, newdata = sim_preds, local = TRUE)</pre>
```

The predictions are visualized (Figure 7, right) by running

They display a similar pattern as the observed data.

Instead of using local = TRUE, we can explicitly set local. For example, we make predictions using the distance method, subsets of 30 observations, and parallel processing with 2 cores by running

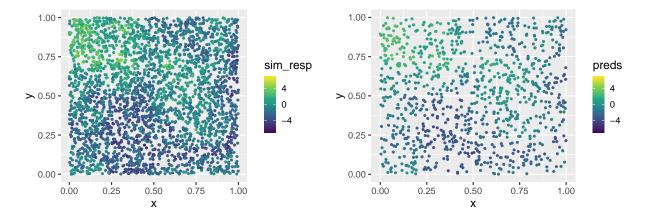


Figure 7: Observed data and big data predictions at unobserved locations. In the left figure, spatial data are simulated in the unit square. A spatial linear model is fit using the default big data approximation for model-fitting. In the right figure, predictions are made using the fitted model and the default big data approximation for prediction.

```
R> pred_list <- list(method = "distance", size = 30, parallel = TRUE, ncores = 2)
R> predict(local1, newdata = sim_preds, local = pred_list)
```

For areal data, no local neighborhood approximation exists because of the data's underlying neighborhood structure. Thus all of the data must be used to compute predictions and by consequence, method and distance are not components of the local list. The only components of the local list for areal data are parallel and ncores:

R> predict(sealmod, local = list(parallel = TRUE, ncores = 2))

## 6 Discussion

Throughout this vignette, we have shown how to use spmodel to fit, summarize, and predict for a variety of spatial statistical models. Spatial linear models for point-referenced data (i.e., geostatistical models) are fit using the splm() function. Spatial linear models for areal data (i.e., spatial autoregressive models) are fit using the spautor() function. Several model-fit statistics and diagnostics are available. The broom functions tidy() and glance() are used to tidy and glance at a fitted model. The broom function augment() is used to augment data with model diagnostics and augment newdata with predictions. Several advanced features are available to accommodate fixed covariance parameter values, random effects, partition factors, anisotropy, simulated data, and big data approximations for model fitting and prediction.

We appreciate feedback from users regarding spmodel. To learn more about how to provide feedback or contribute to spmodel, please visit our GitHub repository at https://github.com/USEPA/spmodel.

## References

Bates, Douglas, Martin Mächler, Ben Bolker, and Steve Walker. 2015. "Fitting Linear Mixed-Effects Models Using lme4." *Journal of Statistical Software* 67 (1): 1–48. https://doi.org/10.18637/jss.v067.i01.

Cook, R Dennis, and Sanford Weisberg. 1982. Residuals and Influence in Regression. New York: Chapman; Hall.

Cressie, Noel. 1985. "Fitting Variogram Models by Weighted Least Squares." Journal of the International Association for Mathematical Geology 17 (5): 563–86.

Curriero, Frank C, and Subhash Lele. 1999. "A Composite Likelihood Approach to Semivariogram Estimation." *Journal of Agricultural, Biological, and Environmental Statistics*, 9–28.

Harville, David A. 1977. "Maximum Likelihood Approaches to Variance Component Estimation and to Related Problems." *Journal of the American Statistical Association* 72 (358): 320–38.

Hoeting, Jennifer A, Richard A Davis, Andrew A Merton, and Sandra E Thompson. 2006. "Model Selection for Geostatistical Models." *Ecological Applications* 16 (1): 87–98.

MacQueen, James, and others. 1967. "Some Methods for Classification and Analysis of Multivariate Observations." In *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability*, 1:281–97. 14. Oakland, CA, USA.

Montgomery, Douglas C, Elizabeth A Peck, and G Geoffrey Vining. 2021. Introduction to Linear Regression Analysis. John Wiley & Sons.

Patterson, H Desmond, and Robin Thompson. 1971. "Recovery of Inter-Block Information When Block Sizes Are Unequal." *Biometrika* 58 (3): 545–54.

Pebesma, Edzer. 2018. "Simple Features for R: Standardized Support for Spatial Vector Data." The R Journal 10 (1): 439–46. https://doi.org/10.32614/RJ-2018-009.

Pinheiro, José, and Douglas Bates. 2006. Mixed-Effects Models in S and S-Plus. Springer science & business media.

Robinson, David, Alex Hayes, and Simon Couch. 2021. Broom: Convert Statistical Objects into Tidy Tibbles. https://CRAN.R-project.org/package=broom.

Tobler, Waldo R. 1970. "A Computer Movie Simulating Urban Growth in the Detroit Region." *Economic Geography* 46 (sup1): 234–40.

Wickham, Hadley. 2016. *Ggplot2: Elegant Graphics for Data Analysis*. Springer-Verlag New York. https://ggplot2.tidyverse.org.

Wolfinger, Russ, Randy Tobias, and John Sall. 1994. "Computing Gaussian Likelihoods and Their Derivatives for General Linear Mixed Models." SIAM Journal on Scientific Computing 15 (6): 1294–1310.

# **Appendices**

## A An Additional Example Using caribou

The caribou data are observed on an equally spaced lattice and can be analyzed as point-referenced or areal data. We view the first few rows of caribou by running

#### R> caribou

```
# A tibble: 30 x 5
   water tarp
   <fct> <fct> <dbl> <dbl> <dbl>
 1 Y
         clear 2.42
                          1
 2 Y
         shade 2.44
                                6
 3 Y
         none
                1.81
                          3
                                6
 4 N
         clear 1.97
                          4
                                6
 5 N
         shade 2.38
                          5
                                6
 6 Y
         none
                2.22
                          1
                                5
7 N
         clear 2.10
                          2
                                5
8 Y
         clear
                1.80
                          3
                                5
9 Y
         shade
                1.96
                          4
                                5
10 Y
         none
                2.10
                          5
                                5
# ... with 20 more rows
```

First we analyze caribou as point-referenced data. Because caribou is not an sf object, we must provide the columns in caribou that represent the x-coordinates and y-coordinates. We fit a spatial linear model regressing nitrogen percentage (z) on water presence (water) and tarp cover (tarp) by running

```
R> cariboumod <- splm(z ~ water + tarp, data = caribou,
+ spcov_type = "exponential", xcoord = x, ycoord = y)
```

An analysis of variance can be conducted to assess the overall impact of the tarp variable, which has three levels (clear, shade, and none), and the water variable, which has two levels (water and no water). We perform an analysis of variance and tidy the results by running

#### R> tidy(anova(cariboumod))

```
# A tibble: 3 x 4
  effects
                df statistic p.value
  <chr>
              <int>
                        <dbl>
                                 <dbl>
1 (Intercept)
                        43.5 4.33e-11
                1
                         1.66 1.98e- 1
2 water
                  1
3 tarp
                  2
                        15.4 4.51e- 4
```

There is significant evidence that at least one tarp cover impacts nitrogen. Note that, like in summary(), these p-values are associated with an asymptotic hypothesis test (here, an asymptotic Chi-squared test).

Next we analyze caribou as areal data. Because caribou is not an sf object, we must create a weights matrix. We define two observations as neighbors if they are adjacent (directly east, west, north, or south) to one another. Two observations in caribou are adjacent if the distance between them equals one (recall that observations are not neighbors with themselves):

```
R> coords <- cbind(caribou$x, caribou$y)
R> dists <- as.matrix(dist(coords))
R> W <- dists == 1</pre>
```

Currently, W is a logical matrix with TRUEs and FALSEs. We coerce it to a numeric matrix by running

```
R> W <- W * 1
```

The ijth value in W is 1 if the observation in the ith row is neighbors with the observation in the jth row and 0 otherwise. We fit a spatial autoregressive model regressing the nitrogen percentage (z) on water presence (water) and tarp cover (tarp) by running

```
R> cariboumod <- spautor(z ~ water + tarp, data = caribou,
+ spcov_type = "car", W = W)
```

We perform an analysis of variance and tidy the results by running

R> tidy(anova(cariboumod))

```
# A tibble: 3 x 4
  effects
                 df statistic
                                p.value
  <chr>
              <int>
                        <dbl>
                                  <dbl>
1 (Intercept)
                            2.36e-157
                  1
                       714.
2 water
                         1.82 1.77e- 1
                  1
3 tarp
                        15.1 5.17e- 4
```

There is significant evidence that at least one tarp cover impacts nitrogen. Note that, like in summary(), these p-values are associated with an asymptotic hypothesis test (here, an asymptotic Chi-squared test).

## B Random Effect Syntax

A couple of common ways to specify random effects in the random argument to splm() or spautor() include:

- ~ (1 | group) : Random intercepts for each level of group. ~ group is shorthand for ~ (1 | group).
- ~ (var | group): Random intercepts for each level of group and random slopes that depend on the variable var for each level of group.

Some additional syntax for more complicated random effects structures include:

- ~ (var 1 | group): Random slopes (without intercepts) that depend on the variable var for each level of group.
- ~ (1 | group:subgroup): Random intercepts for each combination of levels in group and levels in subgroup. ~ group:subgroup is shorthand for ~ (1 | group:subgroup).
- ~ (var | group:subgroup): Random intercepts for each combination of levels in group and levels in subgroup and random slopes that depend on the variable var for each combination of levels in group and levels in subgroup.
- ~ (var 1 | group:subgroup): Random slopes (without intercepts) that depend on the variable var for each combination of levels in group and levels in subgroup.
- ~ (1 | group/subgroup): Shorthand for ~ (1 | group) + (1 | group:subgroup). Commonly, the group/subgroup notation implies subgroup is nested within group.
- ~ (var | group/subgroup): Shorthand for ~ (var | group) + (var | group:subgroup). Commonly, the group/subgroup notation implies subgroup is nested within group.
- ~ (var 1 | group/subgroup): Shorthand for ~ (var 1 | group) + (var 1 | group:subgroup). Commonly, the group/subgroup notation implies subgroup is nested within group.

Distinct random effects terms are separated in random by +. Each term must be wrapped in parentheses. For example, to incorporate random intercepts for group and subgroup, random looks like ~ (1 | group) + (1 | subgroup). For random intercepts, recall that ~ group is shorthand for ~ (1 | group). Thus, an equivalent representation of ~ (1 | group) + (1 | subgroup) is ~ group + subgroup. Note that for both random intercepts and random slopes, the variable on the right-hand side of | (i.e., group, subgroup, group:subgroup) must be a factor (or character) variable.