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REGIONALIZED MODELS WITH SPATIALLY CONTINUOUS PREDICTIONS AT
THE BORDERS

by

Jadon S. Wagstaff

A thesis submitted in partial fulfillment
of the requirements for the degree

of

MASTER OF SCIENCE

in

Mathematical Sciences

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2021

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ABSTRACT

Regionalized Models with Spatially Continuous Predictions at the Borders

by

Jadon S. Wagstaff, Master of Science

Utah State University, 2021

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Department: Mathematics and Statistics

Traditional spatial modeling approaches assume that data are second-order stationary, which is rarely true over large geographical areas. A simple way to model nonstationary data is to partition the space and build models for each region in the partition. This has the side effect of creating discontinuities in the prediction surface at region borders. The regional border smoothing approach described in this thesis ensures continuous predictions by using a weighted average of predictions from regional models. The weights are based on the shortest distance from the observation to each region boundary, with greater weight given to observations that are within or near the boundaries of a region. The R package **remap** is an implementation of the regional border smoothing method that builds a collection of spatial models given a data set with spatial points, a set of polygon regions, and a modeling approach to apply in each region. Special consideration is given to distance calculations that make **remap** package scalable to large problems. Improvements in accuracy using the **remap** package, as opposed to global spatial models, are illustrated using one national-level and one state-level dataset. These accuracy improvements, coupled with their computational feasibility, illustrate the efficacy of the **remap** approach to modeling nonstationary data.

(61 pages)

PUBLIC ABSTRACT

Regionalized Models with Spatially Continuous Predictions at the Borders

Jadon S. Wagstaff

Creating maps of continuous variables involves estimating values between measurement locations scattered throughout a geographic region. These maps often leverage observed similarities between geographically close measurements, but may also make predictions using other geographic information such as elevation. The relationship between the available geographic information and the variable of interest can vary with location, especially when mapping large areas like a continent. A simple way to account for the changing relationship is to divide the space into different sub-regions and model the relationship at each region. The naive implementation of this approach has the side effect of making sudden changes in predictions at the borders of each region. This thesis describes a novel regional border smoothing method that allows for the formation of a continuous map built with regional models. The method is implemented and available to the public through the open source R package **remap**. Improvements in model accuracy are demonstrated using a national scale and a state scale dataset.

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Jadon S. Wagstaff

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ACRONYMS

CRAN	Comprehensive R Archive Network
EPA	Environmental Protection Agency
GAM	Generalized Additive Model
HUC	Hydrologic Unit Code
MSE	Mean Squared Error
NOAA	National Oceanic and Atmospheric Administration
OLS	Ordinary Least Squares
PRISM	Parameter-elevation Regressions on Independent Slopes Model
SNOTEL	Snowpack Telemetry
USGS	United States Geological Survey
WESD	Water Equivalent of Snow Depth

CHAPTER 1

INTRODUCTION

Regression methods attempt to characterize the relationship between predictor variables and a response variable. When observations exhibit spatial autocorrelation, geographic location can be leveraged to improve predictions of the response variable by considering observed values of the response variable at nearby measurement locations. Typical spatial statistical models assume that the covariance between two observations can be modeled as a function of location difference, i.e., the relationship needs to be second-order stationary. For sufficiently large distances, the stationarity assumption often fails.

The simplest way to effectively employ traditional spatial modeling approaches using nonstationary data is to partition the global region into smaller sub-regions that are locally stationary and create separate statistical models for each region. The naive implementation of this approach leads to noncontinuous predictions at the borders of each region. Previous attempts to smooth out discontinuities at region boundaries often involved taking weighted averages of local regional model output where the weights of each local model prediction or covariance structure are a function of the distance between a new observation and the centers of each region (Fuentes, 2001; Fuentes & Smith, 2001; Gosoniu et al., 2009; Gosoniu et al., 2006; Konomi et al., 2014). While the center based approach may be appropriate for symmetrical regions, it may not be appropriate for oddly shaped or disjoint regions not well approximated by their centers. In some cases, a region may not even contain its center. The center based approach also fails to respect major geographic features that can cause sharp changes in response variables over very short distances.

The regional border smoothing approach described in this thesis is a novel method that uses a weighted average of predictions from local models, but gives weight to regional models based on the nearest distance to the *border* of each region rather than distance to the center of each region. With this method, regions may be chosen that more naturally

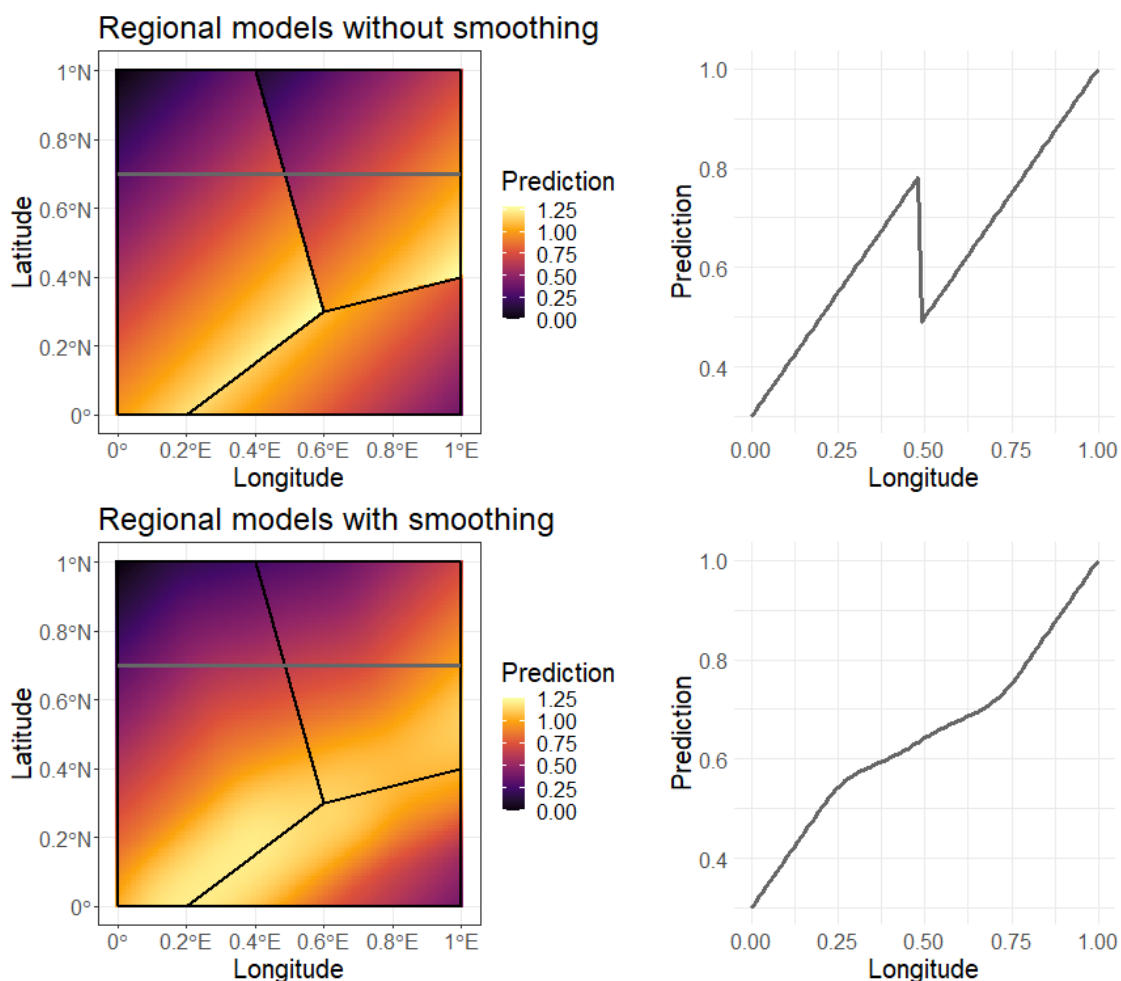


Fig. 1.1: Before (top) and after (bottom) regional border smoothing is applied to regional models where predictions are linear combinations of longitude and latitude. The gray line shows predicted values along the 0.7°N transect. Left region predicts $lon - lat + 1$, bottom region predicts $lat - lon + 1.4$, and right region predicts $lon - lat + 0.7$. Smoothing zone is 30 km ($\approx 0.27^\circ$).

reflect local climate and topography with smoothing only occurring near the borders of each region. Figure 1.1 shows an example of the regional border smoothing approach applied to three regions with different spatial models.

The R package **remap** is a General Public License implementation of this regional border smoothing method that scales well to large problems (Wagstaff, 2021). Using **remap**, regional border smoothing is applied to two different modeling problems. The first problem is a national set of 50-year ground snow loads and the second problem is modeling April

1st snow water content for Utah. Mapped values from both projects show improvement in model accuracy using the regional border smoothing approach over global models for a variety of spatial modeling approaches.

The figures and tables in this thesis are made using the R programming language (R Core Team, 2020). Figures are created with the **tidyverse** (Wickham et al., 2019), **gridExtra** (Auguie, 2017), **cowplot** (Wilke, 2020), and **maps** (Becker et al., 2018) packages. The **sf** (Pebesma, 2018), **mgeo** (Dorman, 2020), and **raster** (Hijmans, 2020) packages are used to manipulate spatial data. Kriging models are built with **automap** (Hiemstra et al., 2009) and generalized additive models are built with **mgcv** (Wood, 2011).

1.1 Background

There are many proposed methods to model nonstationary data using locally stationary models. Haas (1990a, 1990b) describes a moving window approach where only data within a pre-specified bounding box are used to fit a local dependence structure and then make predictions. This process is computationally intensive and may not result in continuous predictions.

Fuentes (2001) and Fuentes and Smith (2001) propose a method for nonstationary problems where a global covariance structure that changes continuously as a function of location is used in a Gaussian process model. The data are first partitioned into locally stationary regions. A global covariance structure is calculated by taking a weighted average of regional covariance structures. Weights are based on the distance from the prediction location to a point in each region, usually the center. Regions are either given *a priori* or by using subgrids chosen using the Bayesian information criterion.

Applications of local partition modeling approaches include Kim et al. (2005), who describe a method to deal with sudden changes in spatial covariance structure that occur between layers of rock strata. The spatial domain is partitioned into independent regions using Voronoi Tessellations (Green & Sibson, 1978), with each region fit using an independent Gaussian model. The resulting global model has sharp changes at the borders of each region, which was desirable in that context. Konomi et al. (2014) illustrate a decision

tree based method for partitioning the spatial domain when modeling global Ozone levels. Heaton et al. (2017) use a hierarchical clustering method to partition the spatial domain for temperature data in Houston, TX. The hierarchical clustering method has the benefit of creating a partition that more naturally follows changes in the covariance structure rather than partitioning the space into symmetrical blocks or spheres.

Gosoni et al. (2009) and Gosoni et al. (2006) provide an additional application of local partitioning models mapping malaria risk using *a priori* partitions of West Africa. The 2006 study uses three large rectangular regions and the 2009 study uses agro-ecological regions to partition the spatial domain. In these studies, spatial random effects are modeled as a weighted sum of regional stationary effects based on the distance to region centroids. The authors note problems with sudden changes at region borders as a result of using region centroids for the weighted sum of effects.

Most of the methods discussed so far create a global covariance structure from local covariance structures of Gaussian process models (Fuentes, 2001; Fuentes & Smith, 2001; Heaton et al., 2017; Kim et al., 2005; Konomi et al., 2014). Each method has a different way of smoothing regional transitions that are specifically tied to their methodology. Many of the methods use a Bayesian framework that requires computationally expensive Markov chain Monte Carlo simulations (Gosoni et al., 2009; Gosoni et al., 2006; Heaton et al., 2017; Kim et al., 2005; Konomi et al., 2014). Many of the techniques are only applied to purely spatial data rather than multivariate data (Heaton et al., 2017; Kim et al., 2005; Konomi et al., 2014). This literature review highlights the lack of methodologies that allow for smooth transitions between partitions and works for multiple modeling techniques. There is also a general lack of software available to handle nonstationary data.

The regional border smoothing method described in this thesis can be thought of as stitching together images to form a larger image with no sharp changes. The approach is similar to those used to combine black and white images from microscopes into a larger image (Thévenaz & Unser, 2007). Individual microscope images are aligned and the overlapping regions are smoothed by taking a weighted average of the overlapping pixel brightness.

The weights are based on the distance from the pixel to the outer edge of each image with more weight being applied to pixels closer to the center of an image.

The process described in this thesis provides a simple way of combining regional model predictions to form a continuous global prediction surface. The method can be applied to problems that are not strictly spatial. For example, Osborne and Suárez-Seoane (2002) show that building models for partitioned space can improve the accuracy of large scale species distribution models. The regional border smoothing method works for any model that produces a continuous prediction. A software implementation of the method described in this thesis is available through the R package **remap** on the Comprehensive R Archive Network (CRAN) (Wagstaff, 2021).

The remainder of this thesis proceeds with a description of the regional border smoothing approach in Chapter 2. This is followed by Chapter 3 which describes the available functions and tools in the **remap** package and Chapter 4 with two demonstrations of the software on a state and national-level dataset. These demonstrations show the utility of the **remap** package in producing smooth estimates when applied to large geographical problems with irregularly shaped partitions.

CHAPTER 2

THE REGIONAL BORDER SMOOTHING APPROACH

Regional border smoothing is the process of using regional models to make predictions that are globally continuous. Regional border smoothing may be used on any spatially referenced data (\mathbf{X}) in conjunction with a modeling approach and a finite set of regions \mathcal{R}_p where each $\mathcal{R}_{p_i} \in \mathcal{R}_p, i = 1 \dots m$, is a closed set of points contained in the region of interest \mathcal{R} . The intention is that \mathcal{R}_p is a set of non-overlapping polygons with shared borders and $\bigcup_{i=1}^m \mathcal{R}_{p_i} = \mathcal{R}$, but these are not necessary conditions. While \mathcal{R}_p does not meet the strict definition of a partition, \mathcal{R}_p will be referred to as a partition throughout this thesis.

The border smoothing approach described in this thesis was originally designed for regression-based models (such as kriging), but can be used with virtually any modeling approach that predicts a continuous response. This technically includes classification techniques that make continuous probability predictions prior to classifying based on a probability threshold. Presumably, the predictions from a chosen modeling approach will result in continuous predictions as a function of location.

Modeling regions are defined by the borders of \mathcal{R}_p . The data contained by a modeling region \mathcal{R}_{p_i} are used to inform a distinct regression model ($f_{p_i}(\mathbf{X})$) for that region. In some cases it may be desirable to include observations near each \mathcal{R}_{p_i} when building regional regression models. In these cases, data within \mathcal{R}_{p_i} and possibly within a buffer zone around each modeling region $\mathcal{R}_{p_i}^*$ are used to build each $f_{p_i}(\mathbf{X})$ (Figure 2.1). Using points within a buffer zone that extends beyond the region boundaries avoids edge extrapolation when using a regional model for interpolation in the smoothing zones of neighboring regions. See Section 2.1 for additional details.

Simply making predictions within each \mathcal{R}_{p_i} using each corresponding $f_{p_i}(\mathbf{X})$ results in noncontinuous predictions at region boundaries. Regional border smoothing results in continuous predictions for the entire space by taking a weighted average of the predictions

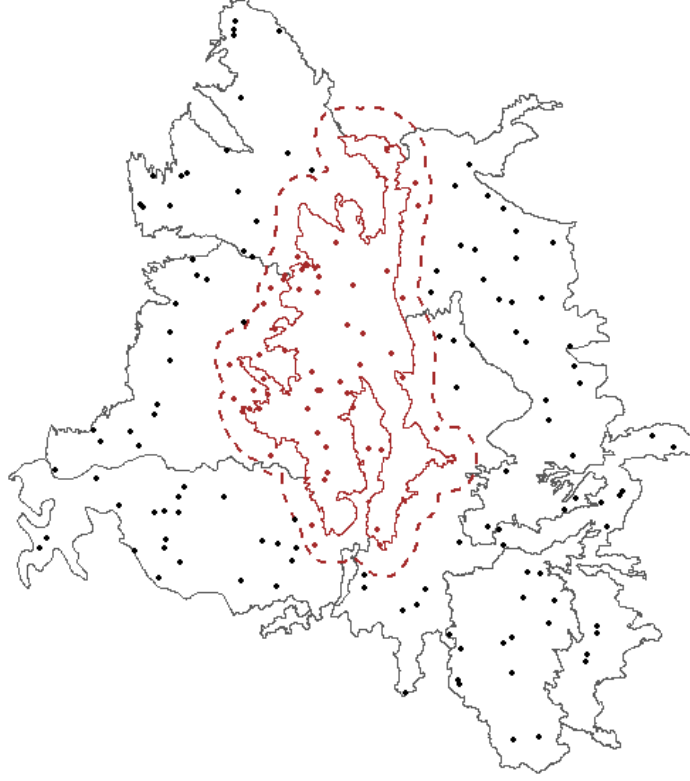


Fig. 2.1: Example of a region's buffer zone. A model is built for the red region using all observations within a buffer zone (red dashed line). Red dots are observations used to build the red region's model.

provided by each $f_{p_i}(\mathbf{X})$. The smoothed global prediction surface is continuous, but not necessarily differentiable (see Section 2.2).

2.1 Smoothing at Borders

Let $\hat{y}_1, \hat{y}_2, \dots, \hat{y}_m$ represent predictions from regional models $f_{p_1}(\mathbf{x}^*), f_{p_2}(\mathbf{x}^*), \dots, f_{p_m}(\mathbf{x}^*)$ for location of interest \mathbf{x}^* where \mathbf{x}^* represents both spatial and non-spatial information. A final prediction \hat{y}' is calculated by the weighted average of each \hat{y} , i.e.,

$$\hat{y}' = \frac{w(d_1|S)\hat{y}_1 + w(d_2|S)\hat{y}_2 + \dots + w(d_m|S)\hat{y}_m}{w(d_1|S) + w(d_2|S) + \dots + w(d_m|S)}. \quad (2.1)$$

The weights are calculated based on the smallest great-circle distances (d_1, d_2, \dots, d_m)

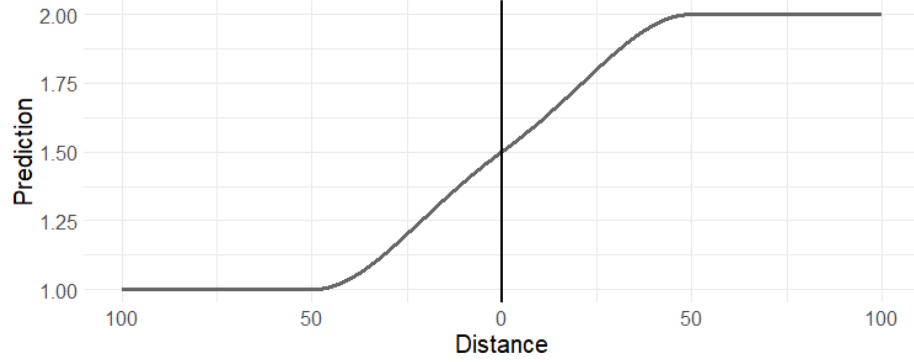


Fig. 2.2: Example of how predictions change as location approaches a region border. In this example $S = 50$, the region on the “left” side of the border predicts a constant value of one and the region on the “right” side of the border predicts a constant value of two.

between the location of \mathbf{x}^* and the boundaries of $\mathcal{R}_{p_1}, \mathcal{R}_{p_2}, \dots, \mathcal{R}_{p_m}$. If \mathbf{x}^* is located within a region, the distance between \mathbf{x}^* and that region is 0. The weight $w(d_i|S)$ given to \hat{y}_i is non-zero when d_i is within some threshold S , i.e.,

$$w(d_i|S) = \begin{cases} \left(\frac{S-d_i}{S}\right)^2 & d_i \leq S \\ 0 & d_i > S. \end{cases} \quad (2.2)$$

Consider now the special case when a prediction is made in region j and $d_{i \neq j} > S$, then $w(d_{i \neq j}|S) = 0$ and Equation 2.1 reduces to $\hat{y}' = \hat{y}_j$. As prediction locations in region j approach \mathcal{R}_{p_k} , then the weight of \hat{y}_k increases gradually and $\hat{y}' = \frac{\hat{y}_j + ((S-d_k)/S)^2 \hat{y}_k}{1 + ((S-d_k)/S)^2}$. At the border of regions j and k , $\hat{y} = \frac{\hat{y}_j + \hat{y}_k}{2}$. Finally, as prediction locations progress into \mathcal{R}_{p_k} , weights for y_{i_j} decrease gradually to zero and $\hat{y}' = \frac{((S-d_j)/S)^2 \hat{y}_j + \hat{y}_k}{((S-d_j)/S)^2 + 1}$. Figure 2.2 shows a simple example of how predictions change across region borders. All locations within S of a region are referred to as the smoothing zone for that region.

2.2 A Note on Smoothing

The “smoothing” described throughout this thesis refers to smoothing in the colloquial sense. A continuous prediction surface is created with a steady transition between regions. The prediction surface is not always differentially smooth. If a region is not convex, the rate of change in the distance to a region can shift suddenly at locations that are equidistant

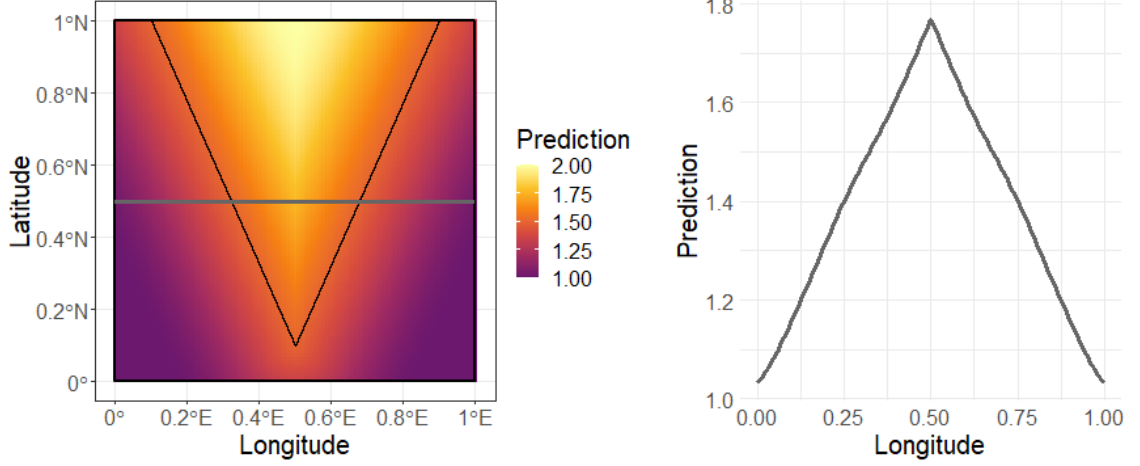


Fig. 2.3: Example of where predictions are not differentiable near non-convex regions. The gray line shows predicted values along the 0.5°N transect. The bottom region predicts a constant value of one and the top region predicts a constant value of two. Smoothing zone is 40 km ($\approx 0.36^\circ$).

to different parts of the region. Figure 2.3 shows an example of a prediction surface near a non-convex region where the prediction surface is not differentiable smooth.

Since each region is a closed set of points, d_i is continuous. It therefore follows that the weight function $w(d_i|S)$ described in Equation 2.2 is continuous as $\lim_{x \rightarrow 0^+} w(x|S) = w(0|S) = 1$ and $\lim_{x \rightarrow S^-} w(x|S) = w(S|S) = 0$ for $x \in [0, \infty)$ and $S > 0$. Since Equation 2.1 includes the multiplication and addition of continuous functions, it is guaranteed to have $\max(w(d_i|S)) > 0$ as long as \mathbf{x}_s^* is within S units of any \mathcal{R}_p and it follows that \hat{y}' is also continuous. Given continuous predictions as a function of location for each region, the regional border smoothing method is guaranteed to be continuous for any location within the smoothing zone of at least one region. Once all $d_i > S$, then the denominator of y' is equal to zero, which means y' is no longer well-defined. As long as all of the data \mathbf{X} are located within \mathcal{R}_p , any prediction location outside of \mathcal{R}_p is spatial extrapolation that is generally discouraged.

CHAPTER 3

REMAP

The R package **remap** (Wagstaff, 2021) is an implementation of the regional border smoothing approach to spatial modeling. The function **remap** creates a set of regionalized models given:

- A set of spatially referenced observations (projected or geographic).
- A set of spatially referenced polygons defining the regions.
- A desired buffer zone distance.
- A modeling function to apply to observations in each region.

Predictions can be made on new observations given a regionalized model and the smoothing parameter **smooth** used for weighted averages in smoothing zones (variable S in Equation 2.2). Detailed descriptions of function parameters can be found in the package documentation which is also available in Appendix A.1. Some working examples using the **remap** package are provided via the vignette which accompanies the package and available in Appendix A.2. The development version of the code for **remap** can be found at <https://github.com/jadonwagstaff/remap>.

3.1 Calculating Distances

The weights for regional predictions require the distances from all observations to the boundary of each region. The modeling process of the **remap** function also requires the distances from all observations to the boundary of each region to assign the correct observations to each regional model. The process of fine-tuning a model can result in recalculating these distances many times. To avoid recalculating distances, the function **redist** is included in the **remap** package to pre-compute the distances from a given set of

observations to a given set of regions. These pre-computed distances can be supplied as a parameter to the `remap` function to reduce computational time while fine-tuning models.

Calculating distances in the `remap` package takes advantage of tools already available for spatial analysis in the R package `sf` (Pebesma, 2018). The function `sf::st_distance` is used to find either Euclidean or great-circle distances depending on the spatial projection of the locations and regions. The `sf::st_distance` function uses the `S2` library (Google, 2020) when calculating great-circle distances. The `S2` library is designed specifically to efficiently compute distances between nearby objects given large sets of geographic data. Regardless, calculating distances can still take a lot of computational time if the regions are complex and/or there are a lot of observations.

The naïve approach to regional border smoothing is to find all distances between each location and each region. This approach may be necessary during the modeling process if any region does not contain a required minimum number of observations (see Section 3.2). If predictions are being made using new observations, then distances do not need to be calculated between every observation and every region.

Because the weight for predictions in different regions is zero when the distance to those regions is greater than the smoothing parameter (Equation 2.2), distances do not need to be calculated between *every* region and *every* prediction location. To determine which observations require distance calculations, an approximate polygon is constructed that encompasses the original region plus the smoothing zone around the region. The function `sf::st_within` is used to determine which observations are within the new polygon and equivalently, which observations are within the smoothing zone of the original region. Observations in the approximate polygon become candidates for precise distance calculations.

An approximate polygon that contains a region and the region’s smoothing zone is created using the `sf::st_buffer` function. For geographic coordinates, `sf::st_buffer` requires a buffer value in degrees. Since the great-circle distance between a unit degree of longitude changes with latitude, Equation 3.1 is used to find c : the shortest distance

(measured in kilometers) required to move one degree longitude at the observation in the dataset that is nearest to a geographical pole. λ represents the vector of latitudes for each observation and 6350 km is the radius of the earth at a pole (rounded down). A sufficient buffer value in degrees for `sf::st_buffer` is calculated by dividing the smoothing zone length in km by c . The resulting buffered polygon contains all of the observations within the smoothing zone of the original polygon.

$$c = \frac{\pi * 6350}{180} * \cos\left(\frac{\pi * \max(|\lambda|)}{180}\right) \quad (3.1)$$

Assuming each region contains a sufficient number of observations to fit each regional model, the same process used for reducing the number of distance calculations for model training can be used to reduce the number of distance calculations required for model predictions. (See Section 3.2 for a description of what happens when the observations in a region fall below a minimum sample size threshold.) The function `redist` is able to restrict distance calculations to only observations within a certain buffer or smoothing zone of each region using the `max_dist` parameter. This eliminates the need to calculate distances to points with a known weight of zero when smoothing.

3.2 Practical Implementation Considerations

Reliable regression results depend upon sufficient sample sizes, which differ based on the variability of the response and dimensionality of the inputs. A strict (and obvious) minimum sample size for the `remap` function is one observation per region, though this threshold will rarely, if ever, ensure reasonable results. An additional parameter `min_n` is included in the `remap` function to specify a minimum number of observations used to build each model. If a region and the buffer around that region do not contain the minimum number of observations specified, the `min_n` observations closest to the boundaries of the region are used to train that region's model.

The `remap` package has the ability to make predictions outside of all modeling regions. If the prediction location is within the smoothing zone of a region, then Equation 2.1 is still

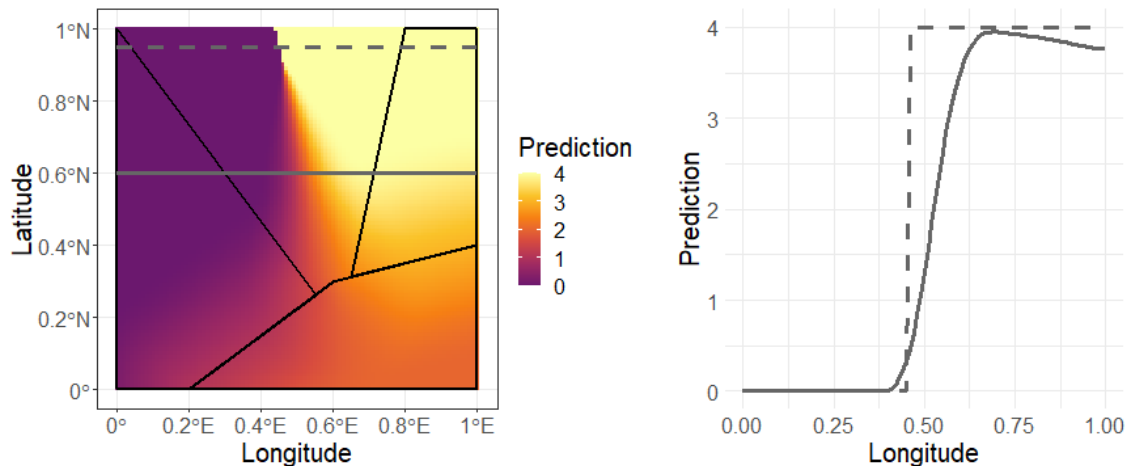


Fig. 3.1: Example of what happens when predictions are made outside of any modeling region. The gray line shows predicted values along the 0.6°N transect. The dashed gray line shows predicted values along the 0.95°N transect. The left region predicts a constant 0, the bottom region predicts a constant 2, and the right region predicts a constant 4. Smoothing zone is 35 km ($\approx 0.32^\circ$).

used and the nearest region will have the most weight. If the prediction location is outside the smoothing zone of all regions, then the model from the closest region is used to make a prediction. This may result in non-continuous transitions in predictions when the closest region changes across geographic space, but this is only possible at locations outside of the smoothing zone of all regions. As a general rule, extrapolation of predictions to locations beyond those represented in the input data is not recommended. See Figure 3.1 for a visual depiction of how predictions behave outside of all modeling regions.

The ability to predict outside of all regions means that the **remap** package can make smooth predictions across small gaps at polygon borders, provided the gaps are no larger than two times the smoothing zone distance. This encourages the use of `rgeos::gSimplify` (Bivand & Rundel, 2020) or `sf::st_simplify` (Pebesma, 2018) to simplify complex polygons and ease the computational burden associated with distance calculations, even if those simplifications slightly compromise the topology of the original geometry.

CHAPTER 4

APPLICATIONS

4.1 National Snow Load Example

Snow loads are obtained from weather stations throughout the United States in the National Oceanic and Atmospheric Administration's (NOAA) Global Historical Climatology Network (Menne et al., 2012). Snow loads are either measured directly, or estimated from measured snow depth using a depth to load conversion model. Engineers have historically used estimates of 50-year ground snow loads when designing structures. The 50-year snow load is traditionally obtained by fitting a probability distribution to yearly maximum snow load measurements and extracting the 98th percentile. A recent effort by the American Society of Civil Engineers has resulted in a new set of 50-year ground snow loads at 7964 measurement locations. The 50-year loads are calculated in a similar manner to Bean et al. (2018), except yearly maximum snow loads are fit to the generalized extreme value distribution instead of the log-normal distribution.

4.1.1 Building a Geospatial Snow Load Model

Building design requirements call for continuous maps that estimate design loads between measurement locations. This has historically been accomplished using various mapping techniques (Bean et al., 2019; Liel et al., 2017; Tobiasson et al., 2002). The problem is that the relationship between predictor variables and snow load can change drastically on a continental scale. For example, the typical loads at 5000 feet elevation in the Rocky Mountains of Colorado are much lower than typical loads at 5000 feet in the Cascade Mountains of Washington State. Commonly used geospatial models for mapping are not well suited for the nonstationary nature of this problem.

Geographic regions defined by the US Environmental Protection Agency (EPA) define

regions with similar ecology and climate called eco-regions (Commission for Environmental Cooperation, 1997). The eco-regions provide a natural partition of the conterminous United States and give no regard to political boundaries. Snow load can be modeled using observations within each eco-region where the relationship between predictor variables and the response is more consistent on a local level. The **remap** package facilitates modeling in separate eco-regions and creates a smooth model on the national scale.

Snow loads are typically assumed to share a log-linear relationship with elevation. This relationship is modeled directly using ordinary least squares (OLS). A generalized additive model (GAM) built with the **mgcv** R package (Wood, 2011) characterizes the log of 50-year loads as a function of elevation and a spatial smoother called splines on the sphere (Wood, 2003). Universal kriging interpolates values using a Gaussian process model after accounting for the log-linear trend in elevation with the **automap** R package (Hiemstra et al., 2009). Parameter-elevation regressions on independent slopes model (PRISM) is a modeling method that uses a form of weighted linear regression to model loads as a function of elevation (Daly et al., 2002; Daly et al., 2008). The adaptation of PRISM to estimate snow loads in this thesis is described in Bean et al. (2017).

Some of the methods for mapping snow loads are compared in Table 4.1 using national scale models and models built with the **remap** package on EPA Level III Eco-Regions (Commission for Environmental Cooperation, 1997). There are 86 eco-regions that fall within the conterminous United States, so 86 separate models are built using the **remap** function with a buffer zone of 50 km and a `min_n` of 150 observations. The regional models are smoothed to a single continuous model using a `smooth` parameter of 25 km.

The results in Table 4.1 show that the **remap** package framework improves the cross validated accuracy of every spatial modeling method. This demonstrates that the **remap** package has the ability to generally improve modeling results, as improvements are not isolated to a single spatial modeling case. Even though the regional models are made up of 86 different regional models, the estimated 50-year loads are smooth across the prediction surface (see Figure 4.1).

Model	MSE $\times 10^2$		Improvement
	National	Regional	
GAM	8.2	5.5	33%
Kriging	7.2	5.9	18%
PRISM	21.0	7.9	62%
OLS	89.3	17.8	80%

Table 4.1: Ten fold cross-validation results from modeling the log of 50-year snow loads. Mean squared error (MSE) is multiplied by 10^2 for readability. Improvement is (national - regional) / national.

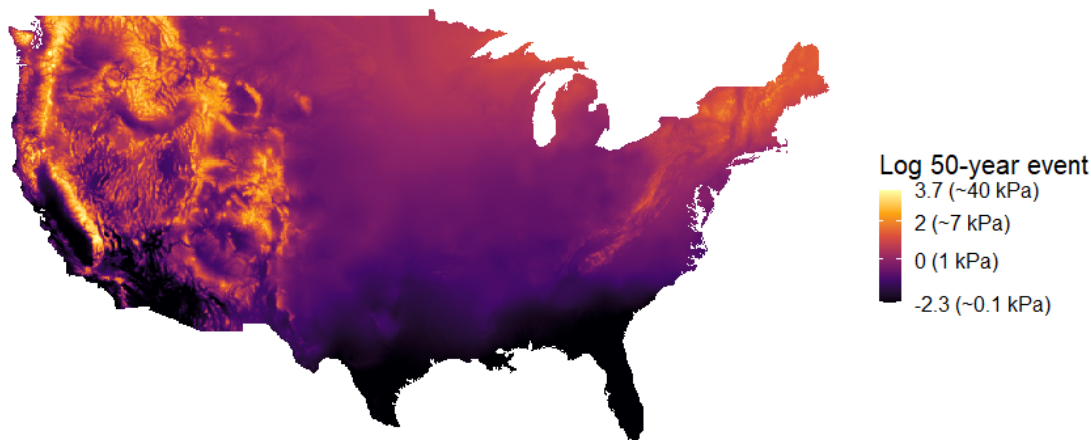


Fig. 4.1: Prediction map for 50-year loads from the regional GAM model built with the **remap** package. Loads are shown on the log scale. Values are restricted to be within the range of values observed in the load data.

4.1.2 Building a Snow Load Prediction Grid

National snow load maps require a sufficiently fine resolution to be feasibly used to design buildings in topographically complex areas. To accomplish this, snow load maps are created that match the resolution of PRISM climate output (PRISM Climate Group, 2020), which maps at a 0.8 km resolution for the conterminous United States. This means that predicted snow loads are calculated at 12,113,556 locations using a model created by the **remap** package with 86 different regions. Elevation values for the grid are obtained from the United States Geological Survey (United States Geological Survey, 2020b).

Since the **remap** package uses the distances between prediction locations and regions to make a smooth model, calculating these distances is a potential bottleneck in the prediction

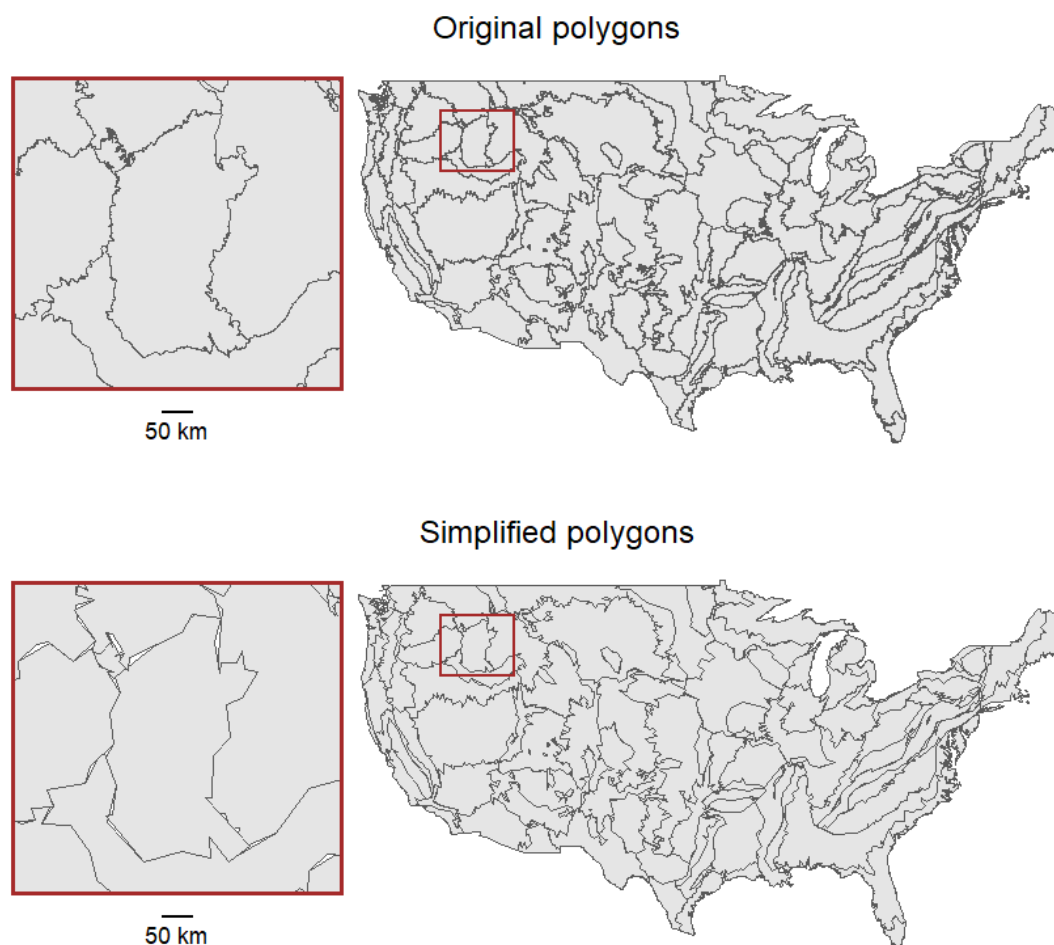


Fig. 4.2: Results of simplification of eco-regions. The highlighted region is an area with some of the most severe gaps between polygons. Notice that the width of the gaps are still much smaller than two times the smoothing parameter (2×25 km).

process. Also, since the prediction area is so large, geographic coordinates rather than projected coordinates must be used to find distances. This further increases the bottleneck since great circle distances require more resources to compute than Euclidean distances. Simply calculating all distances would have taken over a year to run on a typical desktop computer, as illustrated in Table 4.2. The test computer used for Table 4.2 has 16 GB of RAM and an Intel Core I5-4590 CPU which runs at 3.3 GHz.

The first step to reduce the run time for distance calculations is to simplify the polygons as discussed in Section 3.2. Using a tolerance of 0.1° with the function `sf::st_simplify`, the

Remedial steps	Run time in hours	
	Geographic	Projected
None	15000.0*	200.0*
Simplify polygons	44.0*	1.4
+ set <code>max_dist</code> to 25 km	1.8	1.0
+ run in parallel on 4 cores	1.3	1.0

Table 4.2: Run times for `redist` to calculate geographic and projected distances from 0.8 km grid points to 86 different eco-regions (polygons) in the conterminous US. Remedial steps are additive, i.e., each row in the table includes all previous remedial steps. * Approximate run time based on random sample of 10,000 grid points.

size of the polygons are reduced from 21 MB to 0.2 MB. The results of polygon simplification are visualized in Figure 4.2. When making predictions, the `smooth` parameter is set to 25 km; therefore, the `max_dist` parameter of `redist` can be set to 25 km to further reduce run time. Finally, combining the previous steps and running in parallel on four cores, the relevant distances are calculated for all points using great circle distance in about 1.3 hours (Table 4.2). This tremendous computational speed-up is made possible by the ability of the `remap` package to smoothly fill in the gaps that occur in aggressively simplified polygons.

4.2 Utah Snowpack Example

The state of Utah assesses snow water content or snowpack every April 1st to plan for yearly water resource availability. These measurements are much more variable than the 50-year snow loads since the values are based on a single measurement at each location instead of the 98th percentile of a distribution fit to annual maximum values at each location. This example uses direct measurements of the water content made via Snowpack Telemetry (SNOTEL) stations included in NOAA’s Global Historical Climatology Network (Menne et al., 2012). In addition to SNOTEL station data, Snow Course data collected by the National Water and Climate Center are also included in the dataset (Natural Resources Conservation Service, 2017). SNOTEL and Snow Course data measure the water equivalent of snow depth (WESD) and are located in the mountainous areas of Utah above 1777 m elevation. This negates the need to estimate water content from snow depth, which is typically the case when measuring snow at non-mountainous locations in the state.

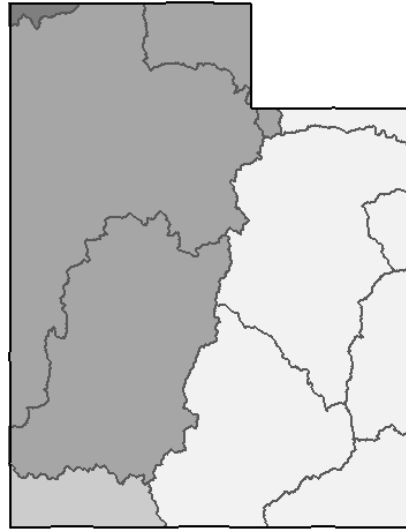


Fig. 4.3: HUC4 regions (lines) and HUC2 regions (shades) in Utah.

SNOTEL stations and Snow Course data within 100 km of the border of Utah are included in the dataset. There are 3511 April 1st WESD observations available for modeling which range from 0 to 1746 mm of water. The observations have 178 unique locations and span 30 years (1986-2015). Each year is modeled separately with no regard for any temporal correlations and each year has at least 97 observations.

Models for GAM, kriging, PRISM, and OLS are created using the same model structure as the national snow load example, but a different response variable. Since there are 142 zero values for WESD within the data, the log of $(WESD + 1)$ is used as the response variable for the April 1st snowpack. Predictions are also constrained to be between $[1, \max(WESD)]$ to avoid excessive extrapolation. The regions used for regional modeling are watershed boundaries defined by the USGS (United States Geological Survey, 2020a). Watersheds are defined by a hierarchy of hydrologic unit codes (HUC) with a two-digit designation for continental scale watersheds (HUC2) and a four-digit designation that partitions each HUC2 region (HUC4). There are four HUC2 regions and 12 HUC4 regions within the boundaries of the state of Utah (see Figure 4.3). A buffer zone of 20 km, a smoothing parameter of 10 km, and a `min_n` of 30 observations are used when modeling both HUC2 and HUC4 regions with the `remap` function.

Model	MSE $\times 10^2$		
	State	HUC2	HUC4
GAM	85	74(13%)	79 (7%)
Kriging	92	90 (2%)	85 (8%)
PRISM	93	86 (7%)	81(13%)
OLS	140	109(22%)	89(36%)

Table 4.3: Ten fold cross-validation mean squared error from modeling $\log(\text{WESD} + 1)$ for Utah snowpack. Mean squared error (MSE) is multiplied by 10^2 for readability. Improvement in parenthesis is calculated with $(\text{state} - \text{HUC}) / \text{state}$.

Table 4.3 shows that the gains in accuracy are more modest in this application than in the national example shown previously. This is expected as the partitions are on the state level instead of the national level. Nevertheless, the consistent improvement in accuracy at various scales using different polygons and input data highlight the general ability of the **remap** package to improve predictive accuracy without sacrificing continuity.

CHAPTER 5

CONCLUSIONS

Partitioning a space for geospatial modeling is a practical approach for handling non-stationary data; however, smooth transitions in mapped values are a desirable constraint of many data products, such as the design snow load requirements set forth by the American Society of Engineers. The **remap** R package provides a ready-to-use framework for regional models with smooth transitions at region borders that overcomes the computational difficulties of naive implementations. This package is available on the Comprehensive R Archive Network (see <https://cran.r-project.org/web/packages/remap/index.html>) with the most current version available at <https://github.com/jadonwagstaff/remap>.

The **remap** package creates continuous prediction surfaces by weighting regional predictions based on the proximity to region borders. Smoothing at region borders makes the package particularly equipped to handle irregularly shaped regions not well represented by their geographic centers. Because the **remap** package has the ability to smooth over small gaps formed when simplifying polygons, computation times can be drastically reduced without sacrificing the continuity of the predictions. Methods that automatically subset the number of required distance calculations further reduce computational times. This thesis has demonstrated accuracy improvements using the **remap** package on two separate datasets with two sets of polygon inputs. These examples highlight the feasibility of applying the **remap** framework to spatial regression modeling problems.

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APPENDICES

APPENDIX A

remap Documentation

A.1 Package Manual

The package manual describes all of the functions in **remap**, describes their parameters, and describes the output objects. The manual is printed as it appears at <https://cran.r-project.org/web/packages/remap/remap.pdf>.

Package ‘remap’

January 14, 2021

Type Package

Title Regional Spatial Modeling with Continuous Borders

Version 0.2.0

Description Automatically creates separate regression models for different spatial regions. The prediction surface is smoothed using a novel method developed by the package creator. If regional models are continuous, the resulting prediction surface is continuous across the spatial dimensions, even at region borders.

License GPL-3

URL <https://github.com/jadonwagstaff/remap>

BugReports <https://github.com/jadonwagstaff/remap/issues>

Encoding UTF-8

LazyData true

Imports graphics (>= 3.6.0), parallel (>= 3.6.0), sf (>= 0.9.6), stats (>= 3.6.0), units (>= 0.6.7), utils (>= 3.6.0)

RoxygenNote 7.1.1

Suggests dplyr (>= 1.0.2), ggplot2 (>= 3.3.2), knitr (>= 1.30), lwgeom (>= 0.2.5), magrittr (>= 2.0.1), maps (>= 3.3.0), mgcv (>= 1.8.33), rmarkdown (>= 2.5), tibble (>= 3.0.4)

VignetteBuilder knitr

Depends R (>= 3.6.0)

NeedsCompilation no

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Repository CRAN

Date/Publication 2021-01-14 10:30:02 UTC

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*predict.remap***R topics documented:**

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plot.remap	<i>Plot method for remap object.</i>
------------	--------------------------------------

Description

Plots the regions used for modeling.

Usage

```
## S3 method for class 'remap'
plot(x, ...)
```

Arguments

x	S3 object output from remap.
...	Arguments to pass to regions plot.

Value

A list that plots a map of the regions used for modeling.

predict.remap	<i>Make predictions given a set of data and smooths predictions at region borders. If an observation is outside of all regions and smoothing distances, the closest region will be used to predict.</i>
---------------	---

Description

Make predictions given a set of data and smooths predictions at region borders. If an observation is outside of all regions and smoothing distances, the closest region will be used to predict.

Usage

```
## S3 method for class 'remap'
predict(object, data, smooth, distances, cores = 1, progress = FALSE, ...)
```


print.remap

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Arguments

<code>object</code>	S3 object output from <code>remap</code> .
<code>data</code>	An sf dataframe with point geometry.
<code>smooth</code>	The distance in km within a region where a smooth transition to the next region starts. If <code>smooth = 0</code> , no smoothing occurs between regions unless an observation falls on the border of two or more polygons. (Can be a named vector with different values for each unique <code>object\$region_id</code> in <code>'object\$region'</code> .)
<code>distances</code>	An optional matrix of distances between <code>'data'</code> and <code>'object\$regions'</code> generated by <code>redist()</code> function (calculated internally if not provided).
<code>cores</code>	Number of cores for parallel computing. <code>'cores'</code> above default of 1 will require more memory.
<code>progress</code>	If true, a text progress bar is printed to the console. (Progress bar only appears if <code>'cores' = 1</code> .)
<code>...</code>	Arguments to pass to individual model prediction functions.

Value

Predictions in the form of a numeric vector.

See Also

[remap](#) building a regional model.

`print.remap` *Print method for remap object.*

Description

Print method for `remap` object.

Usage

```
## S3 method for class 'remap'
print(x, ...)
```

Arguments

<code>x</code>	S3 object output from <code>remap</code> .
<code>...</code>	Extra arguments.

Value

No return value, a description of the `remap` object is printed in the console.

redist	<i>Get distances between data and regions.</i>
--------	--

Description

Finds distances in km between data provided as sf dataframe with point geometry and regions provided as sf dataframe with polygon or multipolygon geometry.

Usage

```
redist(data, regions, region_id, max_dist, cores = 1, progress = FALSE)
```

Arguments

<code>data</code>	An sf data frame with point geometry.
<code>regions</code>	An sf dataframe with polygon or multipolygon geometry.
<code>region_id</code>	Optional name of column in 'regions' that contains the id that each region belongs to (no quotes). If null, it will be assumed that each row is its own region.
<code>max_dist</code>	a maximum distance that is needed for future calculations. (Set equal to maximum 'smooth' when predicting on new observations.)
<code>cores</code>	Number of cores for parallel computing. 'cores' above default of 1 will require more memory. (Progress bar only appears if 'cores' = 1.)
<code>progress</code>	If true, a text progress bar is printed to the console. Progress set to FALSE will find distances quicker if max_dist is not specified.

Value

A matrix where each row corresponds one-to-one with each row in provided 'data'. Matrix columns are either named with regions from 'region_id' column of 'regions' or the row numbers of 'regions' if 'region_id' is missing. Values are in kilometers.

See Also

[remap](#) - uses redist for regional models.

Examples

```
library(remap)
library(sf)
data(utsnow)
data(utws)

# Reset CRS in case user has old version of GDAL
sf::st_crs(utsnow) <- 4326
sf::st_crs(utws) <- 4326

# Simplify polygons to run example faster
```

remap

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```

utws_simp <- sf::st_simplify(utws, dTolerance = 0.01)

# Build a matrix of distances between objects of utsnow and utws
# We will not set max_dist, so all distances will be found
dists <- redist(data = utsnow,
               regions = utws_simp,
               region_id = HUC2)

head(dists)

```

*remap**Build separate models for mapping multiple regions.***Description**

Separate models are built for each given region and combined into one S3 object that can be used to predict on new data using generic function `predict()`. If a model fails for a region, a warning is given but the modeling process will continue.

Usage

```

remap(
  data,
  regions,
  region_id,
  model_function,
  buffer,
  min_n = 0,
  distances,
  cores = 1,
  progress = FALSE,
  ...
)

```

Arguments

<code>data</code>	An sf data frame with point geometry.
<code>regions</code>	An sf dataframe with polygon or multipolygon geometry.
<code>region_id</code>	Optional name of column in 'regions' that contains the id that each region belongs to (no quotes). If null, it will be assumed that each row of 'regions' is its own region.
<code>model_function</code>	A function that can take a subset of 'data' and output a model that can be used to predict new values when passed to generic function <code>predict()</code> .
<code>buffer</code>	The length of the buffer zone around each region in km where observations are included in the data used to build models for each region. (Can be a named vector with different values for each unique 'region_id' in 'region'.)

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remap

<code>min_n</code>	The minimum number of observations to use when building a model. If there are not enough observations in the region and buffer, then the closest <code>min_n</code> observations are used. No minimum if set to 0.
<code>distances</code>	An optional matrix of distances between 'data' and 'regions' generated by <code>redist()</code> function (calculated internally if not provided). Note that unless you know that you have <code>min_n</code> within a certain distance, no <code>max_dist</code> parameter should be used in <code>redist()</code> .
<code>cores</code>	Number of cores for parallel computing. 'cores' above default of 1 will require more memory.
<code>progress</code>	If true, a text progress bar is printed to the console. (Progress bar only appears if 'cores' = 1.)
<code>...</code>	Extra arguments to pass to 'model_function' function.

Value

A *remap* S3 object containing:

models A list of models containing a model output by 'model_function' for each region.

regions 'regions' object passed to the function (used for prediction). The first column is 'region_id' or the row number of 'regions' if 'region_id' is missing. The second column is the region geometry.

call Shows the parameters that were passed to the function.

See Also

[predict.remap](#) - used for predicting on new data. [redist](#) - used for pre-computing distances.

Examples

```
library(remap)
library(sf)
data(utsnow)
data(utws)

# Reset CRS in case user has old version of GDAL
sf::st_crs(utsnow) <- 4326
sf::st_crs(utws) <- 4326

# Simplify polygons to run example faster
utws_simp <- sf::st_simplify(utws, dTolerance = 0.01)

# Build a remap model with lm that has formula snow_water = elevation
# The buffer to collect data around each region is 30km
# The minimum number of observations per region is 10
remap_model <- remap(data = utsnow,
  regions = utws_simp,
  region_id = HUC2,
  model_function = lm,
  formula = WESD ~ ELEVATION,
```

utsnow

7

```

        buffer = 20,
        min_n = 10,
        progress = TRUE)

# Resubstitution predictions
remap_preds <- predict(remap_model, utsnow, smooth = 10)
head(remap_preds)

```

*utsnow**Snowpack at weather stations in Utah on April 1st, 2011.*

Description

Water equivalent of snow density (WESD) in mm of water at various location within and surrounding the state of Utah. WESD are measured at weather stations within the Daily Global Historical Climatology Network. April first measurements are used to estimate snowpack for the state of Utah.

Usage

```
utsnow
```

Format

An sf points object with 394 rows and 9 variables:

ID Weather station identification code.

STATION_NAME Weather station name.

LATITUDE Latitude of weather station.

LONGITUDE Longitude of weather station.

ELEVATION Elevation of weather station.

HUC2 Largest watershed region containing this weather station (see [utws](#) data).

WESD Water equivalent of snow density in mm of water.

geometry sfc points in geographic coordinates.

Source

<ftp://ftp.ncdc.noaa.gov/pub/data/ghcn/daily>

8

utws

`utws`*Watershed polygons within the state of Utah.*

Description

Watersheds are defined by the United States Geological Survey. Only the largest defines watersheds are used.

Usage`utws`**Format**

An sf object with 394 rows and 2 variables:

HUC2 Largest watershed ID's defined by the USGS.

geometry sfc multipolygon object in geographic coordinates.

Source

https://www.usgs.gov/core-science-systems/ngp/national-hydrography/watershed-boundary-dataset?qt-science_support_page_related_con=4#qt-science_support_page_related_con

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A.2 Package Vignette

The package vignette for **remap** serves as an extended instruction manual with example problems. The vignette is provided as it appears on https://cran.r-project.org/web/packages/remap/vignettes/Introduction_to_remap.html.

Introduction to remap

Jadon S. Wagstaff and Brennan Bean

2021-01-03

Introduction

Most spatial modeling approaches work under the assumption that the data used for modeling are stationary. That is to say, the mean and variance of the response variable are constant in space. This assumption is often violated, especially when modeling large areas. Sometimes, a nonstationary process can be transformed into a stationary one by modeling external trends; however, this is not possible to achieve if the external trends are not constant over space. In such cases, an alternative approach is to partition the space into stationary sub-regions and model each region separately. The problem with this approach is that continuous response variables will have discontinuities in the prediction surface at the borders of the regions.

The package `remap` is an implementation of a regional modeling with border smoothing method that results in a continuous global model. Border smoothing is accomplished by taking a weighted average of regional model predictions near region borders. The `remap` function is also a convenient way to build independent models in a partitioned space, even if no border smoothing is required for the problem.

```
library(magrittr) # For pipe %>% functionality
library(tibble)  # For light data wrangling
library(dplyr)   # For light data wrangling
library(ggplot2) # For plots
library(maps)    # For a polygon of the state of Utah
library(sf)      # For spatial data manipulation
library(mgcv)    # For GAM modeling

library(remap)
data(utsnow)
data(utws)

# Reset CRS in case user has old version of GDAL
sf::st_crs(utsnow) <- 4326
sf::st_crs(utws) <- 4326
```

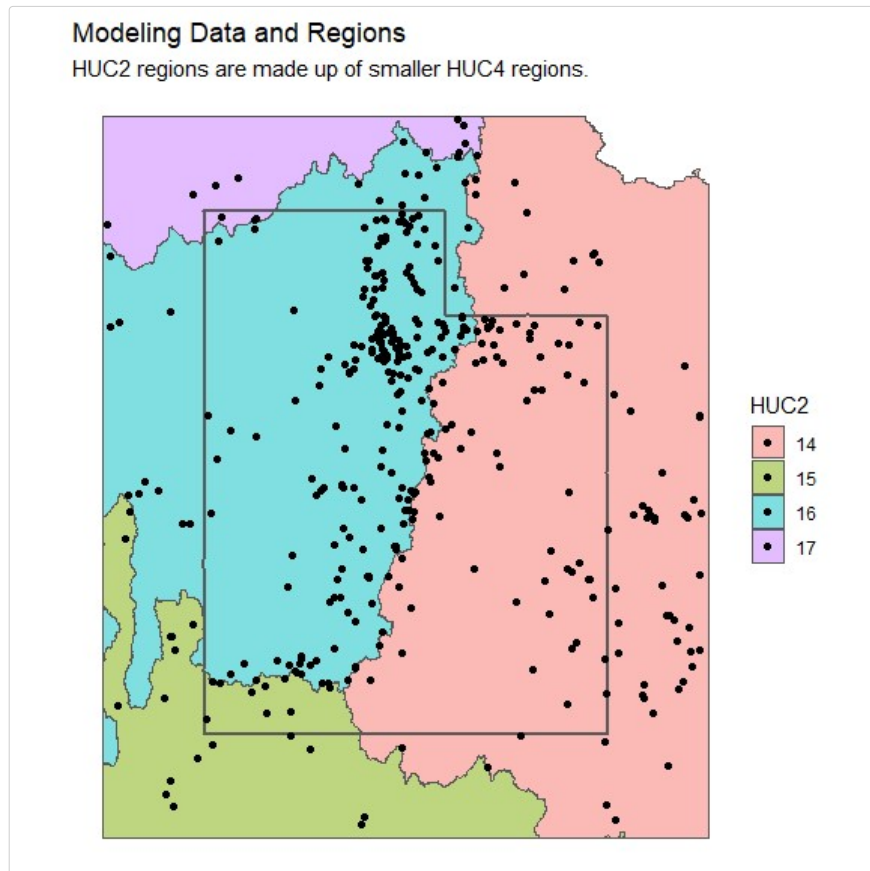
Data

To introduce the functionality of `remap`, we will look at a modeling problem for estimating snow water content in the state of Utah using water equivalent of snow density (WESD) measurements. The `utsnow` data that is part of the package `remap` contains WESD in mm water measured on April 1st, 2011 at 394 locations within and near the state of Utah. The `utws` data in `remap` is a set of polygons representing watersheds defined by the US Geological Survey. These watersheds are defined by a hierarchy of hydrologic unit codes (HUC) with a two-digit designation for continental scale watersheds (HUC2). We will build a regionalized model with `remap` using HUC2 watershed regions.

```
utstate <- maps::map("state", plot = FALSE, fill = TRUE) %>%
  sf::st_as_sf() %>%
  dplyr::filter(ID == "utah") %>%
```

```
sf::st_transform(crs = 4326)

ggplot(utws, aes(fill = HUC2)) +
  geom_sf(alpha = 0.5) +
  geom_sf(data = utstate, fill = "NA", size = 1) +
  geom_sf(data = utsnow) +
  ggtitle("Modeling Data and Regions",
          "HUC2 regions are made up of smaller HUC4 regions.") +
  theme_void()
```



Basic Models

The `remap` function requires the following 4 parameters:

- o `data` - Observations with a spatial component used for modeling.
- o `regions` - Polygons describing the regions used to build each model.
- o `model_function` - A function that takes a subset of the `data` and returns a model.
- o `buffer` - Observations are located within and near a region are used to build each model. The `buffer` parameter dictates how near an observation must be to a location to be included in that region's model.

The following parameters are optional:

- `region_id` - A column name of `regions` which describes which polygons to include in each region. This is helpful if any region has polygons described in multiple rows in the `sf` object. The `region_id` allows for combinations of smaller polygons into larger regions.
- `min_n` - The minimum number of observations required to build a model in each region. If a region does not contain enough observations within its border and buffer zone, the nearest `min_n` observations will be used for modeling.

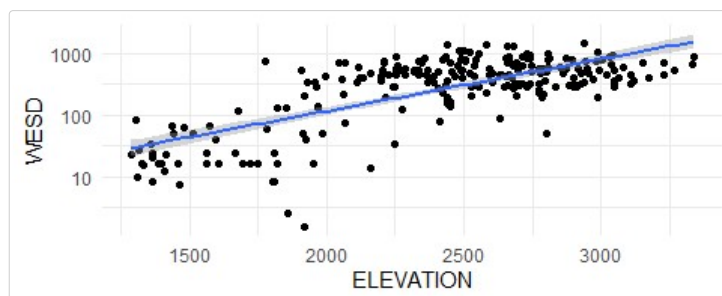
In this section, we use some simple linear models to model snow water content in Utah. First a global model using all data, then a regional model using `remap`. The WESD measurement in our example data commonly shares a log-linear relationship with elevation in mountainous western states. Many locations in Utah have a value of 0 for WESD on April first. Since zero snow values in log transformed variables add another level of complexity to the modeling process, we remove them for now and make a new dataset called `utsnz`.

```
utsnz <- utsnow %>% dplyr::filter(WESD > 0)
```

Global Linear Model

The relationship between the log transformed WESD and elevation of `utsnz` is visualized as:

```
ggplot(utsnz, aes(x = ELEVATION, y = WESD)) +
  geom_point() +
  geom_smooth(method = "lm") +
  scale_y_log10() +
  theme_minimal()
#> `geom_smooth()` using formula 'y ~ x'
```



The resubstitution mean squared error (MSE) for such a model is:

```
lm_global <- lm(log(WESD) ~ ELEVATION, data = utsnz)

lm_global_mse <- mean((utsnz$WESD - exp(predict(lm_global, utsnz)))^2)
lm_global_mse
#> [1] 121370.7
```

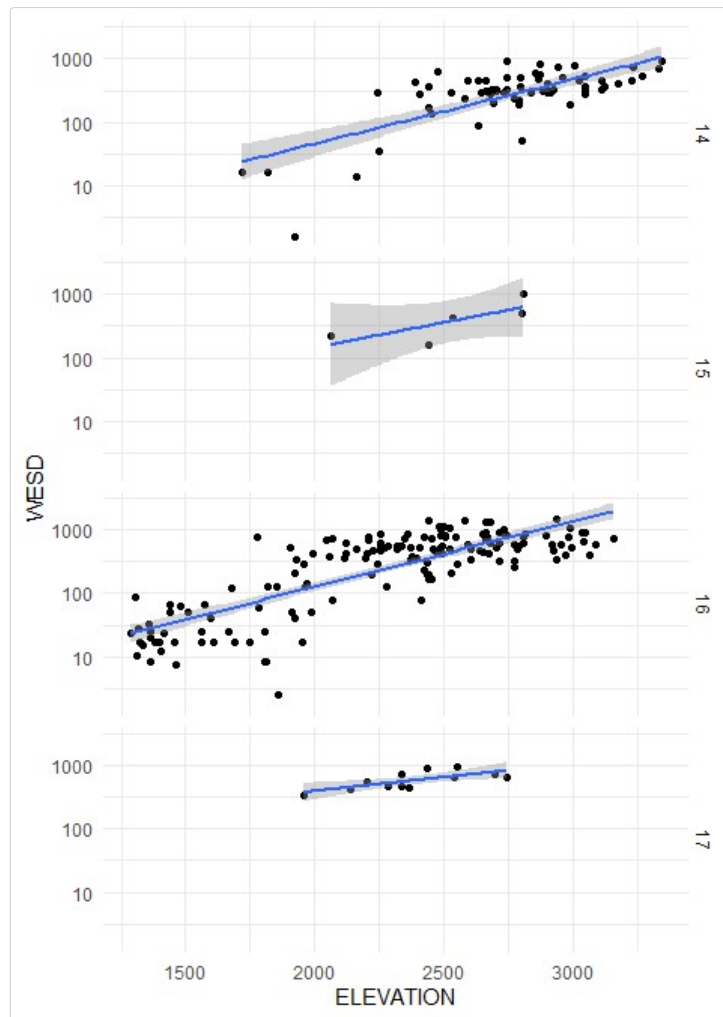
Regionalized Linear Models

The `utsnz` data describes which watersheds each location falls in with the `HUC2` columns. (Note that `remap` does not require these columns in the data when building models using the `utws` regions.) Here is what the relationship between `log(WESD)` and elevation looks like for each of the `HUC2` regions:

```

ggplot(utsnz, aes(x = ELEVATION, y = WESD)) +
  facet_grid(HUC2 ~ .) +
  geom_point() +
  geom_smooth(method = "lm") +
  scale_y_log10() +
  theme_minimal()
#> `geom_smooth()` using formula 'y ~ x'

```



The linear models for each HUC2 region seem to fit a little better than the global linear model; however, it looks like HUC2 region 15 does not have enough data to build a very confident model. Using `remap` to build models for each region, some of the nearest observations to HUC2 region 15 are added to build a better model by using the `min_n` parameter to set the minimum number of observations per region to 10.

For this modeling task, any observation within 20km of a region is to be included in that region's model using the `buffer` parameter. The `lm` function requires a `formula`, so `formula` is added as an extra parameter in `remap`. Since `remap` makes smooth predictions over the entire surface, a `smooth` parameter is required in the `predict` function that dictates the distance from region borders where the smoothing process will start. We set `smooth` to 10km for this example.

```

t1 <- Sys.time()
lm_huc2 <- remap::remap(
  utsnz, utws, region_id = HUC2,
  buffer = 20, min_n = 10,
  model_function = lm,
  formula = log(WESD) ~ ELEVATION
)

lm_huc2_mse <- mean((utsnz$WESD - exp(predict(lm_huc2, utsnz, smooth = 10)))^2)
t2 <- Sys.time()

# mse
lm_huc2_mse
#> [1] 85725.36

# runtime
round(difftime(t2, t1), 1)
#> Time difference of 25.1 secs

```

The output of `remap` returns a list that contains a list of models built in each region and an `sf` data frame storing the region polygons. The models for each region can be accessed directly. For example, the coefficients for each model can be accessed with the following code:

```

sapply(lm_huc2$models, function(x) x$coefficients)
#>      14      15      16      17
#> (Intercept) 0.557864695 -2.292085274 0.564719359 1.8300546
#> ELEVATION   0.001914744 0.003114987 0.002140786 0.0018686

```

The resulting `remap` model has a 29.4% reduction in resubstitution MSE using separate linear models for each of the HUC2 regions rather than the global linear model. This increase in accuracy is likely to be even more drastic when problems span greater areas, such as a model for an entire continent.

Computational Speedup

Many modeling techniques that partition space depend on the distance between prediction locations and the *center* of each region. However, the center is a poor characterization of irregularly shaped regions. The border smoothing method in `remap` uses the distances to region *borders* rather than region centers. This allows for regions of any shape being used for modeling. Building models and predicting with `remap` runs fairly slowly for something as simple as linear models. This is because `remap` requires distance calculations between each observation and the region boundaries in both the modeling and prediction steps. This tends to be computationally expensive with large numbers of points and/or complex region boundaries. This section outlines the steps taken to ameliorate the computational burden of `remap` which allow `remap` to scale to large problems.

Simplifying Regions

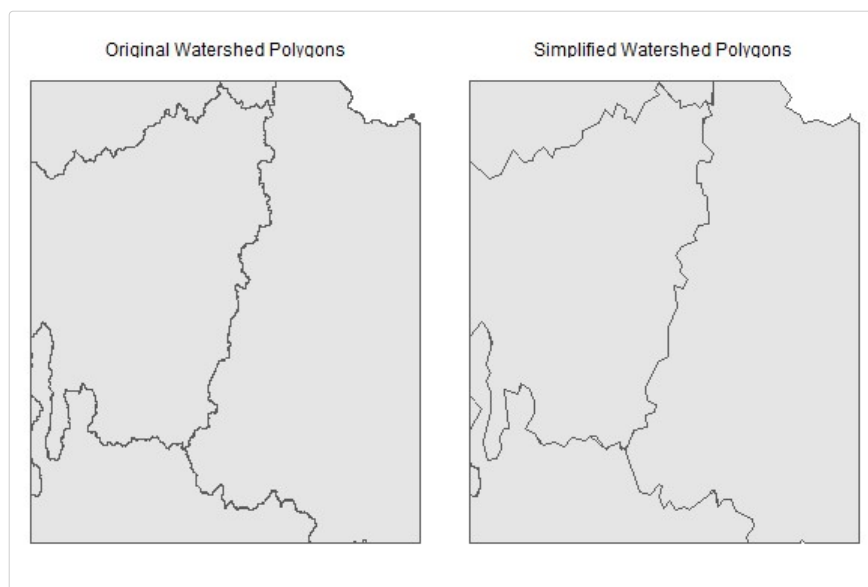
Many spatial processes require continuous polygons (i.e. no gaps in region boundaries), which limits the degree of polygon simplification that can be achieved. One desirable feature of `remap` is the ability of each model to make smooth predict outside of polygons within a smoothing zone, which smooths over any small gaps in

polygons that occurs in an aggressive geometrical simplification. Thus, by only preserving the macro structure of the input polygons, we can greatly speed up distance computations without losing fidelity in model predictions.

Distance calculation time can be dramatically reduced by simplifying the polygons passed to `remap` using the `sf` package `st_simplify` function. The function gives a warning that can be ignored for our purposes, we are only trying to preserve the macro structure and the regions are not near any poles. Gaps at region borders appear, but `remap` has the ability to predict outside of regions and predictions will remain smooth as long as the gaps aren't wider than two times the `smooth` parameter. Notice how the simplified polygons retain the basic structure of the original regions:

```
utws_simp <- utws %>% sf::st_simplify(dTolerance = 0.05)
#> Warning in st_simplify.sfc(st_geometry(x), preserveTopology, dTolerance):
#> st_simplify does not correctly simplify Longitude/Latitude data, dTolerance
#> needs to be in decimal degrees

rbind(
  utws %>% dplyr::mutate(TYPE = "Original Watershed Polygons"),
  utws_simp %>% dplyr::mutate(TYPE = "Simplified Watershed Polygons")
) %>%
ggplot() +
  facet_grid(.~TYPE) +
  geom_sf() +
  theme_void()
```



Simplifying the polygons doesn't drastically change the computation time in this particular example, but some regions can contain massive polygons with details that are unnecessary for regional modeling.

redist

The `remap` and `predict` functions both internally call a function called `redist` to calculate distances from points to polygons. The user can directly use the function `redist` to pre-compute distances from points to polygons and use the pre-computed distances as direct inputs in the `remap` function. The pre-computing step greatly reduces computational costs if multiple regional models must be made with the same input data and polygons.

Distances from prediction locations need only be computed to polygon boundaries for which the prediction location falls within their smoothing zone. Buffered polygons can be used to quickly determine candidate observations for distance calculations in each region. The `max_dist` parameter of `redist` can be used to make these buffered polygons. This drastically reduces the number of points for which distance calculations must be performed and greatly improves computation times.

```
huc2_dist_nz <- remap::redist(utsnz, utws_simp, region_id = HUC2)
head(huc2_dist_nz)
#> Units: [km]
#>      14      15      16      17
#> [1,] 0.00000 330.5847 272.5228 437.81560
#> [2,] 0.00000 428.2982 247.8652 358.01516
#> [3,] 0.00000 236.7842 285.3623 526.89371
#> [4,] 74.03409 386.9778  0.0000  64.61556
#> [5,] 76.54282 324.1539  0.0000 152.82797
#> [6,] 97.67083 175.9193  0.0000 284.43786
```

The newly created distance matrix can be sent to `remap` and `predict` as a parameter. Run the following code and notice how much faster the `remap` and `predict` functions run when the distances are pre-calculated.

```
t1 <- Sys.time()
lm_huc2 <- remap(
  utsnz, utws_simp, region_id = HUC2,
  buffer = 20, min_n = 10,
  model_function = lm,
  formula = log(WESD) ~ ELEVATION,
  distances = huc2_dist_nz
)

lm_huc2_mse <- mean(
  (utsnz$WESD -
   exp(predict(lm_huc2, utsnz, smooth = 10,
               distances = huc2_dist_nz)))^2
)
t2 <- Sys.time()

# mse
lm_huc2_mse
#> [1] 86925.69

# runtime
round(difftime(t2, t1), 1)
#> Time difference of 0.1 secs
```

The MSE for this model is slightly different than previous regional linear model since the simplified polygons are being used.

Parallel Code

Since calculating distances to polygons is independent for each polygon, `redist` can be run in parallel by setting the `cores` to a number greater than one. Models are built and make predictions independent of one another so the `remap` function and `predict` method also have a `cores` parameter for parallel computing. This means that distance calculations, modeling, and predicting processes can all be run in parallel.

Custom Models

While linear models are great for illustration, many spatial modeling approaches will require more complex regional model forms. The `remap` function is flexible enough to handle arbitrary model inputs and outputs, with the only requirement being that the model output must be compatible for use with the generic `predict` function and return a numeric output.

The `remap` function takes a `model_function` as a parameter. The `model_function` must have the following two features:

- Its first unnamed function argument must take a subset of an `sf` data point object,
- The function must output an object with a generic `predict` function that returns a vector of numeric values.

Note that named function arguments can be supplied at the end of the `remap` function, as was the case with the `formula` argument in the linear model example shown previously. The key is that the first unnamed parameter be dedicated to data input.

Suppose we want to make a generalized additive model (GAM) that is limited to only making positive predictions. We also don't want to predict a number greater than the highest observed response in each region to avoid over extrapolation. This can be accomplished through wrapper functions for both `gam` and `predict.gam` that restrict predicted values to a specified range.

```
gam_limit <- function(data, fml) {
  g_model <- mgcv::gam(fml, data = data)
  upper_lim <- max(data$WESD)

  out <- list(g_model = g_model, upper_lim = upper_lim)
  class(out) <- "gam_limit"
  return(out)
}

predict.gam_limit <- function(object, newobs) {
  if (nrow(newobs) != 0) {
    preds <- predict(object$g_model, newobs)

    preds[preds < 0] <- 0
    preds[preds > object$upper_lim] <- object$upper_lim

    return(preds)
  }
  return(NULL)
}
```

Global GAM Model

The following code tests a GAM model where elevation and splines on the sphere are used as predictors. We can use the functions written to do a GAM with `remap` to easily do cross validation on a global model:

```
# Create vector for cross-validation
set.seed(42)
```



```

cv_k <- sample(1:10, nrow(utsnow), replace = TRUE)

# Initialize predictions
gam_global_preds <- rep(as.numeric(NA), nrow(utsnow))

# Formula for global GAM
global_fm1 <- WESD ~ s(ELEVATION, k = 5) + s(LATITUDE, LONGITUDE, bs = "sos", k = 50)

# Build and test models with 10 fold cross-validation
for (i in 1:10) {
  index <- cv_k == i
  gam_global <- gam_limit(utsnow[!index, ], fm1 = global_fm1)
  gam_global_preds[index] <- predict(gam_global, utsnow[index, ])
}

# Calculate MSE
gam_global_mse <- mean((utsnow$WESD - gam_global_preds)^2)
gam_global_mse
#> [1] 23875.94

```

This model is much better than either of the basic linear models, even though the GAM accuracy is measured on cross-validation rather than resubstitution error and the GAM model is also modeling the zero valued observations.

Regionalized GAM Model

First, the distances are pre-calculated so the distance calculations aren't repeated 10 different times when doing cross validation. The distances return a matrix where each row corresponds to each observation in the data. The cross validation only uses a subset of the data, so the corresponding subset of distances should be passed to `remap` during each modeling step.

```

huc2_dist <- remap::redist(utsnow, utws, region_id = HUC2)

```

HUC2 regions are used to build a regionalized GAM models with `remap`. We will reduce the knots on the splines on the sphere from 50 to 25 so we don't need so many degrees of freedom for each model. The `min_n` can be set to 35 to allow at least 5 degrees of freedom per model.

```

# Initialize predictions
gam_huc2_preds <- rep(as.numeric(NA), nrow(utsnow))

# Formula for regional GAMs
gam_huc2_fm1 <- WESD ~ s(ELEVATION, k = 5) + s(LATITUDE, LONGITUDE, bs = "sos", k = 25)

# Build and test models with 10 fold cross-validation
for (i in 1:10) {
  index <- cv_k == i

  gam_huc2 <- remap::remap(
    utsnow[!index, ], utws, region_id = HUC2,
    model_function = gam_limit,
    buffer = 20, min_n = 35,
    distances = huc2_dist[!index, ],
    fm1 = gam_huc2_fm1
  )
}

```

```

)

gam_huc2_preds[index] <- predict(
  gam_huc2, utsnow[index, ],
  smooth = 10,
  distances = huc2_dist[index, ]
)
}

# Calculate MSE
gam_huc2_mse <- mean((utsnow$WESD - gam_huc2_preds)^2)
gam_huc2_mse
#> [1] 16620.54

```

The HUC2 regionalized GAM has 30.4% better MSE than the global GAM model.

Smooth Predictions

A toy model is best used to show how smooth predictions work since the Utah snow water content models have extreme values and sharp changes with elevation. The toy model has 3 regional models with contrived response variables that consists of an affine combination of longitude and latitude values. The left region predicts $lat - lon$, the bottom region predicts $lon - lat - 0.4$, and the right region predicts $lat - lon + 0.3$

```

# Make regions
toy_regions <- tibble::tribble(
  ~id, ~geometry,
  "a", sf::st_polygon(list(matrix(c(0, 0, 2, 0, 6, 3, 4, 10, 0, 10, 0, 0)*.1, ncol = 2, byrow =
    TRUE))),
  "b", sf::st_polygon(list(matrix(c(2, 0, 10, 0, 10, 4, 6, 3, 2, 0)*.1, ncol = 2, byrow = TRUE))),
  "c", sf::st_polygon(list(matrix(c(4, 10, 6, 3, 10, 4, 10, 10, 4, 10)*.1, ncol = 2, byrow = TRUE)))
) %>%
  sf::st_as_sf(crs = 4326)

# Manually make a toy remap model
make_toy <- function(x) {
  class(x) <- "toy_model"
  return(x)
}
remap_toy_model <- list(
  models = list("a" = make_toy("a"),
               "b" = make_toy("b"),
               "c" = make_toy("c")),
  regions = toy_regions,
  region_id = "id"
)
class(remap_toy_model) <- "remap"

# Make a prediction method for toy_model
predict.toy_model <- function(object, data) {
  x <- sf::st_coordinates(data)[, "X"]

```

```

y <- sf::st_coordinates(data)[, "Y"]
if (object == "a") {
  y - x
} else if (object == "b") {
  x - y - 0.4
} else {
  y - x + 0.3
}
}

# Make a grid over the regions for predictions
grd <- sf::st_make_grid(toy_regions, cellsize = .01, what = "corners") %>%
  sf::st_sf()

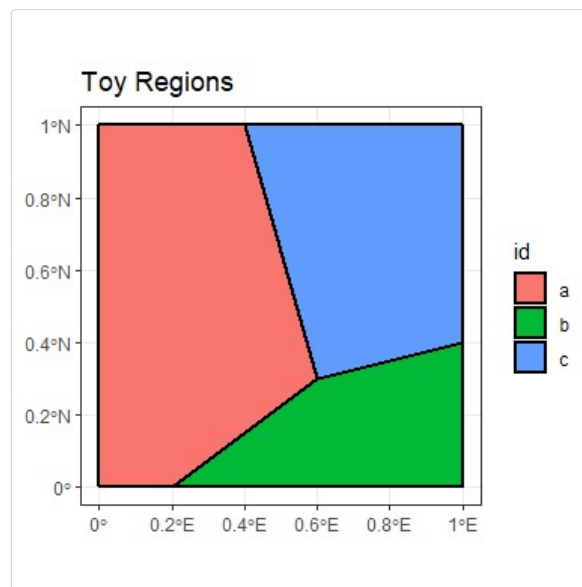
```

The regions cover the following area:

```

ggplot2::ggplot(toy_regions, aes(fill = id)) +
  geom_sf(color = "black", size = 1) +
  ggtitle("Toy Regions") +
  theme_bw()

```



The `remap_toy_model` object can now be used to make predictions on the `grd` object. There are 10201 points in the `grd` object but the regions are simple, so it will not take long to find distances. Two predictions will be made, the `SHARP` predictions will have a smoothing parameter of zero and the `SMOOTH` predictions will have a smoothing parameter set to 30km.

```

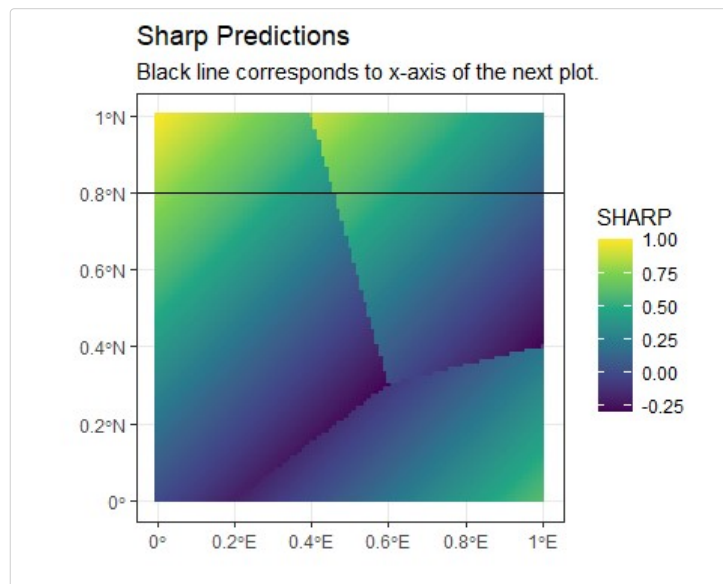
grd_pred <- grd %>%
  dplyr::mutate(SHARP = predict(remap_toy_model, grd, smooth = 0),
               SMOOTH = predict(remap_toy_model, grd, smooth = 30),
               LON = sf::st_coordinates(.)[, "X"],
               LAT = sf::st_coordinates(.)[, "Y"])

```

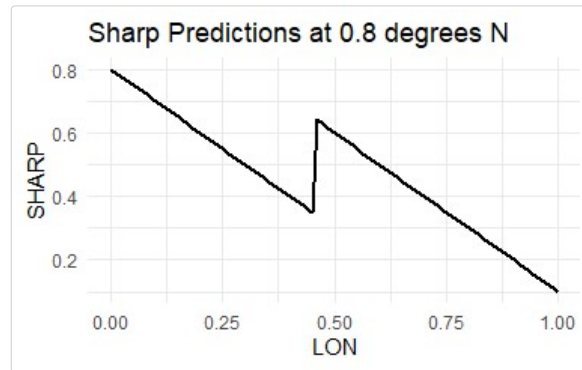
The smooth predictions from the `remap` object start to become a weighted average of regional predictions when

the predictions are within 30km of a region border. The following plots show what is happening with both the SHARP and SMOOTH predictions at predicted values at all locations and specific plots along the 0.8 degree N line. Notice how the predictions at the borders of the toy regions are smoothed:

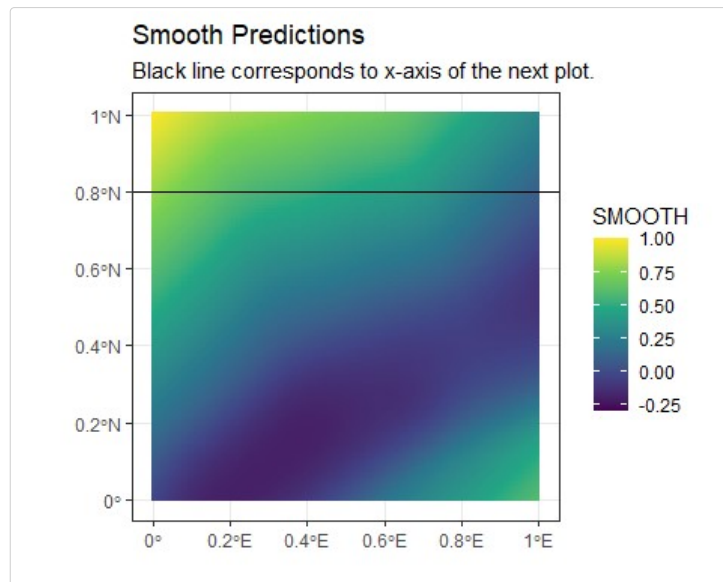
```
ggplot(toy_regions) +
  geom_sf() +
  geom_tile(data = grd_pred, aes(x = LON, y = LAT, fill = SHARP)) +
  scale_fill_viridis_c(limits = c(-0.3, 1)) +
  geom_hline(yintercept = 0.8) +
  ggtitle("Sharp Predictions", "Black line corresponds to x-axis of the next plot.") +
  xlab("") + ylab("") +
  theme_bw()
#> Warning: range backtransformation not implemented in this coord; results may be
#> wrong.
```



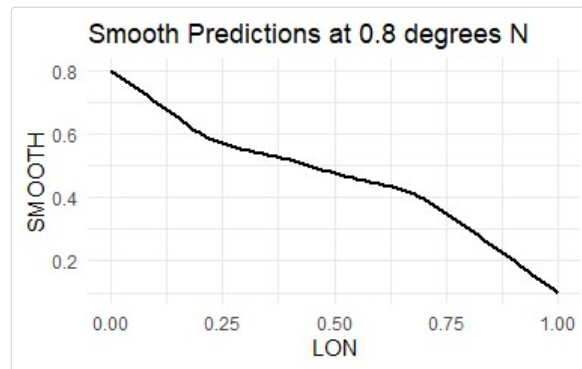
```
ggplot(grd_pred %>% dplyr::filter(LAT == 0.8),
       aes(x = LON, y = SHARP)) +
  geom_line(size = 1) +
  ggtitle("Sharp Predictions at 0.8 degrees N") +
  theme_minimal()
```



```
ggplot(toy_regions) +
  geom_sf() +
  geom_tile(data = grd_pred, aes(x = LON, y = LAT, fill = SMOOTH)) +
  scale_fill_viridis_c(limits = c(-0.3, 1)) +
  geom_hline(yintercept = 0.8) +
  ggtitle("Smooth Predictions", "Black line corresponds to x-axis of the next plot.") +
  xlab("") + ylab("") +
  theme_bw()
#> Warning: range backtransformation not implemented in this coord; results may be
#> wrong.
```



```
ggplot(grd_pred %>% dplyr::filter(LAT == 0.8),  
       aes(x = LON, y = SMOOTH)) +  
  geom_line(size = 1) +  
  ggtitle("Smooth Predictions at 0.8 degrees N") +  
  theme_minimal()
```



The `remap` package provides a way to build regional spatial models given a set of observations and a set of regions. The resulting model can make predictions that have no discontinuities at region borders and scales well to large problems.