LatticeKrig Vignette

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Contents

1 Introduction

In this vignette, we will explore the functions in the LatticeKrig package and show examples of how they can be used to solve problems. The LatticeKrig (LK) model is an example of the spatial statistics method known as kriging, adapted to large data sets.

1.1 What is kriging?

Kriging (named for South African statistician Danie Krige) is a method for making predictions from a spatial data set. By spatial data, we mean the data contains the observed variable and its location, the variable depends on the location, and pairs of observations taken close together have similar values. For example, the current temperature in cities would be spatial data. As such, kriging can be applied to a variety of important data sets, from geological data to atmospheric data.

The standard spatial model for Kriging relates the observation to a sum of three components: a polynomial function of the locations (and covariates, if provided), a spatial process, and measurement error.

1.2 The LatticeKrig model

The key feature of LatticeKrig is that we model a spatial process as the sum of radial basis functions (functions that are symmetric around their center and are 0 for far away points) scaled by coefficients, which we assume are correlated. The smooth basis functions and correlated coefficients create a smooth function representation for the spatial process, and the structure of the basis functions and covariance has some flexibility so you can change the structure to make a more reasonable model for a certain problem. The linear polynomial in the locations and covariates is determined using generalized least squares, following the standard approach of Universal Kriging. To approximate the spatial process, we then fit the basis functions to the residuals from the linear model. In terms of linear algebra, the model is

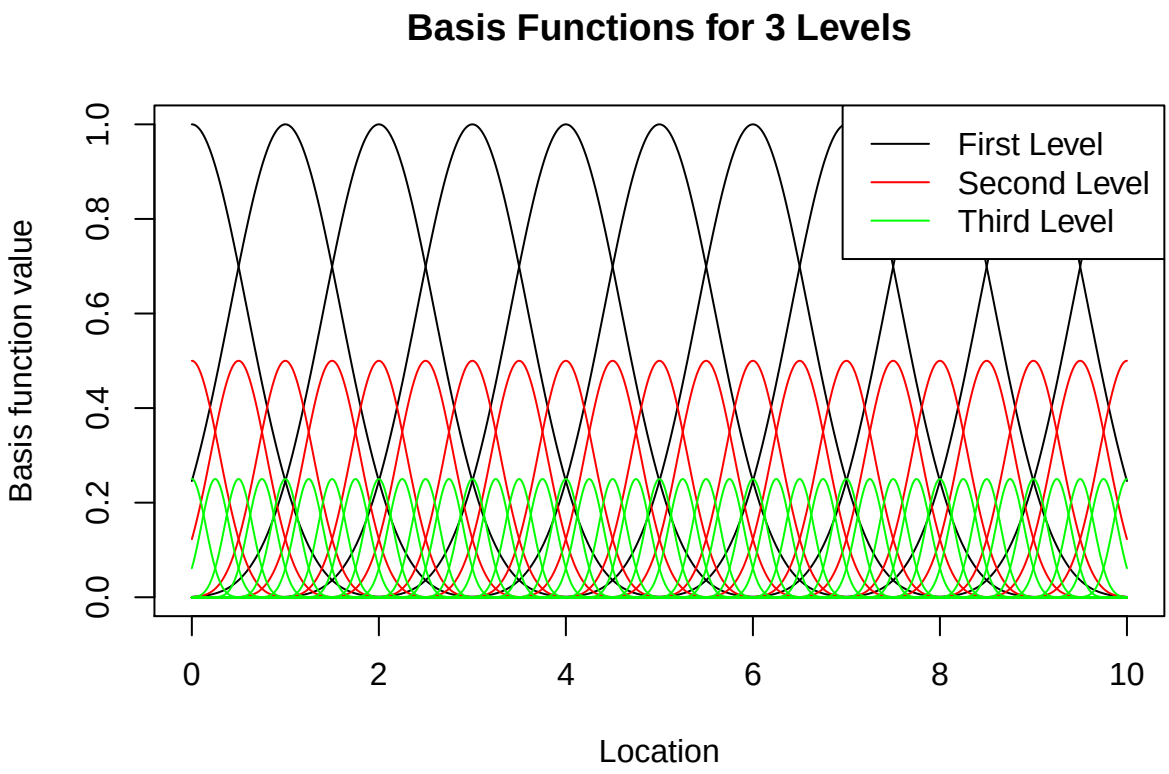
$$\mathbf{y} = X\mathbf{d} + \Phi\mathbf{c} + \mathbf{e}$$

where $\mathbf{y}$ is the vector of variable measurements, X is the matrix of locations and covariates, $\mathbf{d}$ is the vector of coefficients for the linear model, Φ is the matrix of basis functions evaluated at the data points, $\mathbf{c}$ is the vector of coefficients for each basis function, and $\mathbf{e}$ is the measurement error. If we let $\mathbf{g}$ represent the true values of the variable (without measurement error $\mathbf{e}$), we can unroll the matrix multiplications into sums and get the form

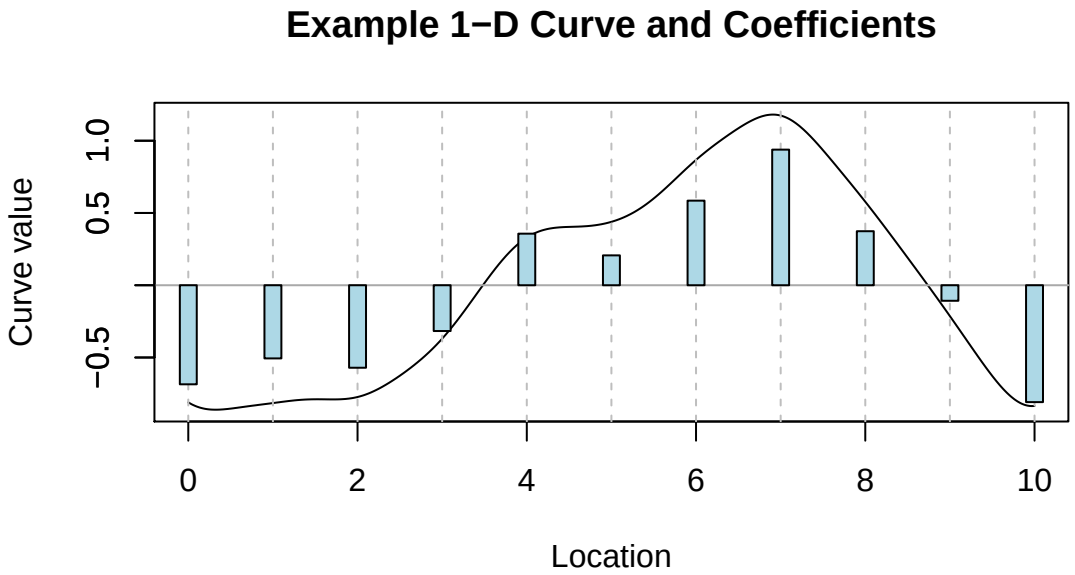
$$g(\mathbf{s}) = \sum_{k=1}^{n} \phi_k(\mathbf{s})\hat{\mathbf{d}}_k + \sum_{k=1}^{m} \psi_k(\mathbf{s})\hat{\mathbf{c}}_k$$

We show the derivations of the equations for $\mathbf{c}$ and $\mathbf{d}$ in Appendix A, and show how all of these calculations are done in Appendix C.

The package is named LatticeKrig because of the placement of the basis functions: they are equally spaced in all dimensions on a lattice. We can also consider multiple different lattice sizes simultaneously to better capture different levels of resolution; by default, each additional level has half as much space between the basis functions in each dimension. The following plot shows the basis functions for each of the three default levels.



To represent a curve, we multiply each basis function by a coefficient and add them together, as shown in the following plot.The blue bars show the coefficient value at each lattice point, and the black line shows the resulting curve from scaling the basis functions with these coefficients and adding them together.



1.3 Glossary of important package functions

- `LatticeKrig`: A top level function that sets up the default spatial model, estimates some key spatial parameters, and uses the `LKrig` function for the kriging computation. `LatticeKrig` can use a minimal set of inputs and is a quick way to fit a kriging model to data.
- `LKrig`: Performs the Kriging computation and evaluates the Gaussian spatial likelihood function for a fixed LatticeKrig model. This is the main computational step in the package, and is common to all choices of geometries and models.
- `LKrigSetup`: Creates an `LKinfo` object, which is used to describe the complete spatial model for a `LatticeKrig` or `LKrig` call; especially useful for examining the effect of changing one parameter on the model.
- `surface`: Plots a fitted surface in 2D space as a color plot and adds contour lines.
- `image.plot`: Plots a dataset or fitted surface in 2D space as an image plot and adds a color bar legend.
- `predictSurface`: Takes a Kriging model and evaluates its fitted function on a grid of locations.

2 Quick Start Guide

In this section, we will lay out the bare essentials of the package as a quick overview for the impatient reader. To fit a surface and interpolate data using `LatticeKrig`, the only required arguments are, naturally, the measurement locations (formatted in a matrix where each row indexes one location) and measurement values. However, we highly recommend using some of the optional parameters to customize the model to your specific data problem - several ways to do this are illustrated in this vignette. Calling the `LatticeKrig` function and passing in the locations and values will produce an `LatticeKrig` object that contains all the information needed to predict the variable at any location. Also, some spatial parameters are estimated by maximum likelihood if not specified.

For a simple, 1-dimensional example, we will take our locations to be 50 randomly spaced points on the interval $[-6, 6]$, and our observations to be the values of $\sin(x)$ at these locations with some added error. The goal of our kriging fit is to estimate this smooth curve from the observations.

2.1 One dimensional LatticeKrig example

```
#Making the synthetic data
set.seed(223)
locations <- runif(50, min=-6, max=6)
locations <- as.matrix(locations)
observations <- sin(locations) + rnorm(50, sd = 1e-1)
#Fit to the data, with parameters sigma and rho found by maximum likelihood.
kFit1D <- LatticeKrig(locations, observations)
```

Now we will print out the `LKrig` object: this list features the data's estimated covariance scale `rho` and estimated standard measurement error `sigma`, and the basis function description: the type of basis function, how distance is measured, and the number and spacing of basis functions. In this example, all of this information is determined by `LatticeKrig` from defaults, but can be changed with optional parameters.

```
print(kFit1D)
```

```
## Call:
## LatticeKrig(x = locations, y = observations)
##
##
##  Number of Observations:                      50
##  Number of parameters in the fixed component 2
##   Effective degrees of freedom (EDF)         10.34
##     Standard Error of EDF estimate:          0.9605
##  MLE sigma                                   0.1062
##  MLE rho                                     91.19
##  MLE lambda = sigma^2/rho                    0.0001237
##
## Fixed part of model is a polynomial of degree 1 (m-1)
## Basis function :  Radial
## Basis function used:  WendlandFunction
## Distance metric:  Euclidean
##
## Lattice summary:
## 3  Level(s) 75 basis functions with overlap of  2.5 (lattice units)
##
##  Level Lattice points   Spacing
##      1             17 1.8592024
```

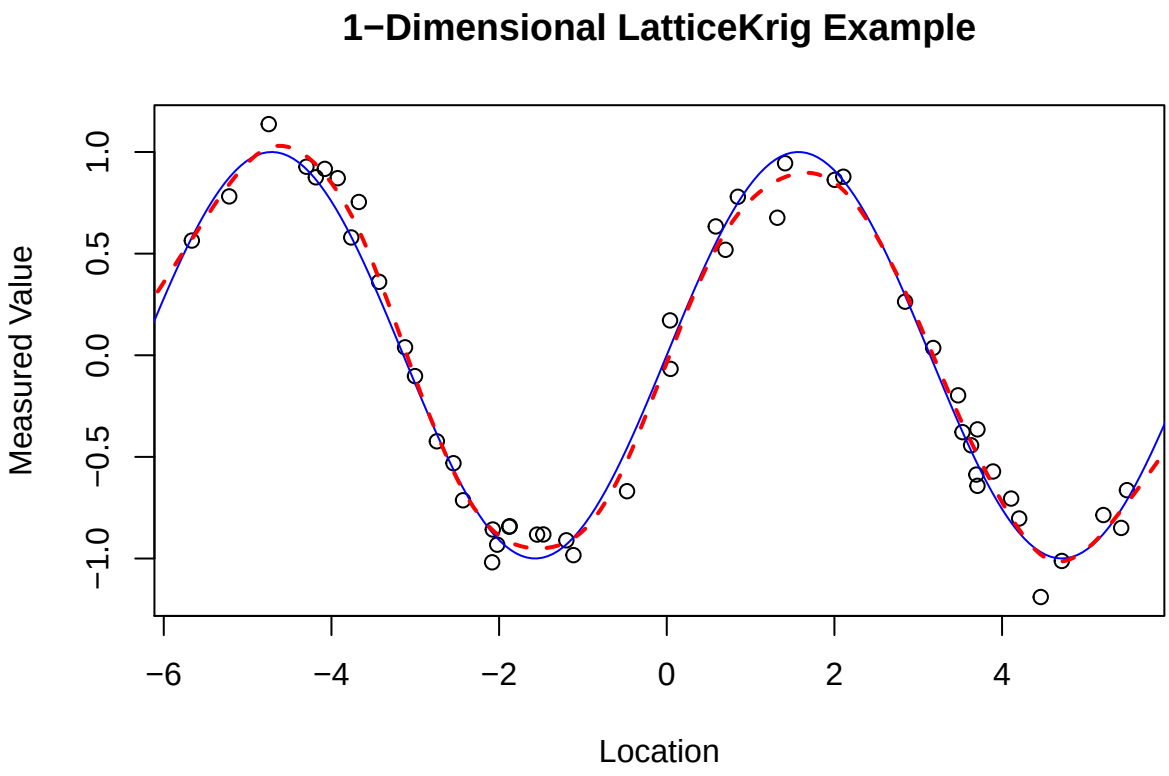
```
##       2             23 0.9296012
##       3             35 0.4648006
##
## Nonzero entries in Ridge regression matrix 806

## NULL
```

In the printout above, `sigma` is the estimated standard deviation of the measurement error; we set it to be 0.1, so the estimate 0.106 is great. EDF is a measurement of how strictly the model matches the original data; when EDF = 1, the model will be a straight line; when EDF equals the number of observations, the model will exactly match each recorded data point. We can also see the type of basis function used: in this case it is the Wendland function. We also have the default 3 levels to capture different effect scales.

2.2 Plotting the results

Now, we'll make a plot of the original 50 data points and the true function ($\sin(x)$) and the `LatticeKrig` fit at 200 equally spaced points to compare them.

```
xGrid <- seq(-2*pi, 2*pi, len=200)
prediction <- predict(kFit1D, xGrid)
plot(locations, observations, main="1-Dimensional LatticeKrig Example",
     xlab="Location", ylab="Measured Value")
lines(xGrid, sin(xGrid), col='blue')
lines(xGrid, prediction, col='red', lty=2, lwd=2)
```



For this example, the fitted curve (in red) matches the true function (in blue) rather closely, though error increases near the endpoints and we underestimate some peaks and troughs.

2.3 Inference and error analysis

Although it is beyond the scope of this Vignette to go into the details of conditional simulation it is useful to explain how the package is designed to do this computation – and what it is good for! Suppose you have fit a model to data, with the results in `MyFit` as an `LKrig` or `LatticeKrig` object and suppose `Z1` are the covariates at the locations `x1`.
The following code generates 10 draws from the distribution of the unknown process *given* (i.e. conditional on) the observations. This random sample is often called an ensemble. As a frequentist-based package, the conditioning in LatticeKrig also assumes that sigma, rho, alpha and a.wght covariance parameters are known. (A Bayesian approach would also sample these from their posterior distribution.)

```
aDraw<- LKrig.sim.conditional( MyFit, M=10, x.grid= x1, Z.grid=Z1)
```

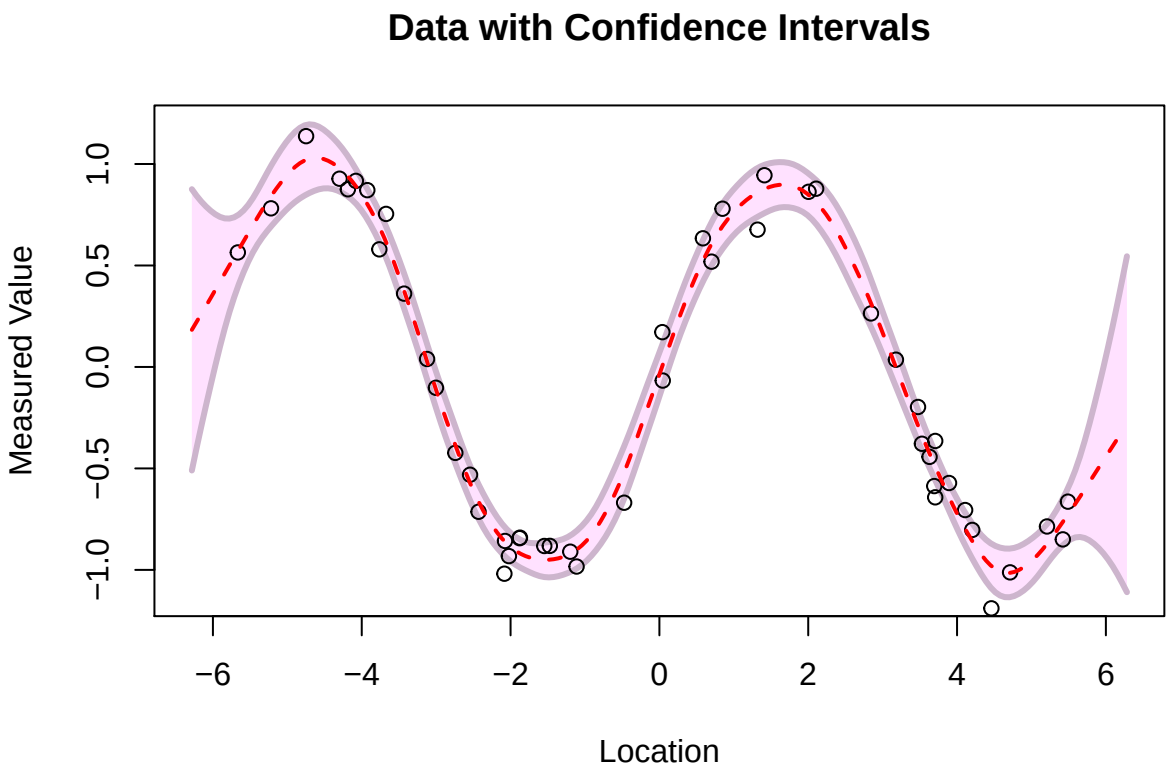
The interpretation of `aDraw` is that each column of aDraw is an equally likely representation of the process and linear model at locations `x1` given the observed data. As M becomes large the sample mean of the ensemble will converge to the estimate from LKrig. These simulations are easier to compute than the standard error for large data sets and so they are used to estimate the standard error of a model in LatticeKrig. The sample covariances of the ensemble will converge to the correct covariance matrix expressing the unceratinty in the estimate.

This first plot shows the 95% confidence intervals for the individual locations, based on a collection of simulations.

```
#simulates 50 curves based on the given data
uncertainty <- LKrig.sim.conditional(kFit1D, x.grid = as.matrix(xGrid), M=50)
```

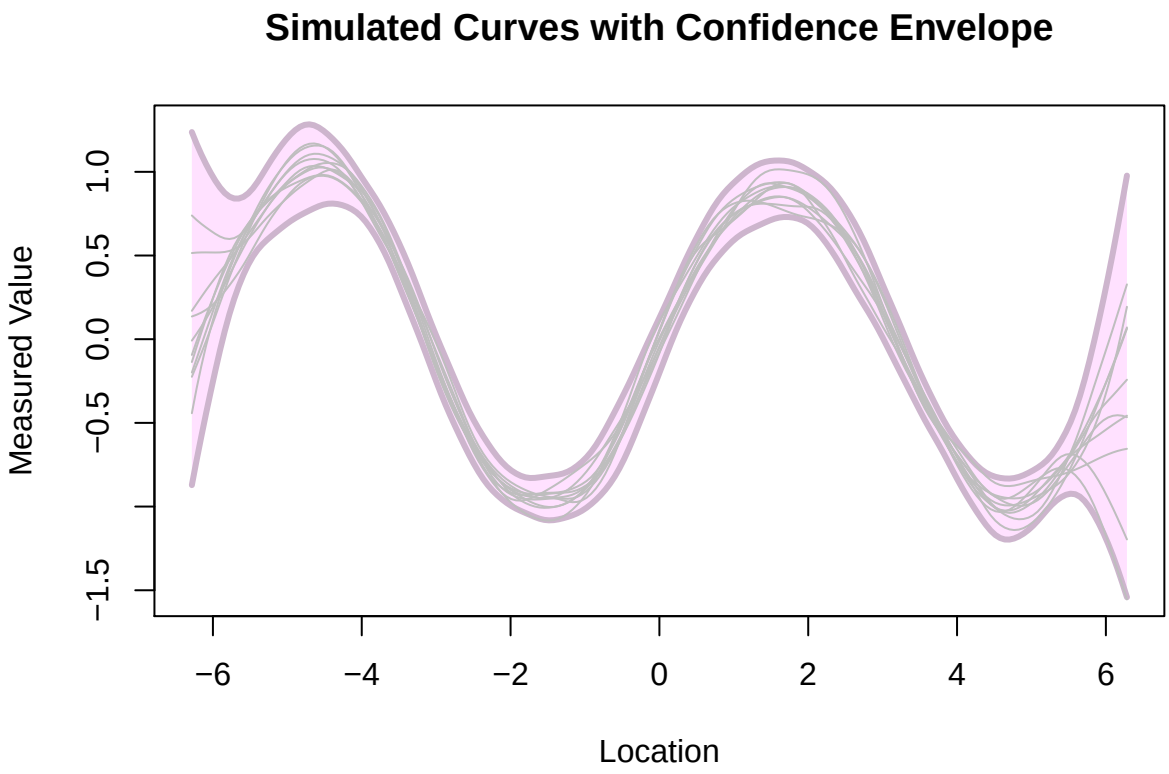
```
## 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23  24  25  26  27  28
```

```
#making a 95% confidence interval for each data point
sdVec <- apply(uncertainty$g.draw, 1, sd)
gamma <- qnorm(0.975)
upperBound <- prediction + gamma*sdVec
lowerBound <- prediction - gamma*sdVec
plot(xGrid, upperBound, type="l", ylim = c(min(lowerBound), max(upperBound)),
     main = "Data with Confidence Intervals", xlab = "Location", ylab = "Measured Value")
EnvelopePlot(xGrid, y1 = lowerBound, y2 = upperBound)
points(locations, observations)
lines(xGrid, prediction, col='red', lty=2, lwd=2)
```



This next plot adds a collection of simulations based on the fitted curve and the 95% confidence envelope for the entire fitted curve.

```
#computing the number of standard deviations needed to make the envelope contain 95% of the data
norm <- (uncertainty$g.draw - as.vector(prediction)) / sdVec
gammas <- apply(abs(norm), 2, max)
gamma <- quantile(gammas, 0.95)
#making the upper and lower bounds and plotting the envelope
upperBound <- prediction + gamma*sdVec
lowerBound <- prediction - gamma*sdVec
plot(xGrid, upperBound, type="l", ylim = c(min(lowerBound), max(upperBound)),
     main = "Simulated Curves with Confidence Envelope", xlab = "Location", ylab = "Measured Value")
EnvelopePlot(xGrid, y1 = lowerBound, y2 = upperBound)
for(i in 1:10) {
  lines(uncertainty$x.grid, uncertainty$g.draw[,i], col="gray")
}
```



We can see that the simulations get farther apart, meaning the confidence envelope gets wider, where there aren't many data points and especially at the edges of the region.

2.4 Fitting the model in two dimensions

For another, more practical example, we will predict the average daily mean spring temperature for locations throughout Colorado. Using the data set `COmonthlyMet`, we can make a surface showing our predictions over a range of longitudes and latitudes, use the `US` function to draw in the USA state borders to show where Colorado is, and draw the points where data was recorded. Notice that `LatticeKrig` will automatically discard any data points with missing values (NAs) if needed.

```
data(COmonthlyMet)
locations <- CO.loc
observations <- CO.tmean.MAM.climate
kFitWeather <- LatticeKrig(locations, observations)
```

```
## Warning in LatticeKrig(locations, observations): NAs removed
```

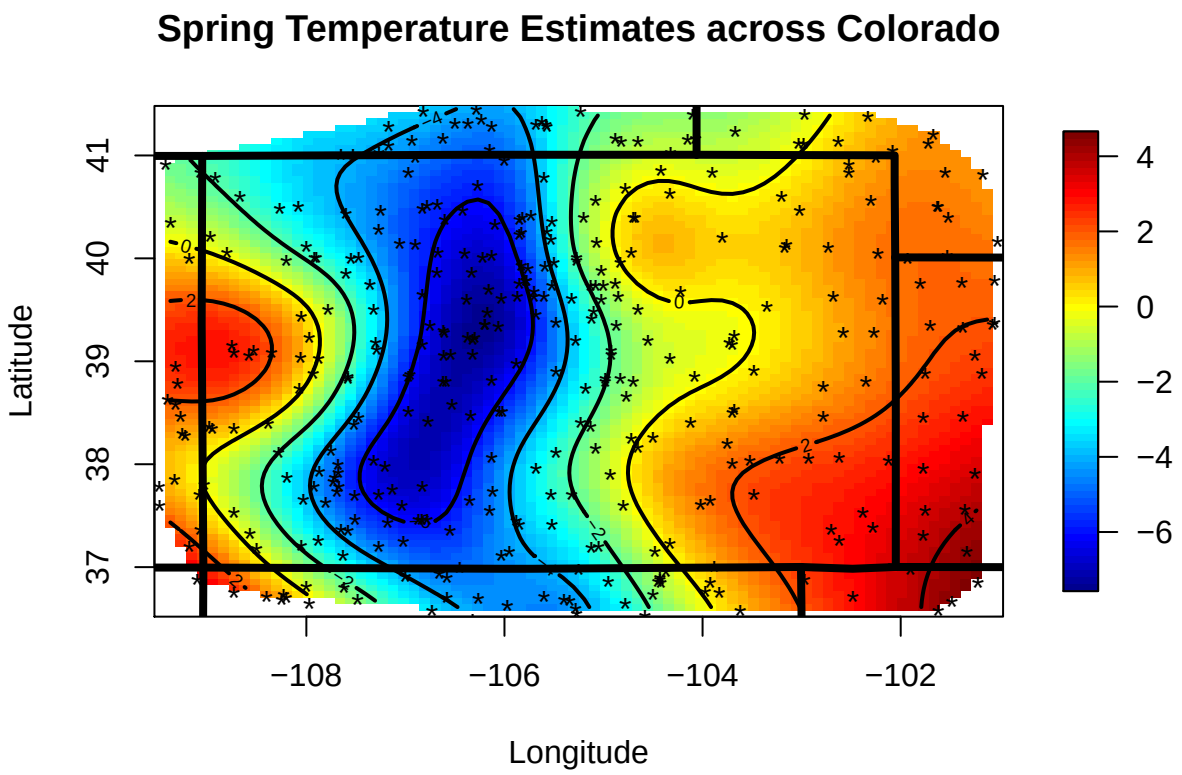
```
print(kFitWeather)
```

```
## Call:
## LatticeKrig(x = locations, y = observations)
##
##
##  Number of Observations:                      213
##  Number of parameters in the fixed component 3
##   Effective degrees of freedom (EDF)         36.96
```

```
##     Standard Error of EDF estimate:          1.685
##  MLE sigma                                   1.566
##  MLE rho                                     1832
##  MLE lambda = sigma^2/rho                    0.001338
##
## Fixed part of model is a polynomial of degree 1 (m-1)
## Basis function :  Radial
## Basis function used:  WendlandFunction
## Distance metric:  Euclidean
##
## Lattice summary:
## 3  Level(s) 797 basis functions with overlap of  2.5 (lattice units)
##
##  Level Lattice points Spacing
##      1            168   2.820
##      2            238   1.410
##      3            391   0.705
##
## Nonzero entries in Ridge regression matrix 51212
```

```
## NULL
```

```
surface(kFitWeather, main = "Spring Temperature Estimates across Colorado",
        xlab="Longitude", ylab="Latitude")
points(locations, pch = '*')
US(add=TRUE, col='black', lwd=4)
```



This plot is useful, but we can do better. We can see that the coldest temperatures are in the Rocky Mountains at higher elevations, which is not surprising. Thus, we might expect that we will get a more accurate fit by having `LatticeKrig` account for the elevation at each location as well. Another way we can improve the plot is by increasing its resolution - the current image is somewhat pixelated. The `surface` function will evaluate the surface at more points if we increase the `nx` and `ny` arguments: setting `nx=200, ny=150` will produce a grid of 30,000 points, which will take longer to compute but produces a nicer looking, more detailed plot. Finally, we can also have `surface` extend the evaluation all the way to the corners of the window by using the `extrap` argument; by default it doesn't extrapolate outside of the existing data, since the error often increases dramatically when predicting outside of the given data. However, extending the plot to the corners will make it look nicer. For the sake of example, we will also change the color scale in the image by setting the `col` parameter.

```
data(COmonthlyMet)
locations <- CO.loc
observations <- CO.tmean.MAM.climate
elevations <- CO.elev
kFitWeather <- LatticeKrig(locations, observations, Z=cbind(elevations))
```

```
## Warning in LatticeKrig(locations, observations, Z = cbind(elevations)): NAs
## removed
```

```
print(kFitWeather)
```

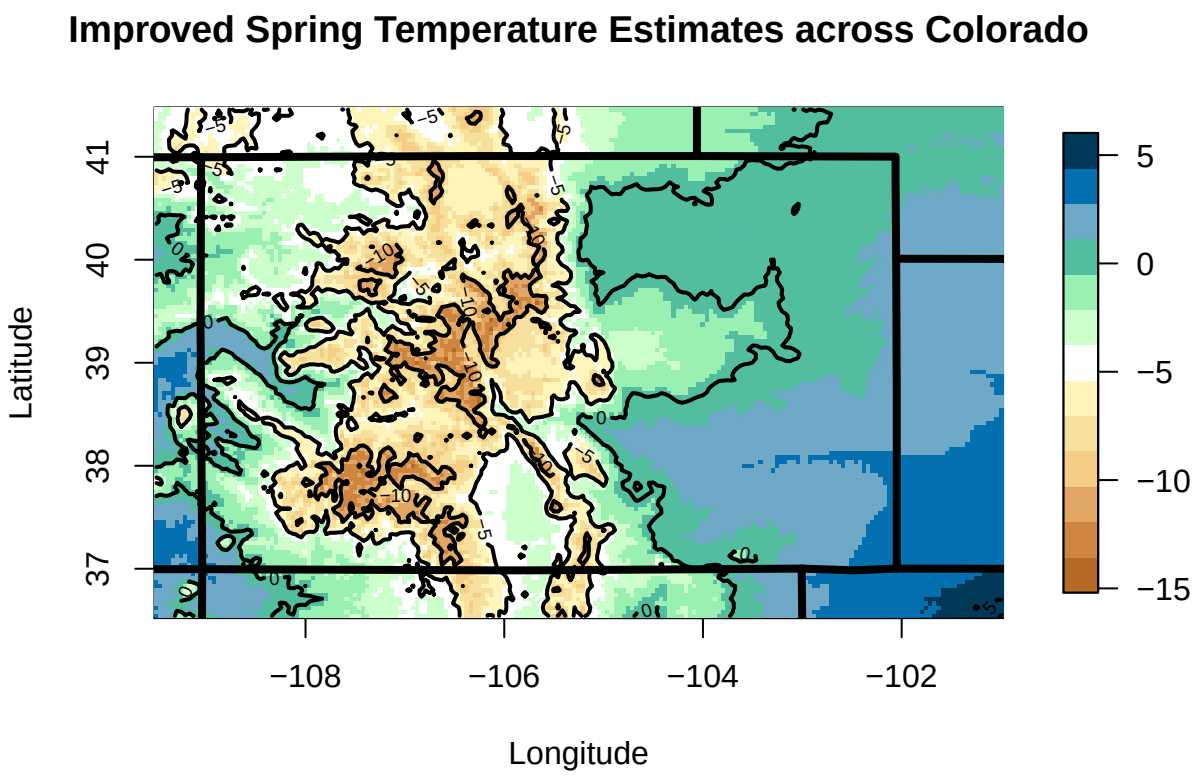
```
## Call:
## LatticeKrig(x = locations, y = observations, Z = cbind(elevations))
##
##
##  Number of Observations:                      213
##  Number of parameters in the fixed component 4
##  Number of covariates                         1
##   Effective degrees of freedom (EDF)         16.69
##     Standard Error of EDF estimate:          1.085
##  MLE sigma                                    1.204
##  MLE rho                                      64.43
##  MLE lambda = sigma^2/rho                     0.02248
##
## Fixed part of model is a polynomial of degree 1 (m-1)
## Basis function :  Radial
## Basis function used:  WendlandFunction
## Distance metric:  Euclidean
##
## Lattice summary:
## 3  Level(s) 797 basis functions with overlap of  2.5 (lattice units)
##
##  Level Lattice points Spacing
##      1            168   2.820
##      2            238   1.410
##      3            391   0.705
##
## Nonzero entries in Ridge regression matrix 51212
```

```
## NULL
```

Compared to the previous fit, we can see that this new fit with the covariate has...

```
# look at the help file in fields for information on the grid.list format
prediction <- predictSurface(kFitWeather, grid.list = CO.Grid, ZGrid = CO.elevGrid,
```

```
                              nx = 200, ny = 150, extrap = TRUE)
surface(prediction, main = "Improved Spring Temperature Estimates across Colorado",
        xlab="Longitude", ylab="Latitude", col=larry.colors())
US(add=TRUE, col='black', lwd=4)
```



This surface is so rough because it accounts for elevation; we can see that the plot is fairly smooth in the eastern half of the state, and extremely rough in the mountains.

Finally, it is important to note some potential issues that `LatticeKrig` calculations won't catch. Because `LatticeKrig` estimates some parameters of the data, the model could be a poor fit if the estimates aren't reasonable. See section 6.4 for more details on this. The `LatticeKrig` model also approximates a thin plate spline by default, which may not be a good fit for a given problem. Finally, as with other curve fitting techniques, you should examine the residuals of the model for any patterns or features that may indicate a poor fit.

2.5 Simulating a spatial process from the LatticeKrig model

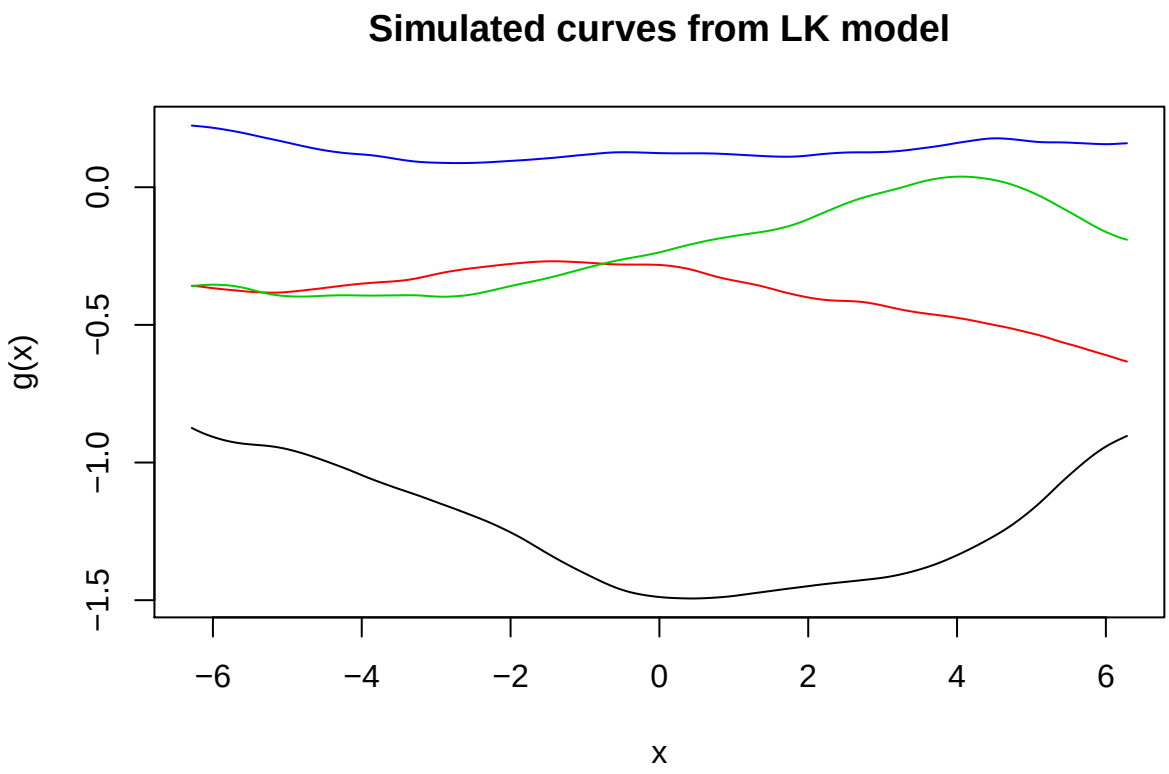
As a final topic we describe how to generate realizations from the Gaussian model in this package. The `LKinfo` object has a full description of the model and so simulation is easy. In the two examples of this section this object was set up from the top level function `LatticeKrig` and is the LKinfo component of the returned results. For more control over the model, however, we recommend that this object be created separately. (See Section 3)

For `kFit1D` from Section 2.1 note that a listing of the full model is shown from.

```
print(kFit1D$LKinfo)
```

Here we simulate 4 sample curves from this model and evaluate them on a finer grid of points than the observations. The random seed is set to reproduce these particular psuedo random draws.

```
set.seed(123)
gSim <- LKrig.sim(xGrid, kFit1D$LKinfo, M=4)
matplot(xGrid, gSim, type="l", lty=1, xlab="x", ylab="g(x)")
title("Simulated curves from LK model")
```



Note that in actually fitting the data a linear function is also included but since this is not a random component it is not part of the simulated process. Also the variance of the process is set to one.

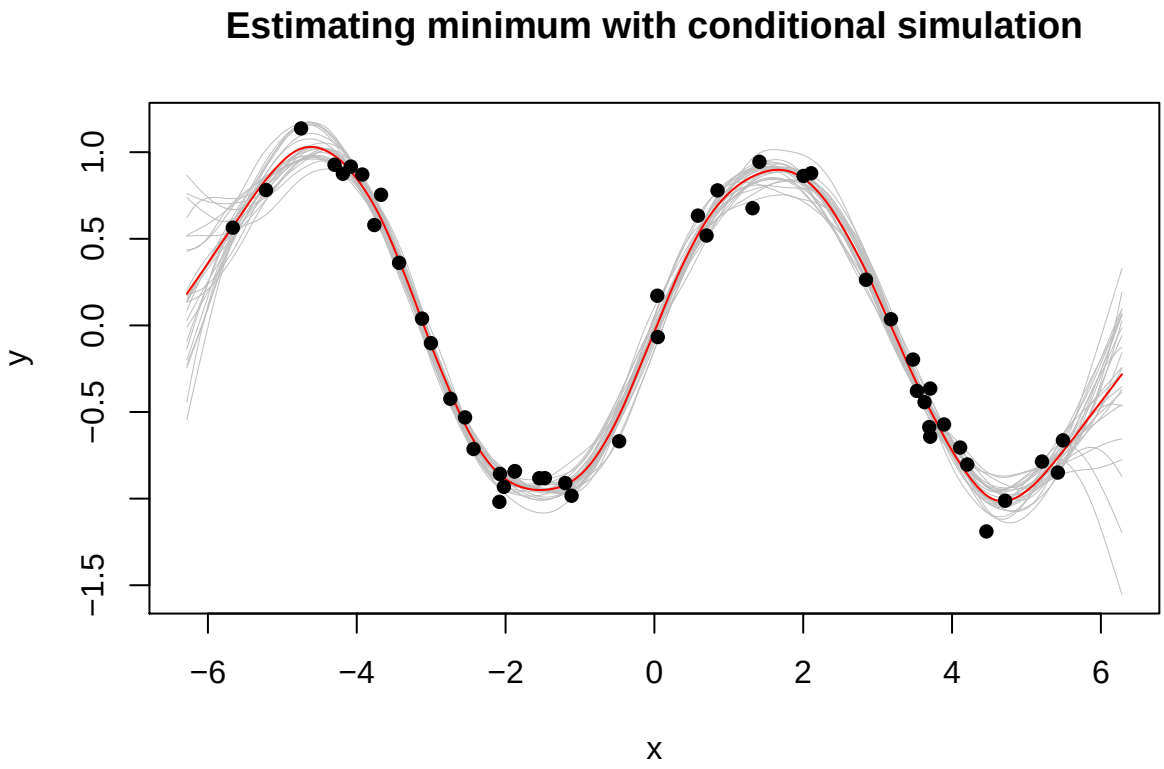
These simulated curves are referred to as *unconditional* because they are unrelated to the actual data except in terms of the range of the x values. Another form of simulation is to generate the process *conditional* on the observed data. This technique turns out to be very useful for quantifying the uncertianty in the curve estimate, and is the Monte Carlo method used to generate standard errors and confidence envelopes in the previous section. The example below creates 25 conditional draws from fitting the 1D example. All these curves are "equally likely" or plausible given the observations. This function returns several different parts of the estimate and so a list format is used. Note the use of the predict function to recover the estimated curve and also that the data is part of the fitted object. Within the range of the data all the conditional curves tend to track the estimate and the data, however, as one might expect beyond on the range of the observations there is much more variability among the simulated curves.

```
set.seed(123)
gCondSim <- LKrig.sim.conditional(kFit1D, M=25, x.grid=as.matrix(xGrid))
```

```
## 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23  24  25  25
```

```
matplot(xGrid, gCondSim$g.draw, type="l", lty=1,xlab="x", ylab="y", col="grey",
        main="Estimating minimum with conditional simulation", lwd=.5)
```

```
lines(xGrid, predict(kFit1D, xGrid), col="red")
points(kFit1D$x, kFit1D$y, pch=16, col="black")
```



2.6 Extra credit!

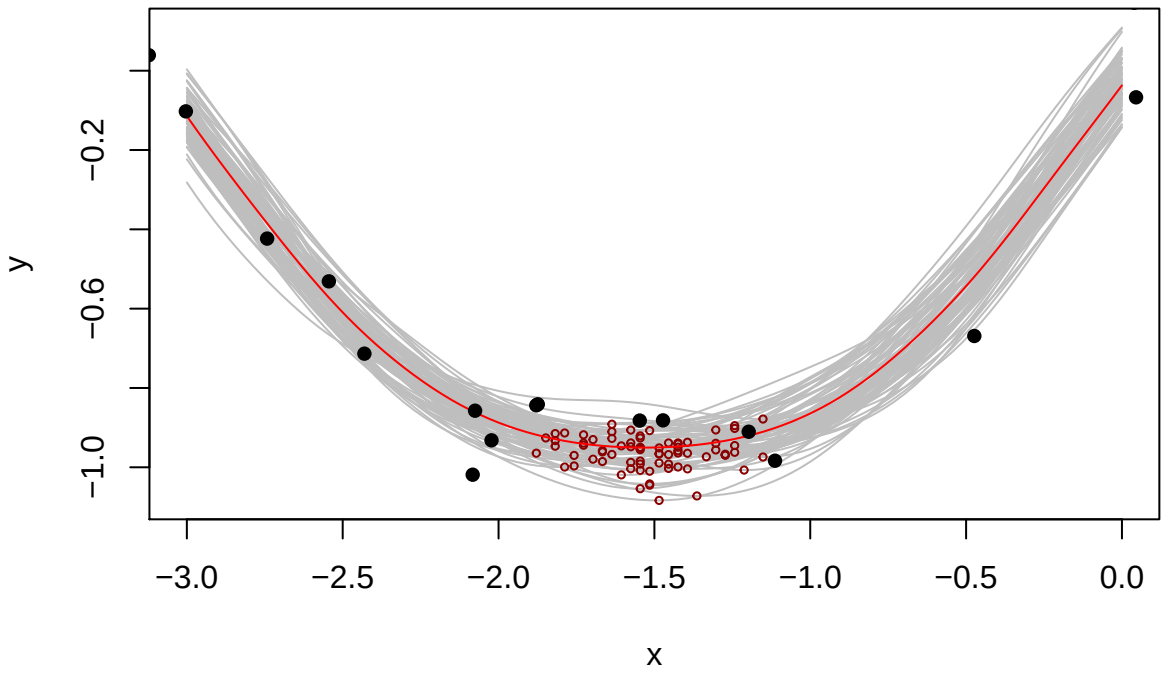
Here is a final example illustrating the power of determining the uncertainty by Monte Carlo. We generate a larger conditional sample over the subinterval [-3,0], find the minimum of each realization and plot the minimum and its location. Note that this represents uncertainty in both the minimum value itself and its location on the x-axis. Of course, because we know the true curve is a sine wave, we know the true minimum is exactly -1 at $x = -\pi/2$. This two dimensional distribution of minima and their locations is a valid approach to approximate the uncertainty of the estimated minimum of the true curve in this range. It would be difficult to derive an analytic formula for this distribution so the Monte Carlo approach is quite useful.

```
xGrid2 <- as.matrix(seq(-3, 0, length.out=100))
set.seed(333)
suppressMessages(
  gCondSim <- LKrig.sim.conditional(kFit1D, x.grid=xGrid2, M=75)
)
```

```
## 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23  24  25  26  27  28
```

```
# index of where minimum occurs in each draw
minXIndex <- apply(gCondSim$g.draw, 2, which.min)
XMin <- xGrid2[minXIndex]
YMin <- apply(gCondSim$g.draw, 2, min)
matplot(xGrid2, gCondSim$g.draw, type="l", lty=1,
```

```
        xlab="x", ylab="y", col="grey", ylim=c())
points(XMin, YMin, col="red4", cex=.5)
lines(xGrid2, predict(kFit1D, xGrid2), col="red")
points(kFit1D$x,kFit1D$y, pch=16, col="black")
```



3 LKrigSetup

The only *required* arguments for the LatticeKrig function are the set of locations and variable observations. However, LatticeKrig also allows for a variety of optional arguments to adapt the model to be more realistic. In this section we will list some of the most important optional parameters that can be passed into LatticeKrig; for a complete list, check the LatticeKrig help page. The LKrigSetup function is a convenient (and, in some cases, the only) way to pass in a group of parameters to LatticeKrig or LKrig. We will cover the required parameters and some of the more important optional parameters here; for full descriptions, check the help pages for LatticeKrig and LKrigSetup. This code will printout of the LKinfo object created by LatticeKrig in the quick start guide's one-dimensional example.

```
print(kFit1D$LKinfo)
```

We could make such an LKinfo object directly from the LKrigSetup function as follows:

```
kFit1DInfo <- LKrigSetup(locations, nlevel = 3, NC = 6, nu = 1, a.wght = 2.01)
```

3.1 Required Parameters for LKrigSetup

- x

The parameter x is used to find the range of the data locations in each dimension for the lattice. As such, it is often easiest to pass in the matrix of observation locations, but you can also just pass in the range directly.

- nlevel

The parameter nlevel is an integer that determines the number of different lattice sizes the computation should run on. This is set to 3 by default in LatticeKrig. Increasing nlevel will increase the potential detail of the fitted surface, and will increase the computation time significantly. The coefficients at each different lattice size is computed independently, and the resulting coefficients are scaled by the weights in alpha.

- NC

The parameter NC is an integer that determines the number of basis functions to put along the largest dimension at the first level. Recall that each basis function is centered on a lattice point, so NC equivalently controls the number of lattice points to set across the region in the longest dimension. Note that the actual number of basis functions may be different. By default, 5 additional basis functions (this can be changed with the optional NC.buffer parameter) are added outside the domain on each side. For example, if the spatial domain is a rectangle whose length is double its width and NC = 6, the first level of basis functions will contain 16x13 = 208 basis functions (6x3 inside the domain with 5 extended from each edge) and the second level will contain 21x15 = 315 basis functions (11x5 inside the domain with 5 extended from each edge).

- alpha or alphaObject or nu

At least one of alpha, alphaObject, and nu must be set. In most cases you will use alpha or nu. The parameter alpha should be a vector of length nlevel that holds the weights that scale the basis functions on each different lattice size; nu is a scalar that controls how quickly the values in alpha decay. When nu is set, alpha will be filled by setting alpha[i] = 2^(-2 * i * nu), then scaling so the sum of the weights in alpha is 1. This scaling should always be done before passing in alpha to make sure the model fits correctly. The alphaObject and a.wghtObject below can be used for nonstationary models, which are not discussed in this vignette.

- a.wght or a.wghtObject

At least one of a.wght and a.wghtObject must be set. In most cases you will use a.wght, which can be either a scalar or a vector of length nlevel. The minimum value for this parameter varies depending on the geometry and the number of dimenions: in the default Euclidean geometry, the minimum value is two times

the number of dimensions. For example, in 2 dimensions, you might set `a.wght = 4.01`. When using the `LKSphere` geometry, the minimum value for `a.wght` is 1, and again a small decimal should be added on.

3.2 Optional parameters

- `lambda`

`Lambda` is an estimate of the noise to signal ratio in the data. If not listed, `LatticeKrig` and `LKrig` will estimate it using maximum likelihood. There is a one-to-one relationship between this parameter and the effective degrees of freedom (EDF) of the curve estimate. However, EDF is more expensive to compute so lambda is preferred for computing.

- `LKGeometry`

The `LKGeometry` specifies the geometry used for the LK model. For example, if the dataset covers the whole earth, it would be more appropriate to base the kriging on a sphere than a rectangle. This is covered in more depth in the next section.

- `distance.type`

When using a different `LKGeometry` than default (Euclidean), you may also need to change the `distance.type`. This is also covered in more depth in the next section.

- `NC.buffer`

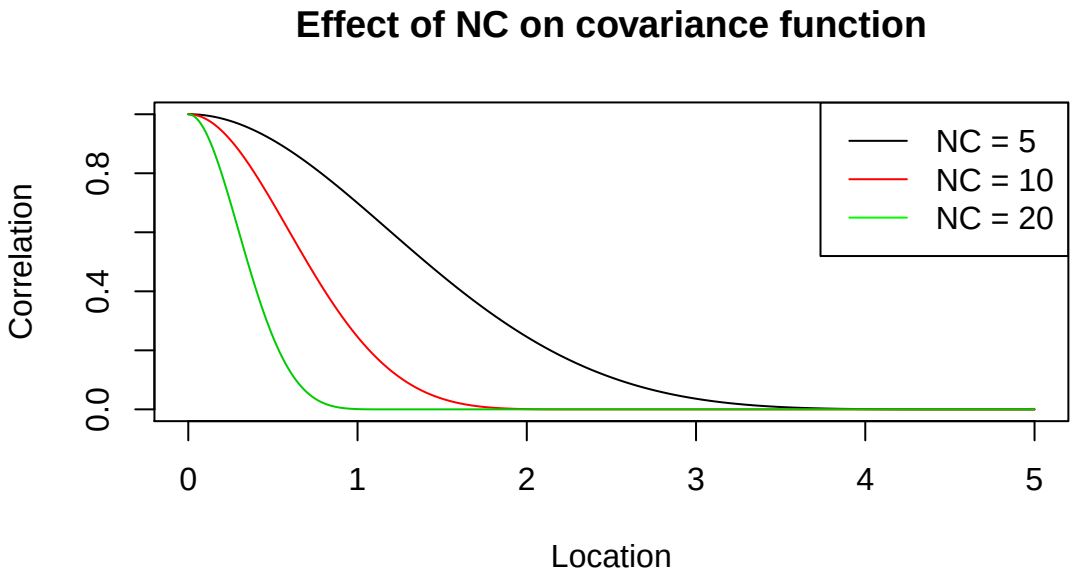
This parameter determines how many lattice points to add outside the range of the data on each side. The effect of changing this parameter is relatively minor compared to the effect of changing `NC`, and it usually will only affect the prediction near the edges of the data.

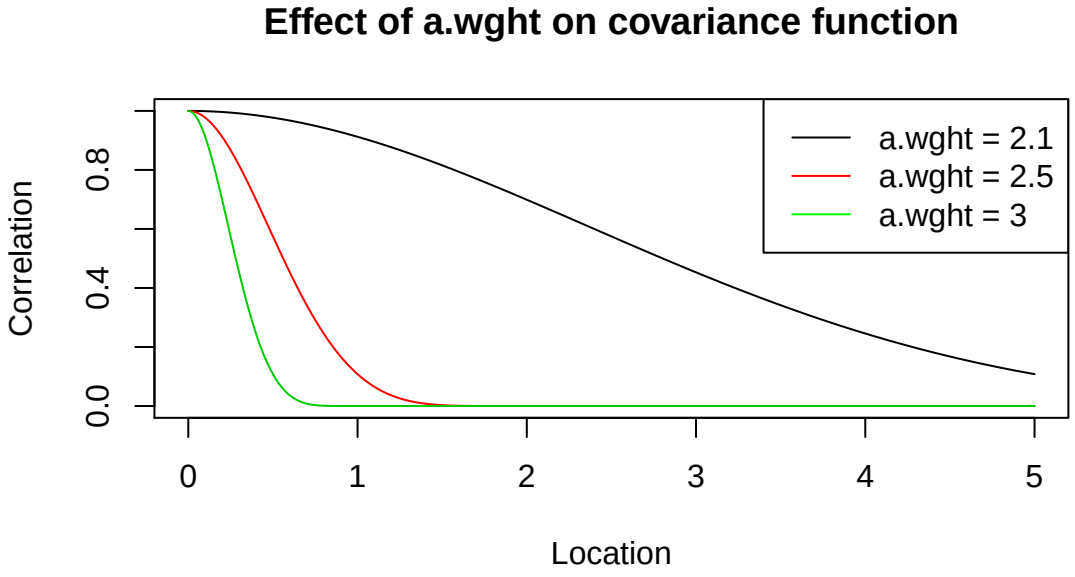
- `normalize`

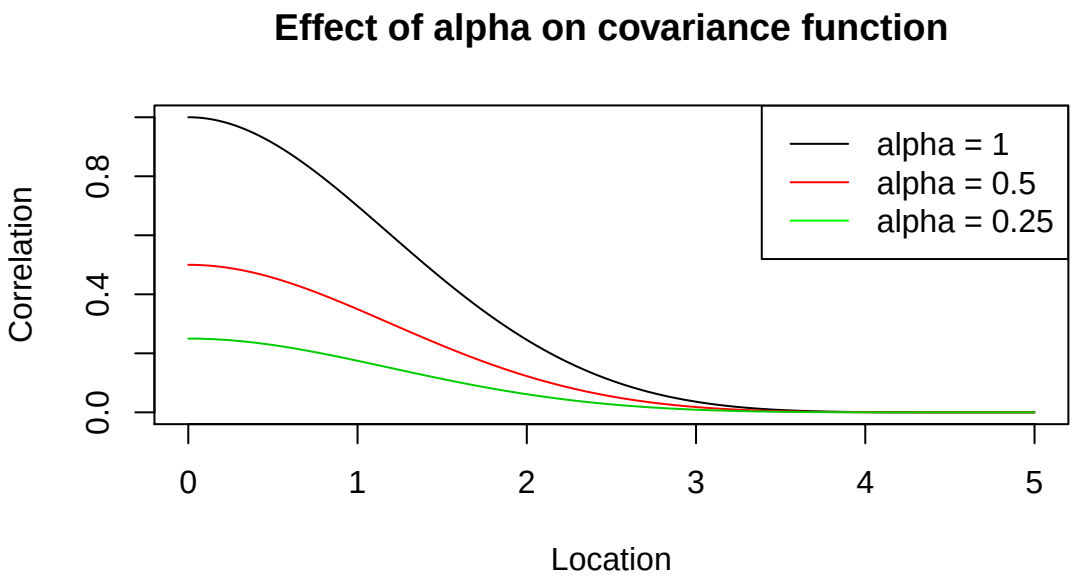
This parameter determines whether or not to normalize the basis functions after computing them, making the variance 1. This is set to `TRUE` by default, sacrificing some computing time to reduce edge and lattice artifacts created by the model that aren't present in the data.

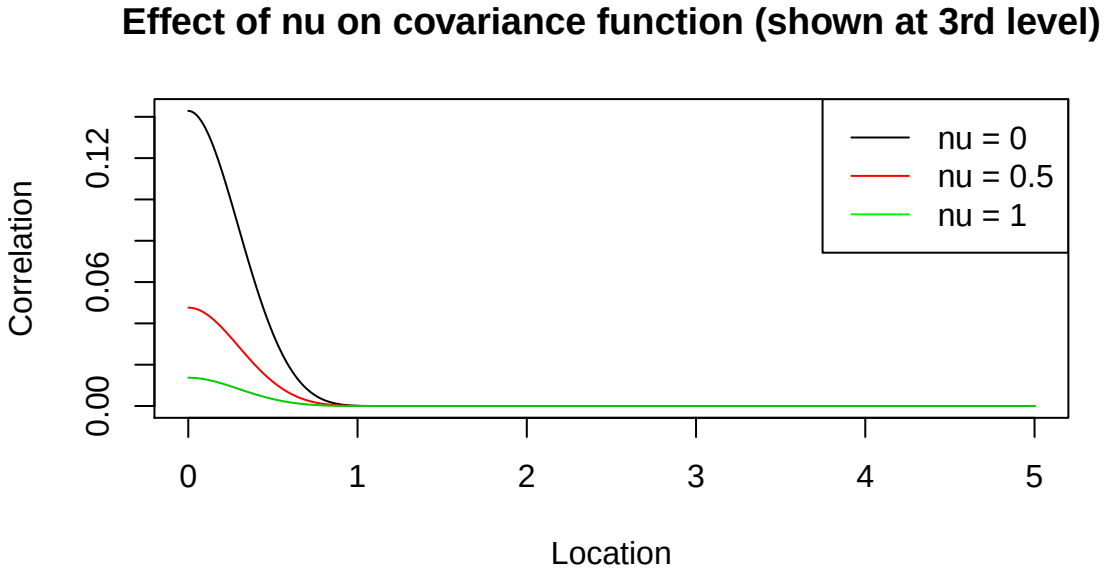
3.3 Relationships between parameters and the covariance function

The following plots show how different values of `NC`, `a.wght`, `alpha`, and `nu` affect the covariance function. These plots are all one dimensional for ease of viewing; the covariance function is radially symmetric in higher dimensions and has similar dependence on these parameters.


Effect of NC on covariance function
Correlation
0.0
0.4
0.8
0
1
2
3
4
5
Location
NC = 5
NC = 10
NC = 20


Effect of a.wght on covariance function
Correlation
0.0
0.4
0.8
0
1
2
3
4
5
Location
a.wght = 2.1
a.wght = 2.5
a.wght = 3


Effect of alpha on covariance function
Correlation
0.0
0.4
0.8
0
1
2
3
4
5
Location
alpha = 1
alpha = 0.5
alpha = 0.25

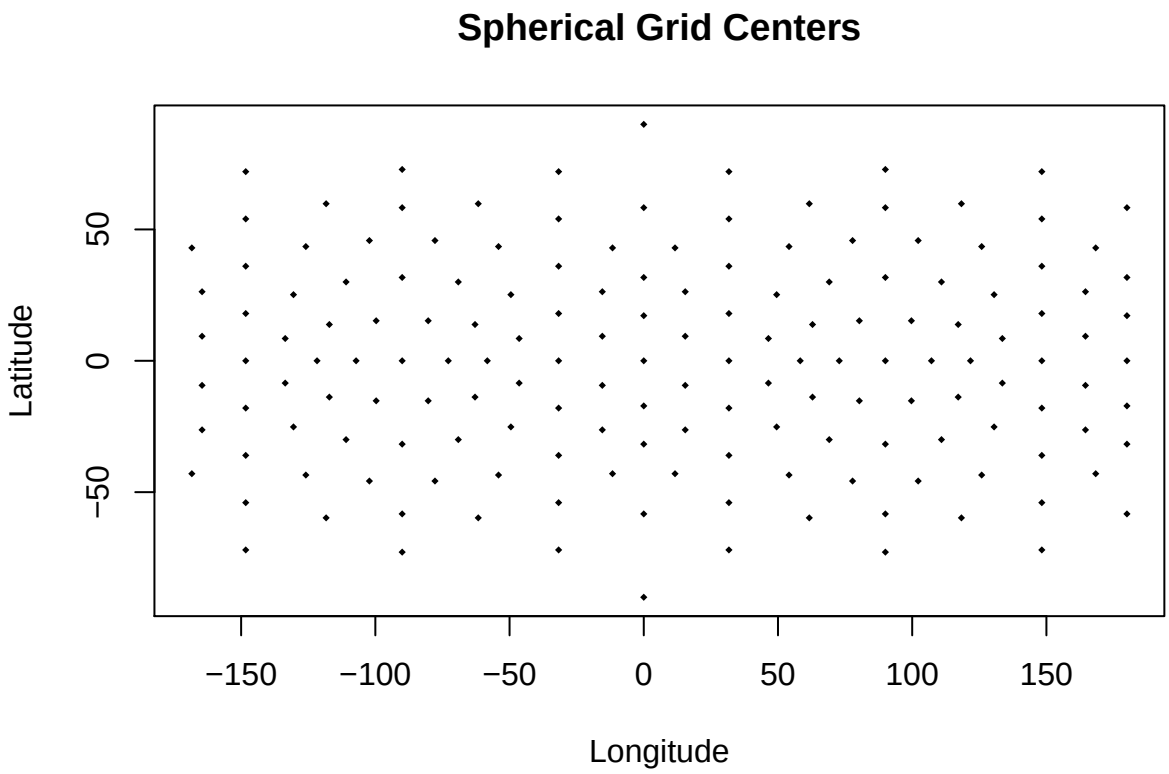

Effect of nu on covariance function (shown at 3rd level)
Correlation
0.00
0.06
0.12
0
1
2
3
4
5
Location
nu = 0
nu = 0.5
nu = 1

4 Kriging in Different Geometries

By default, `LatticeKrig` will interpret the location data it receives as points in n-dimensional Euclidean space, and calculate the distance accordingly. However, this package also supports distance metrics for other geometries. One example is locations on a sphere (e.g. observations on the Earth's surface), expressed as azimuth (longitude) and zenith (latitude). There are also other options for non-Euclidean geometries: a cylinder using 3 dimensional cylindrical coordinates, and a ring using 2 dimensional cylindrical coordinates (z and θ at a fixed radius). To set the geometry, set the `LKGeometry` parameter in `LKrigSetup`. These are the current choices:

- `"LKInterval"`: 1 dimensional Euclidean space
- `"LKRectangle"`: 2 dimensional Euclidean space
- `"LKBox"`: 3 dimensional Euclidean space
- `"LKSphere"`: 2 dimensional spherical coordinates
- `"LKCylinder"`: 3 dimensional cylindrical coordinates
- `"LKRing"`: 2 dimensional cylindrical coordinates

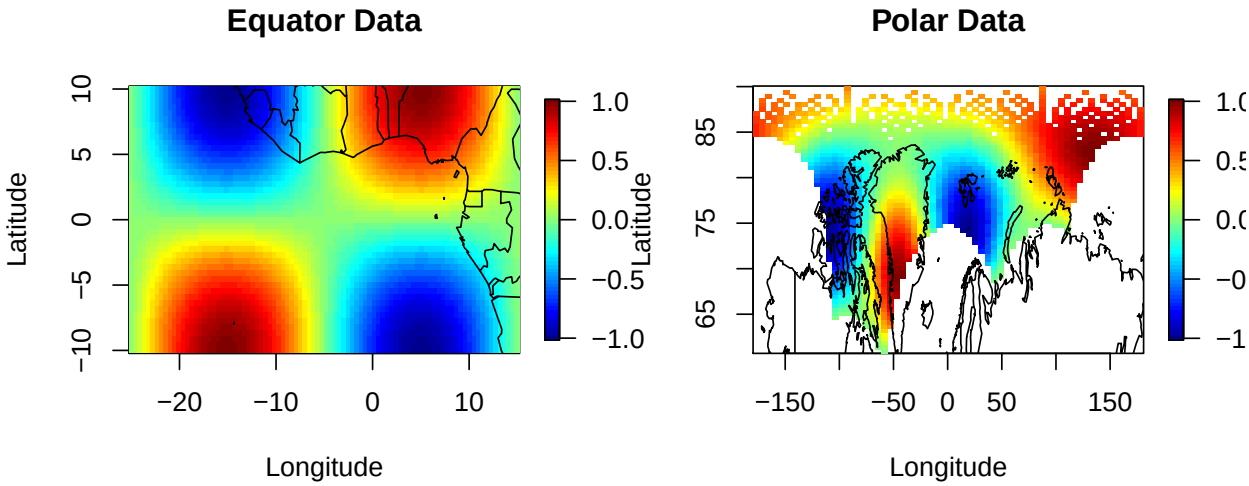
By default, `LKinfo` will use either `LKInterval`, `LKRectangle`, or `LKBox`, depending on the number of columns in the data locations. However, it is best to set `LKGeometry` explicitly; failing to do so can cause errors. When using the `LKSphere` geometry, there are also different ways of measuring distance using the `distance.type` argument of the `LKinfo` object - the default is `"GreatCircle"`, which measures the shortest distance over the surface of the sphere, or you can use `"Chordal"` to measure the straight-line distance, treating the coordinates as 3-dimensional Euclidean locations. Finally, when using the spherical geometry, you need to set `startingLevel`, which serves a similar role to `NC` from the Euclidean space. The `startingLevel` parameter controls how fine of a grid to use at the lowest level of the fit in spherical coordinates. The following plot shows the centers of the basis functions at `startingLevel = 3`, where they are at the vertices of an icosohedron inscribed in the sphere; for more information, check the `LKSphere` help page and the example in the `IcosohedronGrid` help page using the rgl library.



4.1 Working with spherical coordinates

For an example of fitting data taken on the globe using spherical geometry, we will load 2 copies of the same sample data – one near the equator, one near the north pole – and compare the models computed on the `LKRectangle` geometry and `LKSphere` geometry. We compute a kriging fit for the original data and the rotated data using the rectangular geometry and the spherical geometry, and print out the sum of squared errors as a measurement of how accurately the different fits match the data. We will expect to see very similar results for the two spherical models and noticeably different results for the two rectangular models.

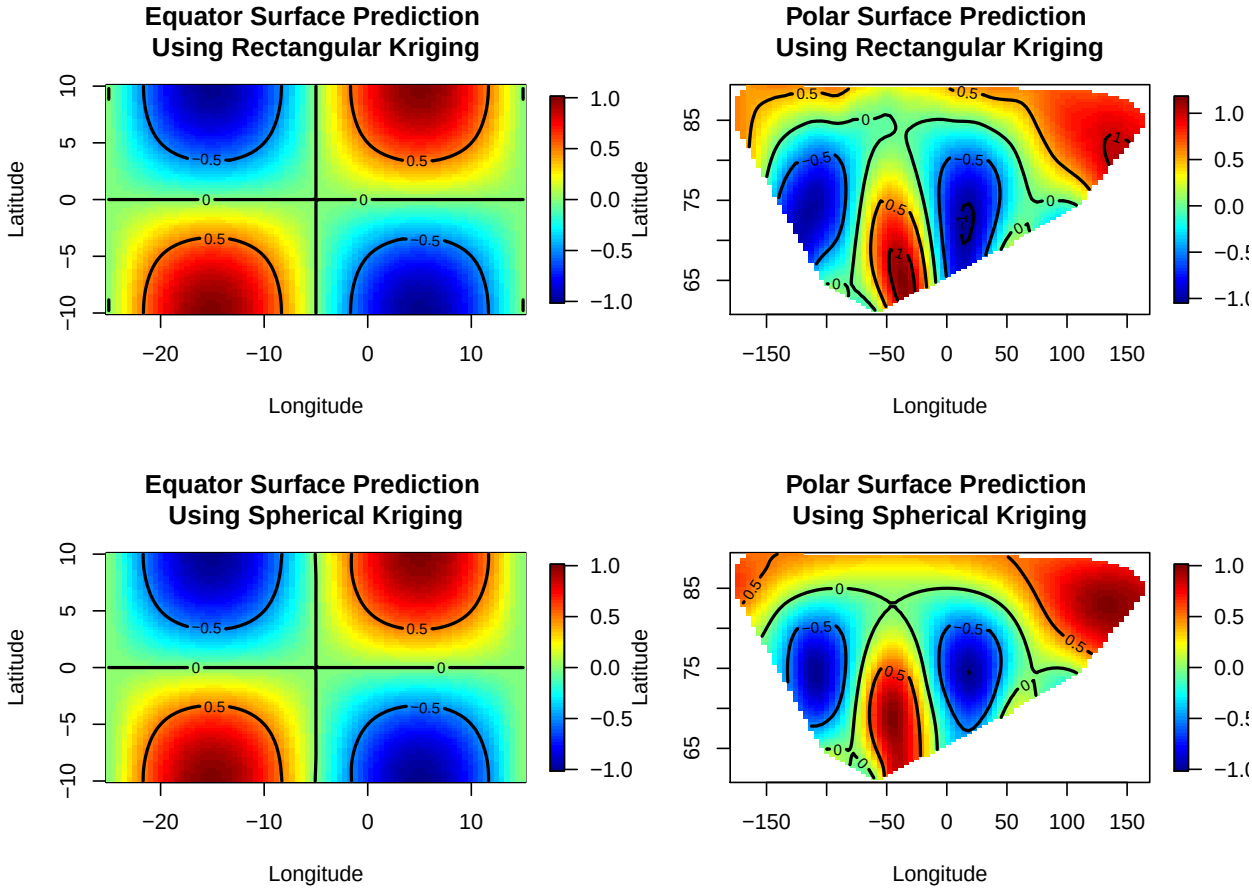
```
library(LatticeKrig)
data(EquatorData)
data(PolarData)

#plot the data at the equator and at the north pole in rectangular coordinates
#note the significant distortion at the north pole
par(mfrow = c(1,2))
quilt.plot(equatorGrid, equatorGridValues, nx = 90, ny = 45,
           main="Equator Data", xlab="Longitude", ylab="Latitude")
world(add=TRUE)
quilt.plot(polarGrid, polarGridValues, main="Polar Data",
           xlab="Longitude", ylab="Latitude")
world(add=TRUE)
```



Now, we will use `LatticeKrig` to approximate the surfaces in both rectangular and spherical geometries, and print out the root mean square error of all four models.

```
par(mfrow = c(2,2))

rectEqInfo <- LKrigSetup(equatorLocations, nlevel = 2, NC = 13,
                         NC.buffer = 2, alpha = c(0.8, 0.2), a.wght = 4.01)
rectEqFit <- LatticeKrig(equatorLocations, equatorValues,
                         LKinfo = rectEqInfo)

rectPoleInfo <- LKrigSetup(polarLocations, nlevel = 2, NC = 13,
                           NC.buffer = 2, alpha = c(0.8, 0.2), a.wght = 4.01)
rectPoleFit <- LatticeKrig(polarLocations, polarValues, LKinfo = rectPoleInfo)


sphereEqInfo <- LKrigSetup(equatorLocations, nlevel = 2, startingLevel = 6,
                    alpha = c(0.8, 0.2), a.wght = 1.01, LKGeometry = "LKSphere")
sphereEqFit <- LatticeKrig(equatorLocations, equatorValues, LKinfo = sphereEqInfo)


spherePoleInfo <- LKrigSetup(polarLocations, nlevel = 2, startingLevel = 6,
                    alpha = c(0.8, 0.2), a.wght = 1.01, LKGeometry = "LKSphere")
spherePoleFit <- LatticeKrig(polarLocations, polarValues, LKinfo = spherePoleInfo)



surface(rectEqFit, main="Equator Surface Prediction \nUsing Rectangular Kriging",
        xlab="Longitude", ylab="Latitude")

surface(rectPoleFit, main="Polar Surface Prediction \nUsing Rectangular Kriging",
        xlab="Longitude", ylab="Latitude")

surface(sphereEqFit, main="Equator Surface Prediction \nUsing Spherical Kriging",
        xlab="Longitude", ylab="Latitude")

surface(spherePoleFit, main="Polar Surface Prediction \nUsing Spherical Kriging",
```

```
        xlab="Longitude", ylab="Latitude")
```



As we can see, the rectangular model fails badly on the data that has been rotated up to the north pole, while the spherical model matches it nicely. At the equator, the two model are nearly indistinguishable.

5 Using Sparse Matrices

LatticeKrig, along with other statistical models for large spatial data sets, make use of sparse linear algebra for efficient computation. Sparse matrices are generated in the LK model in two ways. The basis functions have compact support, meaning they are 0 outside a fixed region, so many of the entries in the basis function matrix will be 0. The precision matrix for the coefficients is also constructed to be sparse.

Computing with sparse matrices can be much faster than the equivalent dense matrices, since one can save memory by only keeping track of the indices and values of the nonzero entries, and algorithms can skip all of the 0 entries. This optimization makes sparse matrix computations on large data sets orders of magnitude faster than the traditional corresponding computations.

In this package, we use the `spam` package for sparse matrices. This package has built-in methods for storing, multiplying, and solving sparse matrices, as well as finding their Cholesky decomposition, all of which are used heavily in LatticeKrig. The Cholesky decomposition of a matrix A finds the lower triangular matrix L such that $LL^T = A$. This is heavily used in LatticeKrig because it is significantly easier to solve a triangular system than a normal system ($\mathcal{O}(n^2)$ v.s. $\mathcal{O}(n^3)$), which combines with the optimization of using sparse matrices to make our calculations practical on very large data sets.

5.1 Timing sparse v.s. dense matrices

To demonstrate the difference sparse matrices can make, we will time how long it takes to compute the Cholesky decomposition with and without taking advantage of the sparsity. We will consider 100×100, 300×300, 1000×1000, and 3000×3000 matrices. For each size, we will first do the Cholesky decomposition on the full matrix representation, then on the sparse representation. Recall that even though many of the matrix entries are 0, the decomposition doesn't take advantage of this feature unless we use the sparse formatting.

```
for(N in c(100, 300, 1000, 3000)) {
  FMat <- LKDiag(c(-1, 5, -1), N)
  SMat <- as.spam(FMat)
  cat("Matrix size: ", N, "\n")
  cat("Full Matrix:\t\t")
  startTime <- Sys.time()
  FChol <- chol(FMat)
  stopTime <- Sys.time()
  delta <- stopTime - startTime
  print(delta)

  cat("Sparse Matrix:\t")
  startTime <- Sys.time()
  SChol <- chol(SMat)
  stopTime <- Sys.time()
  delta <- stopTime - startTime
  print(delta)
  cat("\n")
}
```

```
## Matrix size:  100
## Full Matrix:     Time difference of 0.0009949207 secs
## Sparse Matrix:   Time difference of 0.0009958744 secs
##
## Matrix size:  300
## Full Matrix:     Time difference of 0.002991199 secs
## Sparse Matrix:   Time difference of 0.001995802 secs
```

```
##
## Matrix size:  1000
## Full Matrix:     Time difference of 0.1466072 secs
## Sparse Matrix:   Time difference of 0.0009977818 secs
##
## Matrix size:  3000
## Full Matrix:     Time difference of 4.112037 secs
## Sparse Matrix:   Time difference of 0.0009939671 secs
```

As you can see from the output above, with sizable inputs the sparse matrix computation is thousands of times faster than the traditional dense matrix computation, and this advantage grows even faster with larger inputs.

6 LatticeKrig Implementation Details

This package is designed to be modular and separate the steps of computation, prediction and simulation. It also uses R's function overloading with S3 and S4 objects to simplify the coding. This strategy is especially helpful for different geometries and distance functions. Finally, the use of sparse matrix methods is also implemented as S4 methods through the spam package so much of the linear algebra uses the standard R matrix multiplication operator `%*%` even through sparse computations are being done behind the scenes.

Despite this complexity it is important to keep in mind the computation and statistical results are just the usual ones associated with Kriging and maximum likelihood associated with a Gaussian spatial process model. The difference is that the spatial process is specified in a way that is suited to generating sparse matrices for the computations. Also, overloading function calls makes the code handling different geometries easier to read and write, as demonstrated below.

6.1 An example of classes and methods

To fix some concepts we give a simple illustration of overloading a function using S3 methods. The (trival) operation is to find an equally spaced grid based on some ranges and a spacing delta and we would like this for 1D and 2D. First we define the method `makeGrid` for the two classes: `1D` and `2D`.

```
makeGrid <- function(gridInfo, ...) {
    UseMethod("makeGrid")
}

makeGrid.1DGrid <- function(gridInfo,...) {
  out<- list(x= seq(gridInfo$min, gridInfo$max, gridInfo$delta))
  return(out)
}

makeGrid.2DGrid <- function(gridInfo,...) {
  out<- list(x = seq(gridInfo$minX, gridInfo$maxX, gridInfo$delta),
             y = seq(gridInfo$minY, gridInfo$maxY, gridInfo$delta))
  return(out)
}
```

The first function is a template that is used for dispaching and the two following functions actually handle the two cases. Now to use these we create some objects and just call `makeGrid`. Notice that even though we call the `makeGrid` function both times, the outputs are completely different based on the class of each input.

```
test1 <- list(min=0.0, max=1.0, delta=.2)
class(test1) <- "1DGrid"
out1 <- makeGrid(test1)
print(out1)
```

```
## $x
## [1] 0.0 0.2 0.4 0.6 0.8 1.0
```

```
test2 <- list(minX=0.0, maxX=1.0,
              minY=0.0, maxY=2.0, delta=.2)
class(test2) <- "2DGrid"
out2 <- makeGrid(test2)
print(out2)
```

```
## $x
## [1] 0.0 0.2 0.4 0.6 0.8 1.0
##
```

```
## $y
##  [1] 0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
```

The analogy in the LatticeKrig coding is that there are several generic steps in defining the spatial model that benefit from using a method without haing to add many different cases in the top level functions based on geometry. In this example one could just have a line such as `out <- makeGrid( gridInfo)` and the class of `gridInfo` would direct which function is called.

6.2 LKinfo object

The model computation is controlled by the `LKinfo` object. This is a list of class `LKinfo` that has all the information needed to specify the spatial model. One could build this list directly including all the necessary information although is it is easier to use the function `LKrigSetup` to make sure all the details are filled in correctly. This function will also make some checks on the passed arguments and will fill in some with defaults if not specified. This package provides a print method for this object class and that creates the summary of the model when this object is printed. Printing this object as a raw list would usually be a big mess of output and not very helpful! See the source code for `print.LKinfo` to see how this is done and where different components are located in the object. The `LKinfo` object also has a second class that is the geometry. This controls how other components in this object are filled in. In particular the component `LatticeInfo` will change, reflecting different lattices based on different geometries. See `help(LKGeometry)` for more details on what needs to done for a given geometry.

As a specific example here is how these steps fill in the lattice information for the LKInterval geometry, the 1-D model.

In `LKrigSetup` is the code

```
LKinfo$latticeInfo <- do.call("LKrigSetupLattice", c(list(object = LKinfo,
        verbose = verbose), setupArgs))
```

The LKinfo object in this case has already been given the class "LKInterval" and so the call to `LKrigSetupLattice` branches to the actual function `LKrigSetupLattice.LKInterval`. The interested reader may want to list out this short function to see the details of this lowest code level.

Although all the details of this function are not important for this illustration, there are several key features. First, all the information for constructing the lattice comes from components of LKinfo. Here `NC`, the number of initial lattce points in the spatial interval, is used to determine the grid spacing and a `for` loop is used to fill in the lattice points at each resolution level, if there is more than one level specified. Finally, all the resulting parts describing the lattice are combined as a list: this object becomes the component `latticeInfo` in the `LKinfo` object. These top level components are consistent across the different geometries and so it makes it possible to have a single summary/print method for the `LKinfo` object.

6.3 LKrig function

The basic computation where the basis coefficients are estimated based on locations and data is done in `LKrig`. These steps track the explicit linear algebra in Section 11.1 and as coded, hide the details from different models. As mentioned earlier, `LKrig` is the function that runs all the logic to compute the kriging fit: * creating the covariate matrix, basis function matrix, and precision matrix; * running a series of intermediate calculations; * calculating the estimates for $\mathbf{c}$ and $\mathbf{d}$; * using those coefficients to calculate the fitted values and residuals; * calling a function that estimates the likelihood of the calculated fit; * estimating the effective degrees of freedom in the fitted surface. Essentially the `LKinfo` object is the reference for what needs to be done. And the coding at this level does not have explicit branches to different geometries.

For example the line

```
Q <- LKrig.precision(LKinfo)
```

Creates the correct precision matrix for the basis function coefficients by using the information from `LKinfo`.

This line in `LKrig`

```
G <- t(wX) %*% wX + LKinfo$lambda * (Q)
```

assembles the G matrix (a key part of the intermediate calculations mentioned earlier) from the precision matrix, the value of `lambda` and the weighted basis function matrix. Although these matrices are in sparse format, note that the `%*%` operator is used because the spam package has provided methods for addition and multiplication using the typical operators. Creating the different components of the model in LatticeKrig is also an example of overloading where the class is the value of LKgeometry.

One advantage of this structure is that new features can be added to the LatticeKrig models without having to change the basic `LKrig` function and its computational steps. It also results in many key steps only happening one place. For example, the Cholesky decomposition of the G matrix created above is done only in one place in this package. Moreover, the subsequent steps of finding the basis coefficients (`LKrig.coef`), computing the predicted values, evaluating the likelihood (`LKrig.lnPlike`), and finding the approximate model degrees of freedom (`LKrig.traceA`) are the same for any model. That is, they are unique functions that work for any geometry or configuration of the lattice and SAR weights. Of course the advantage here is that the code base needs to changed in only one place if any of these basic steps are modified or corrected.

6.4 Estimating covariance parameters.

The function `LKrig` is designed to compute the model fit assuming the parameters `a.wght` and `lambda` are known. With these parameters fixed the likelihood can be maximized in closed form for the remaining parameters, `d`, `sigma` and `rho`. By default these values are used in fitting the model in this function. The component `lnProfileLike` returned in the LKrig object is the log likelihood having maximized over `d`, `sigma` and `rho`.

The parameters `lambda` and `a.wght` are estimated using maxmimum liklihood with built in optimizers in R and the wrapper functions `LKrigFindLambda` for a fixed `a.wght` (using `optim`) and `LKrigFindLambdaAwght` for finding both parameters (using `optimize`). In either case, the likelihood is evaluated by calls from the optimizer to `LKrig`. The search over lambda is done in the log scale and over a.wght in a scale (called omega) that is propotional to the log of the correlation range parameter. For a 2-D rectangle this is log(a.wght - 4)/2. (See Awght2Omega)

One useful feature of the optimization code is that each evalution of the likelihood is saved and these are returned as part of the optimization object. This helps to get an idea of the likelihood surface and determine the reliabilty of the result as a global maximum. See the component `MLE$lnLike.eval` in the LatticeKrig output object. Although one could call the LKrig function over a grid of parameters to explore the likelihood surface in finer detail, often the points of opportunity evaluated by the optimizer are enough to interrogate the surface.

6.5 LatticeKrig

The top level function `LatticeKrig` is an easy way to estimate these model parameters from a minimal specification of the model and then to evaluate using these estimates. It is also convenient to setup the LKinfo object. In particular `LatticeKrig` also makes use of the `LatticeKrigEasyDefaults` method depending on `LKGeometry` and provides flexibility of filling in standard model default choices without continually retyping them.

6.6 Prediction

Model predictions at the data locations are returned in the `fitted.values` component of the `LatticeKrig` and `LKrig` objects. Predictions of the fitted curve or surface at arbitrary locations are found by multiplying the new covariate vectors with the `d.coef` linear model parameters and multiplying the basis functions with the `c.coef` coefficients. It is probably no surprise that creating the basis functions depends on the components of the LKinfo object. But with this structure we have a simple form for making predictions, in keeping with other methods in R. In general if `MyLKinfo` is the model fit using `LKrig` or `LatticeKrig` and `x1` are the locations for evaluating the process, we predict the model at the locations with the line

```
gHat <- predict(MyLKinfo,x1)
```

Here the returned vector has the predictions of the smooth function and the low order polynomial terms (if present) at the locations `x1`.

One complication in this process is the need to evaluate the predictions on a grid of covariates. In the Colorado climate example one may want to predict just the smooth function of climate based on latitude and longitude or add to it the linear model adjustment due to elevation. Moreover, one might want to evaluate these on a grid to make it easier to plot the results on a map. In 2 or more dimensions keeping track of the grids adds a step to this process; refer to the help files and the Quick Start example for more details.

6.7 Simulation

A feature of the LatticeKrig model is that it is efficient to simulate realizations of the process. This operation, called *unconditional simulation*, can be then used to generate conditional simulations (conditioned on the data points) to determine approximate prediction standard errors and quantify the estimate's uncertainty.

The LKinfo object contains all the model attributes needed to simulate a realization of the process. In general if `MyLKinfo` is the model specification and `x1` are the locations for evaluating the process,

```
gSim <- LKrig.sim(x1, LKinfo)
```

simulates the process at the locations and returns the values as a vector in `gSim`. Note that this function is designed to only simulate the random process part of the model. The fixed linear part involving the `Z` covariates is not included.

We note that like the unconditional simulation this code depends on the LKinfo object in MyFit, and applies the estimate computation from `LKrig` and the predict function for an LKrig object. In this way the basic computational alogrithms are reused from the code base and appear only in only one place.

7 Common Error Messages and Frequently Asked Questions

7.1 Could not find function

Make sure that the library is installed (`install.packages("LatticeKrig")`) and loaded (`library(LatticeKrig)`).

7.2 Need to specify NC for grid size

7.3 Invalid 'times' argument

7.4 Only one alpha specifed for multiple levels

7.5 Missing value where TRUE/FALSE needed

All of these errors can be caused by using `LKrig` instead of `LatticeKrig`. The `LatticeKrig` function has ways to either supply defaults or estimate all of the optional parameters that `LKrig` doesn't, so `LKrig` will produce errors like the ones above while `LatticeKrig` will work correctly.

7.6 Non-conformable arguments

This error can occur when using `LKrigSetup` (or `LatticeKrig`, by extension) on a 1-dimensional problem if you don't explicitly set `LKGeometry = "LKInterval"` for `LKrigSetup`. More generally, this problem occurs when trying to multiply matrices with incompatible dimensions.

7.7 Argument is of length zero

This error most commonly occurs when using `LKrigSetup` in one dimension and passing in the range of the data explicitly. For example, `LKrigSetup(c(0,1), ...)` will cause this error (assuming the other arguments are provided correctly). The issue is that the `c` function doesn't format the input as a matrix, which is the format `LKrigSetup` expects. To fix this, just call `as.matrix` on the first parameter you give to `LKrigSetup` - so we would correct the example above to `LKrigSetup(as.matrix(c(0,1)), ...)`.

7.8 Does the order of the parameters matter?

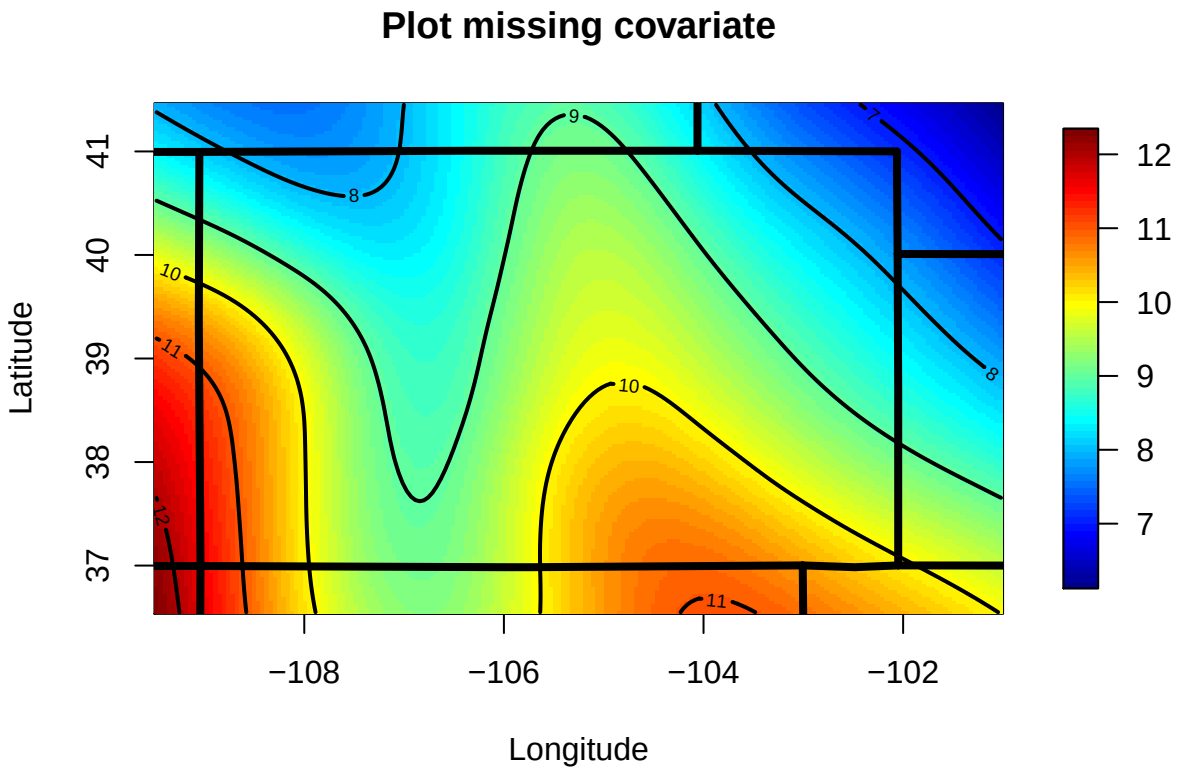
The order of the parameters only matters when you pass them in without specifying their names: for example `LatticeKrig(locations, values)` works, but `LatticeKrig(values, locations)` doesn't. However, if the names are specified, either order will work correctly: both `LatticeKrig(x = locations, y = values)` and `LatticeKrig(y = values, x = locations)` work as intended. The optional parameters can also be listed without their names, but then they would need to be in the correct order and every single one would need to be specified, so it is highly recommended to include the names alongside each optional parameter. For this reason, it is best practice to use the names of the parameters while passing them in, except in cases where it is obvious.

7.9 The predicted values from my Kriging fit are nowhere near the data; what's wrong?

If your model includes covariates (the `Z` parameter of `LatticeKrig` and `LKrig`), your plot may not have included the effect of the covariate. The following code demonstrates this issue using the Colorado temperature

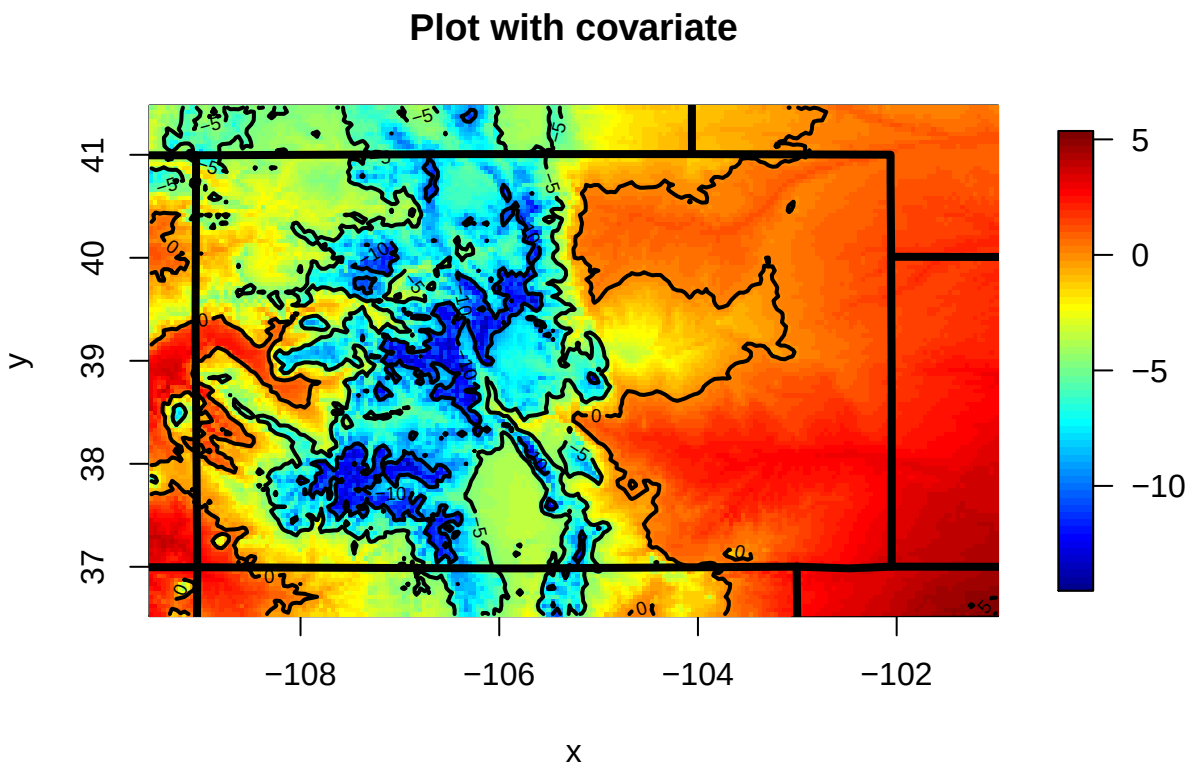
data and kriging fit from the quick start guide, and how to fix the issue. Using the `surface` function will leave out the covariate, resulting in a plot that doesn't match the original data and is smoother than we might expect.

```
surface(kFitWeather, nx = 200, ny = 150, extrap = TRUE, main="Plot missing covariate",
        xlab = "Longitude", ylab="Latitude")
US(add=TRUE, col='black', lwd=4)
```



To fix this, call `surface` on a `predictSurface` object instead of on an `LKrig` object, and make sure to pass in the `grid.list` and `ZGrid` parameters to the `predictSurface` call.

```
prediction <- predictSurface(kFitWeather, grid.list = CO.Grid,
                  ZGrid = CO.elevGrid, nx = 200, ny = 150, extrap = TRUE)
surface(prediction, main="Plot with covariate")
US(add=TRUE, col='black', lwd=4)
```



7.10 Why aren't the settings in my LKrigSetup object being used by the kriging fit?

First, make sure everything is spelled correctly; R variables are case sensitive. For example, `LatticeKrig(x, y, LKInfo = info)` will not work, because the 'i' in "LKinfo" must be lowercase. Next, make sure that every parameter is being set correctly: in particular, don't confuse `x` with `X` or `alpha` with `a.wghts`. Also make sure that parameters that need to be passed as strings are in quotes, e.g. `LKGeometry = "LKSphere", distance.type="GreatCircle"`. If everything is set correctly and spelled correctly, make sure that the list from LKrigSetup is being passed in to your `LatticeKrig` or `LKrig` call.

8 Appendix A: The Linear Algebra of Kriging

Suppose we have a vector $\mathbf{y}$ of observations, where each observation y_i is taken at location $\mathbf{s}_i$ and a covariate vector $\mathbf{X}_i$ containing the coordinates of the locations and possibly other related information. Assuming that the observations are a linear combination of the covariates with a Gaussian process of mean 0, we have

$$y_i = \mathbf{z}_i^T \mathbf{d} + g(\mathbf{s}_i) + \epsilon_i$$

where $\epsilon \sim MN(\mathbf{0}, \sigma^2 I)$ and $g(\mathbf{s})$ is a Gaussian Process with mean zero and covariance function $k(\mathbf{s}, \mathbf{s}')$. The covariance function describes how strongly correlated observations at varying distances are; as such, we would expect that it has a maximum when $\mathbf{s} = \mathbf{s}'$. We can make further assumptions about the covariance function to make computations easier. In LatticeKrig, we assume the covariance function is a Wendland function, which has compact support on $[0, 1]$. This compact support will lead to a sparse Σ, which makes computing with Σ significantly faster and allows us to compute kriging estimates on very large data sets in a reasonable amount of time. Alternatively, in fixed-rank kriging, it is assumed that $\Sigma = S^T K S$, where K is a matrix of fixed size, independent of the number of observations. This form of Σ also makes computations easier, making it another technique for kriging on large data sets.

In LatticeKrig, we assume that $g(\mathbf{s}) = \Phi\mathbf{c} + \epsilon$, where Φ is a matrix of radial basis functions (so ϕ_{ij} is the j^{th} basis function evaluated at the i^{th} point), and $\mathbf{c}$ is the vector of coefficents that scale each basis function. Thus, our total model is $\mathbf{y} = X\mathbf{d} + \Phi\mathbf{c} + \mathbf{e}$. We can't predict measurement error, so instead we focus on predicting $\mathbf{f} = X\mathbf{d} + \Phi\mathbf{c}$ at new locations. The matrix of covariates X and the matrix of basis functions Φ are both determined from the points we choose to predict at: the unknowns we need to estimate are $\mathbf{c}$ and $\mathbf{d}$. We estimate $\mathbf{d}$ by using the generalized least squares estimate: $\mathbf{d} = (X^T\Sigma^{-1}X)^{-1}X^T\Sigma^{-1}$. Estimating $\mathbf{c}$ is more involved. First, we partition X and $\mathbf{y}$ into two parts: the parts corresponding to the known data, X_1 and $\mathbf{y}_1$, and the parts corresponding to the data we want to predict, X_2 and $\mathbf{y}_2$. Since we assume that y follows a Gaussian process, we can write

$$\begin{pmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{pmatrix} \sim N\left(\begin{pmatrix}\mu_1\\ \mu_2\end{pmatrix}, \begin{bmatrix}\Sigma_{11} & \Sigma_{12}\\ \Sigma_{21} & \Sigma_{22}\end{bmatrix}\right).$$

It is known from multivariate probability theory that

$$E[\mathbf{y}_2|\mathbf{y}_1] = \mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1).$$

Where μ_1 and μ_2 are the means of $\mathbf{y}_1$ and $\mathbf{y}_2$, respectively. Since $\epsilon = \Phi\mathbf{c} + \mathbf{e}$ has mean 0, the mean must come from the $X\mathbf{d}$ term: that is, $\mu_1 = X_1\mathbf{d}$ and $\mu_2 = X_2\mathbf{d}$. Since $E[\mathbf{y}_2|\mathbf{y}_1]$ is the best estimator of the values of $\mathbf{y}_2$, we want to find a value of $\mathbf{c}$ that makes our model reproduce this estimator, so we set $E[\mathbf{y}_2|\mathbf{y}_1] = X_2\mathbf{d} + \Phi_2\mathbf{c}$, where Φ_2 is the matrix of all basis functions evaluated at the points where we're trying to predict y. This gives us the equation

$$X_2\mathbf{d} + \Phi_2\mathbf{c} = X_2\mathbf{d} + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1).$$

Now, consider what happens if we make the covariance function and basis function match. Each entry in Σ_{21} is the covariance function of the distance between the j^{th} data point and the i^{th} prediction point, which would be equal to the basis function of the distance between the j^{th} data point and the i^{th} prediction point, which is each entry in Φ_2. This means we can substitute $\Phi_2 = \Sigma_{21}$ into our equation, giving us:

$$\begin{aligned}
X_2\mathbf{d} + \Phi_2\mathbf{c} &= X_2\mathbf{d} + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1)\\
\Phi_2\mathbf{c} &= \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1)\\
\Phi_2\mathbf{c} &= \Phi_2\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1)\\
\mathbf{c} &= \Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1)
\end{aligned}$$

This gives the best coefficient vector if each basis function is centered at a data point. Since our basis functions are instead centered on a lattice, we need $\hat{\mathbf{c}} = P\Phi^T\mathbf{c}$, where P is the covariance matrix for the centers of the basis functions and Φ is the basis function matrix. Thus, our final estimate for $\mathbf{c}$ is $\hat{\mathbf{c}} = P\Phi^T\Sigma_{11}^{-1}(\mathbf{y} - X\mathbf{d})$.

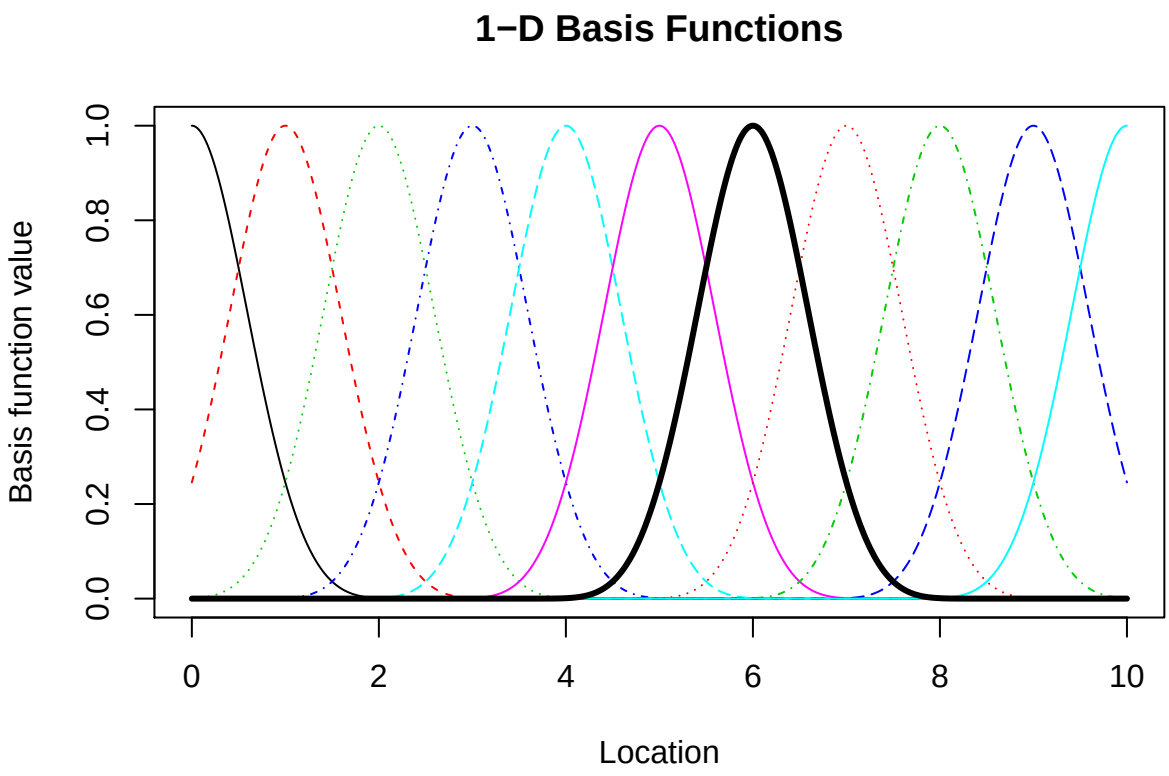
8.1 Sparse Matrix Algorithms

As mentioned earlier, the LatticeKrig package is able to handle large data sets because the covariance function equals 0 for large input. Recall that we make the simplifying assumption that the covariance function is the same as the radial basis function. In LatticeKrig, this function is a Wendland function:

$$\phi(d) = \begin{cases} \frac{1}{3}(1-d)^6(35d^2+18d+3) & 0 \leq d \leq 1 \\ 0 & 1 < d \end{cases}$$

More specifically, a given radial basis function will be 0 at a distance of at least the gap in the lattice multiplied by the parameter `overlap` (which is 2.5 by default). This description is rather opaque, so here is a visualization for the 1-dimensional case.

```
phi <- function(d) {
  return(1/3 * (1-d)^6 * (35*d^2 + 18*d + 3) * (d < 1))
}
overlap <- 2.5
basisCenters <- 0:10
gridPoints <- seq(0, 10, length=1000)
distances <- rdist(gridPoints, basisCenters)
values <- phi(distances / overlap)
matplot(x = gridPoints, values, type="l", xlab="Location",
        ylab = "Basis function value", main="1-D Basis Functions")
lines(values[,7], x=gridPoints, type="l", col="black", lwd=3)
```



We can see that the basis functions all overlap significantly, which is necessary to get a smooth fit. We can see from the highlighted basis function, centered around 6, that the radius of each basis function is 2.5, so the highlighted function is 0 outside of the interval (3.5, 8.5). The graphs appear to reach 0 at a radius of 2

because they go to 0 smoothly, so they don't get far enough from 0 to see the difference near the borders. The basis functions behave similarly in higher dimensions; they are all radially symmetric about their centers.

Since the basis functions and covariance functions are nonzero only on a compact interval, the covariance between many pairs of points will be 0, and equivalently the basis functions will be 0 at many of the points they are evaluated at. This means that the matrices P, Φ, and Σ_{11}^{-1} will all be sparse, which makes the computations much faster. For a further improvement, we can use the Cholesky decomposition of these matrices, which is both triangular and sparse, to speed up calculations even more.

9 Appendix B: Comparison with mKrig function from fields package

In this section we will compare the kriging done in LatticeKrig with ordinary kriging, such as the kriging done in fields. The chief difference is that LatticeKrig assumes a particular covariance function that leads to a sparse precision matrix (the precision matrix is the inverse of the covariance matrix). However, when we do ordinary kriging with this particular covariance function, we will see that the results come out the same for both algorithms, though the ordinary kriging uses dense matrix operations so it takes much longer with large data. To investigate this, we will use `LKrig` (the function that does the computation in `LatticeKrig`) and `mKrig` to compute models for the data. To make sure the parameters match up, we use an `LKinfo` object to store the parameters for the kriging.

After loading in the data, we start by filtering out the NA values in y

```
data(ozone2)
x <- ozone2$lon.lat
y <- ozone2$y[16,]
good <- !is.na(y)
x<- x[good,]
y<- y[good]
lambda <-  1.5
# The covariance "parameters" are all in the list LKinfo
# to create this special list outside of a call to LKrig use
testInfo <- LKrigSetup(x, NC=16, nlevel=1, alpha=1.0, a.wght=5)
obj1 <- LKrig(x, y, lambda=lambda, iseed=122, LKinfo = testInfo)

# this call to mKrig should be identical to the LKrig results
# because it uses the LKrig.cov covariance with all the right parameters.
obj2 <- mKrig(x, y, lambda=lambda, m=2, cov.function="LKrig.cov",
              cov.args=list( LKinfo=testInfo), iseed=122)
```

These two kriging fits produce identical predicted values and standard errors. To make `mKrig` use the same covariance function as `LKrig`, we set the parameter `cov.function="LKrig.cov"`. The `LKrig.cov` function is a top level function that computes the covariance between arbitrary sets of locations according to the model specified by the LKinfo object. Note that `LKrig` uses the (sparse) precision matrix instead of inverting the covariance matrix, which is one of the reasons that `LKrig` is much faster than `mKrig` for large data sets.

10 Appendix C: Sample `LatticeKrig` calculation

The computations inside of `LatticeKrig` and `LKrig` can be hard to understand, so here we will work through several examples showing all of the linear algebra used. Some of the variable names will be changed from the code in the previous section so that they match the names in the linear algebra appendix and in the JCGS article.

10.1 First Example: One level, no normalization

First, we create the data, create the basis/covariance function `basis`, and call `LKrig` to fit the data.

```
lambda = 0.05
overlap = 2.5
psi <- function(d) {
  return(1/3 * (1-d)^6 * (35*d^2 + 18*d + 3) * (d < 1))
}

#clear x and y to make sure our data doesn't get overwritten
rm(x, y)
data(KrigingExampleData)
```

Next, we create an equally spaced lattice of 6 points in [0,1] and add 5 additional points on either side; since we only have 1 level in 1 dimension, this is relatively easy.

```
nc <- 6
ncBuffer <- 5

#finding the spacing for the lattice
delta <- 1/(nc-1)
latInside <- seq(from=0, to=1, by=delta)

#adding the buffer lattice points outside the interval
latBefore <- seq(to=0-delta, by=delta, length.out = ncBuffer)
latAfter <- seq(from=1+delta, by=delta, length.out = ncBuffer)
lattice <- c(latBefore, latInside, latAfter)
m <- length(lattice)
```

Now we create the covariance matrix for $\mathbf{y}$, which is M_λ, and the covariance matrix for the basis functions, which is P.

```
Phi <- psi(rdist(x, lattice) / (overlap*delta))
B <- LKDiag(c(-1, 2.01, -1), m)
Q <- t(B) %*% B
P <- solve(Q)
M <- Phi %*% P %*% t(Phi) + lambda*diag(1, length(x))
Minverse <- solve(M)
```

Finally, we can calculate our estimates for $\mathbf{c}$ and $\mathbf{d}$: `cHat` and `dHat`, respectively.

```
ones <- rep(1, length(x))
Z <- cbind(ones, x)
dHat <- solve(t(Z) %*% Minverse %*% Z, t(Z) %*% Minverse %*% y)
G <- t(Phi)  %*% Phi + lambda*Q
cHat <- solve(G) %*% t(Phi) %*% (y - Z %*% dHat)

info <- LKrigSetup(as.matrix(c(0,1)), NC = 6, NC.buffer = 5, nlevel = 1, a.wght = 2.01,
```

```
                    alpha = 1, lambda = 0.05, normalize = FALSE, LKGeometry = "LKInterval")
krigFit <- LKrig(x, y, LKinfo = info)

#compare kriging prediction with calculated prediction
xGrid <- seq(0,1,length = 200)
krigPredictions <- predict(krigFit, xGrid)
PhiPredict <- psi(rdist(xGrid, lattice) / (overlap*delta))
ZPredict <- cbind(rep(1, length(x)), xGrid)
predictions <- ZPredict %*% dHat + PhiPredict %*% cHat

#making covariance matrix and comparing it to the LKrig one
testCov <- Phi %*% P %*% t(Phi)
targetCov <- LKrig.cov(x, x, info)

test.for.zero(testCov, targetCov)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(dHat, krigFit$d.coef)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(cHat, krigFit$c.coef)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(krigPredictions, predictions)
```

```
## PASSED test at tolerance  1e-08
```

10.2 Second example: One level with normalization

In this example, we normalize `Phi` so that the basis functions have covariance 1 at each data point. This normalization will reduce artifacts in the kriging model that aren't present in the data near the edges of the window. We also print out the diagonal of the covariance matrix, $\Phi P \Phi^T$ - note that it is all ones.

```
D <- Phi %*% P %*% t(Phi)
#discarding the off-diagonal elements of D
DS <- diag(diag(D)^(-1/2))
Phi <- DS %*% Phi
diag(Phi %*% P %*% t(Phi))
```

```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## [36] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

```
#calculating Phi matrix for prediction locations
xGrid <- seq(0,1,length = 200)
PhiPredict <- psi(rdist(xGrid, lattice) / (overlap*delta))
#normalizing PhiPredict too
DPredict <- PhiPredict %*% P %*% t(PhiPredict)
#discarding the off-diagonal elements of D
DPredictS <- diag(diag(DPredict)^(-1/2))
PhiPredict <- DPredictS %*% PhiPredict
```

The rest of the calculations proceed in the same way as the first section without normalization.

```
M <- Phi %*% P %*% t(Phi) + lambda*diag(1, length(x))
Minverse <- solve(M)

Z <- cbind(1, x)
ZPredict <- cbind(1, xGrid)
dHat <- solve(t(Z) %*% Minverse %*% Z, t(Z) %*% Minverse %*% y)
G <- t(Phi)  %*% Phi + lambda*Q
cHat <- solve(G) %*% t(Phi) %*% (y - Z %*% dHat)
predictions <- ZPredict %*% dHat + PhiPredict %*% cHat

info <- LKrigSetup(as.matrix(c(0,1)), NC = 6, NC.buffer = 5, nlevel = 1,
                   a.wght = 2.01, alpha = 1, lambda = 0.05, LKGeometry = "LKInterval")
krigFit <- LKrig(x, y, LKinfo = info)
krigPredictions <- predict(krigFit, xGrid)

#making covariance matrix and comparing it to the LKrig one
testCov <- Phi %*% P %*% t(Phi)
targetCov <- LKrig.cov(x, x, info)

test.for.zero(testCov, targetCov)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(dHat, krigFit$d.coef)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(cHat, krigFit$c.coef)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(krigPredictions, predictions)
```

```
## PASSED test at tolerance  1e-08
```

10.3 Third Example: Three levels, no normalization

The setup in this example is almost the same as in the first one; the only differences are the different random seed and the different values of `nlevel` and `alpha` in the `LKinfo` object. The value of `alpha` is chosen so that each level has half as much weight as the previous and the sum of all the weights is 1.

```
lambda <- 0.05
overlap <- 2.5
```

Making the lattice is now more complicated, since we need to create three different levels. However, note that the first level is the same as before, and the new levels just have lattice points 2x and 4x closer together.

```
nc <- 6
ncBuffer <- 5
delta <- 1 / (nc-1)
L1Inside <- seq(from=0, to=1, by=delta)
L1Before <- seq(to=0-delta, by=delta, length.out = ncBuffer)
L1After <- seq(from=1+delta, by=delta, length.out = ncBuffer)
L1 <- c(L1Before, L1Inside, L1After)

L2Inside <- seq(from=0, to=1, by=delta/2)
```

```
L2Before <- seq(to=0-delta/2, by=delta/2, length.out = ncBuffer)
L2After <- seq(from=1+delta/2, by=delta/2, length.out = ncBuffer)
L2 <- c(L2Before, L2Inside, L2After)

L3Inside <- seq(from=0, to=1, by=delta/4)
L3Before <- seq(to=0-delta/4, by=delta/4, length.out = ncBuffer)
L3After <- seq(from=1+delta/4, by=delta/4, length.out = ncBuffer)
L3 <- c(L3Before, L3Inside, L3After)

s1 <- length(L1)
s2 <- length(L2)
s3 <- length(L3)
c(s1, s2, s3)
```

```
## [1] 16 21 31
```

Note that the values of `s1, s2, s3` don't follow a strict 1:2 ratio as we might expect; this is because of the lattice points outside the region, and because of the boundaries. Specifically, `s1 = 16` because there are `nc = 6` lattice points covering the interval, with 5 gaps between them, and an additional 5 lattice points on each side of the interval. At the second level, the gaps are half as wide, so the 5 gaps become 10; there are now 11 lattice points in the interval and 5 on each side, giving the total `s2 = 21`. Similarly, at the third level the 10 gaps become 20, making 21 lattice points in the interval and 5 on either side, so we have `s3 = 31`.

Now we create the covariance matrix for $\mathbf{y}$, which is M_λ, and the covariance matrix for the basis functions, which is P. Now that we have 3 different lattice sizes, making $Q = P^{-1}$ becomes more difficult, since it's a block-diagonal matrix with a block entry for each different lattice size.

```
alpha <- c(4, 2, 1)/7
Phi1 <- psi(rdist(x, L1) / (overlap*delta)) * sqrt(alpha[1])
Phi2 <- psi(rdist(x, L2) / (overlap*delta/2)) * sqrt(alpha[2])
Phi3 <- psi(rdist(x, L3) / (overlap*delta/4)) * sqrt(alpha[3])
Phi <- cbind(Phi1, Phi2, Phi3)

B1 <- LKDiag(c(-1, 2.01, -1), s1)
B2 <- LKDiag(c(-1, 2.01, -1), s2)
B3 <- LKDiag(c(-1, 2.01, -1), s3)
Q1 <- t(B1) %*% B1
Q2 <- t(B2) %*% B2
Q3 <- t(B3) %*% B3
Q <- matrix(0, nrow = s1+s2+s3, ncol = s1+s2+s3)

#putting Q1, Q2, Q3 into block-diagonal matrix Q
Q[1:s1, 1:s1] <- Q1
Q[(s1+1):(s1+s2), (s1+1):(s1+s2)] <- Q2
Q[(s1+s2+1):(s1+s2+s3), (s1+s2+1):(s1+s2+s3)] <- Q3
P <- solve(Q)
M <- Phi %*% P %*% t(Phi) + lambda*diag(1, length(x))
Minverse <- solve(M)
```

Finding coefficients

```
ones <- rep(1, length(x))
Z <- cbind(ones, x)
dHat <- solve(t(Z) %*% Minverse %*% Z, t(Z) %*% Minverse %*% y)
G <- t(Phi)  %*% Phi + lambda*Q
cHat <- solve(G) %*% t(Phi) %*% (y - Z %*% dHat)
```

```
info <- LKrigSetup(as.matrix(c(0,1)), NC = 6, nlevel = 3, a.wght = 2.01, alpha = c(4,2,1)/7,
                   lambda = 0.05, normalize = FALSE, LKGeometry = "LKInterval")
krigFit <- LKrig(x, y, LKinfo = info)

#making covariance matrix and comparing it to the LKrig one
targetBasis <- spam2full(LKrig.basis(x, info))
test.for.zero(targetBasis, Phi)
```

```
## PASSED test at tolerance  1e-08
```

```
testCov <- Phi %*% P %*% t(Phi)
targetCov <- LKrig.cov(x, x, info)
test.for.zero(testCov, targetCov)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(dHat, krigFit$d.coef)
```

```
## PASSED test at tolerance  1e-08
```

```
test.for.zero(cHat, krigFit$c.coef)
```

```
## PASSED test at tolerance  1e-08
```

```
->
```