LatticeKrig Vignette

Matthew Iverson, Doug Nychka

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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 model is an example of the spatial statistics method known as kriging, adapted to large data sets.

1.1 What is Kriging?

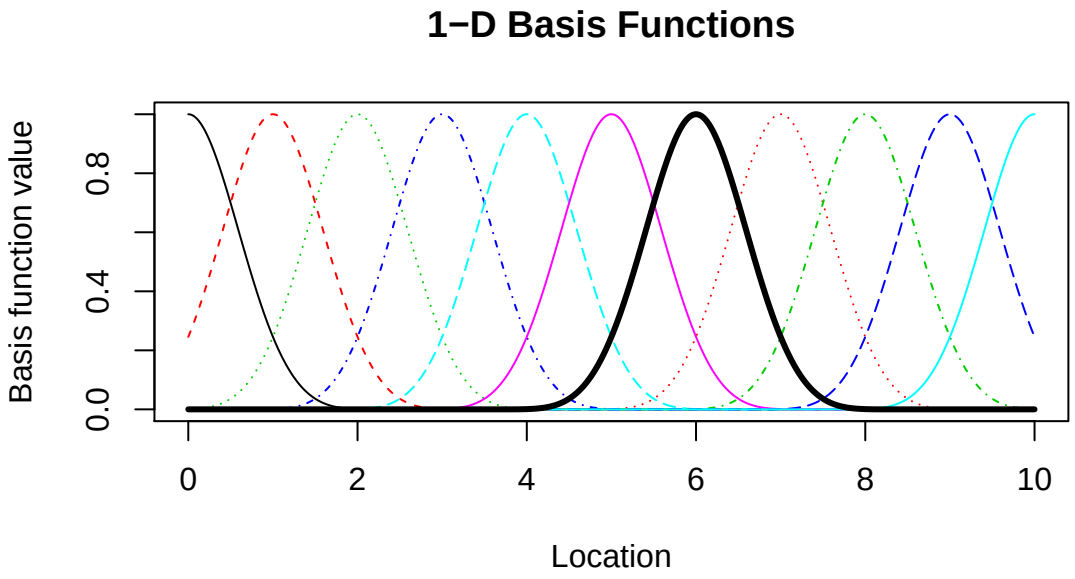
Kriging (named for South African statistician Danie Krige) is a method for making predictions from a spatial data set. A spatial data set means the data contains the observed variable and its location, the variable depends on the location, and pairs of observations taken close together have similar values. 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. In LatticeKrig, we use a linear polynomial for the locations, meaning we start by estimating each data point at location (x, y) with $ax + by + c$, where a, b, and c are constants that don't change between data points.

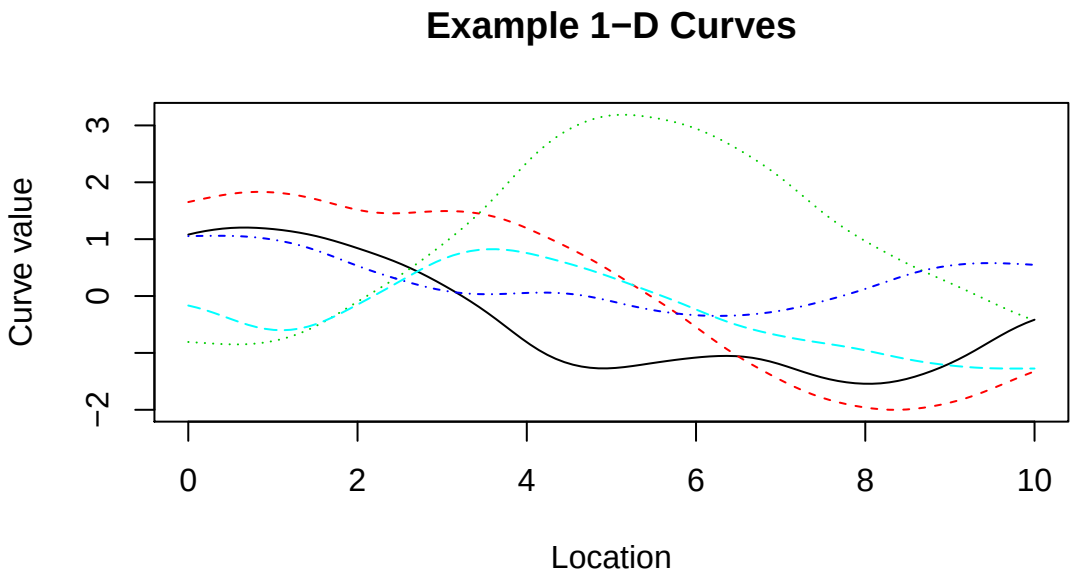
1.2 The LatticeKrig Model

The central method of LatticeKrig is that we model a spatial process as the sum of basis functions scaled by coefficients, which we assume are correlated. The smooth basis functions and correlated coefficients create a smooth function representation for the spatial process. 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, so it will be as close as possible to all of the data. 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 $\mathbf{y} = Z\mathbf{d} + \Phi\mathbf{c} + \mathbf{e}$, where $\mathbf{y}$ is the vector of variable measurements, Z 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. 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; each additional level has half as much space between the basis functions in each dimension. The following plot shows an example of 11 basis functions in the region from 0 to 10, with the one centered around 6 highlighted for emphasis.



The following plot shows some examples of potential curve fits that could be produced from these basis functions, depending on the given data.



1.3 Glossary of Important Functions

- `LatticeKrig`: 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 for a fixed LatticeKrig model. This is the main computational

step in the package.

- `LKrigSetup`: Creates an `LKinfo` object, which is a list to store the parameters to use for a `LatticeKrig` or `LKrig` call; especially useful for examining the effect of changing one parameter on the fit.
- `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 a color plot without contour lines.
- `predictSurface`: Computes the values from a Kriging fit and makes a surface, but doesn't plot it.

2 Quick Start Guide

In this section, we will lay out the bare essentials of the package as a quick overview. 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 is 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 `LKrig` object that contains all the information needed to predict the variable at any location.

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

2.1 Fitting the model in one dimension

```
set.seed(223)
locations <- runif(50, min=-6, max=6)
locations <- as.matrix(locations)
observations <- sin(locations) + rnorm(50, sd = 1e-1)
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 many basis function settings: 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 the defaults, but can be changed with optional parameters.

```
print(kFit1D)
```

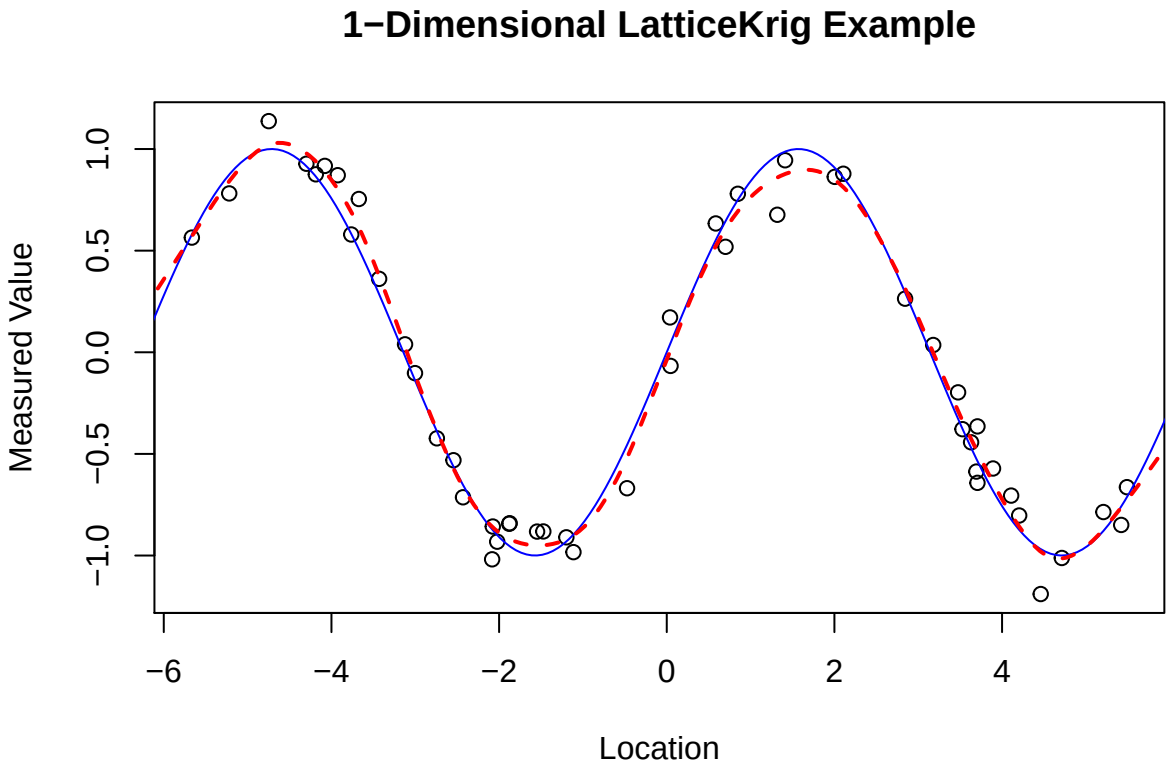
```
## Call:
## LatticeKrig(x = locations, y = observations)
##
##
##  Number of Observations:                      50
##  Number of parameters in the fixed component 2
##   Effective degrees of freedom (EDF)          10.34
##     Standard Error of EDF estimate:           0.9605
##  MLE sigma                                    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
```

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.

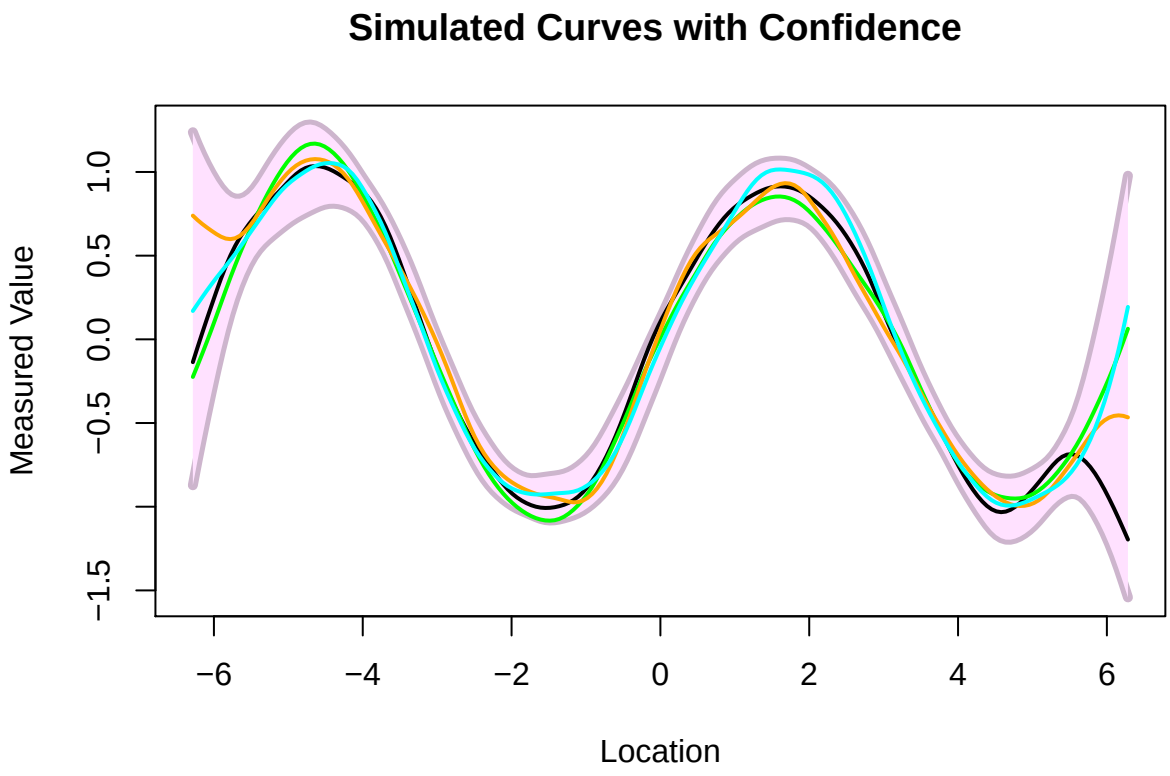
2.3 Inference and Error Analysis

This next plot adds a collection of simulations based on the fitted curve; the simulations get farther apart, meaning the standard error gets larger, where there aren't many data points and especially at the edges of the region. These simulations are easier to compute than the standard error, so they are used to estimate the standard error of a model in LatticeKrig.

```
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
```

```
sdVec <- apply(uncertainty$g.draw, 1, sd)
norm <- (uncertainty$g.draw - as.vector(prediction)) / sdVec
gammas <- apply(abs(norm), 2, max)
gamma <- quantile(gammas, 0.95)
upperBound <- prediction + gamma*sdVec
lowerBound <- prediction - gamma*sdVec
plot(xGrid, upperBound, type="l", ylim = c(min(lowerBound), max(upperBound)),
     main = "Simulated Curves with Confidence ", xlab = "Location", ylab = "Measured Value")
EnvelopePlot(xGrid, lowerBound, xGrid, upperBound)
lines(uncertainty$x.grid, uncertainty$g.draw[,1], lwd = 2)
lines(uncertainty$x.grid, uncertainty$g.draw[,2], lwd = 2, col="green")
lines(uncertainty$x.grid, uncertainty$g.draw[,3], lwd = 2, col="orange")
lines(uncertainty$x.grid, uncertainty$g.draw[,4], lwd = 2, col="cyan")
```



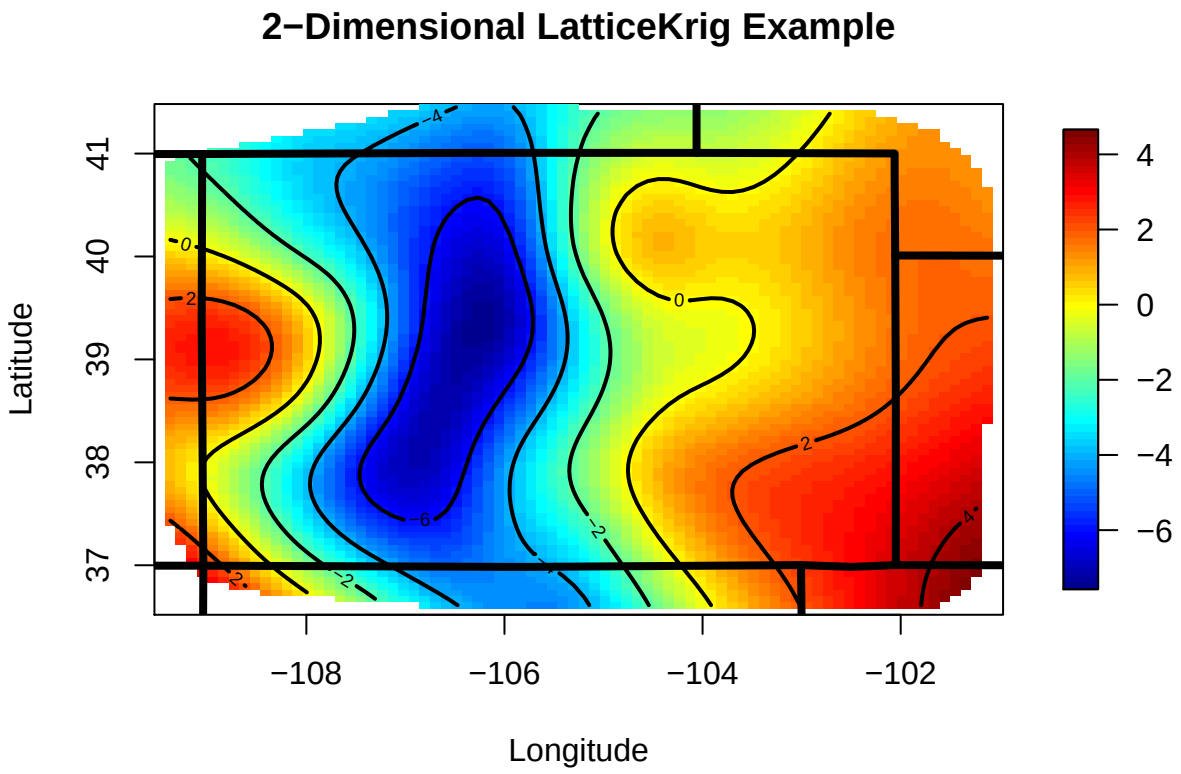
2.4 Fitting the model in two dimensions

For another, more practical example, we will predict the average 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, and use the `US` function to draw in the USA state borders to show where Colorado is. 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
```

```
surface(kFitWeather, main = "2-Dimensional LatticeKrig Example",
        xlab="Longitude", ylab="Latitude")
US(add=TRUE, col='black', lwd=4)
```



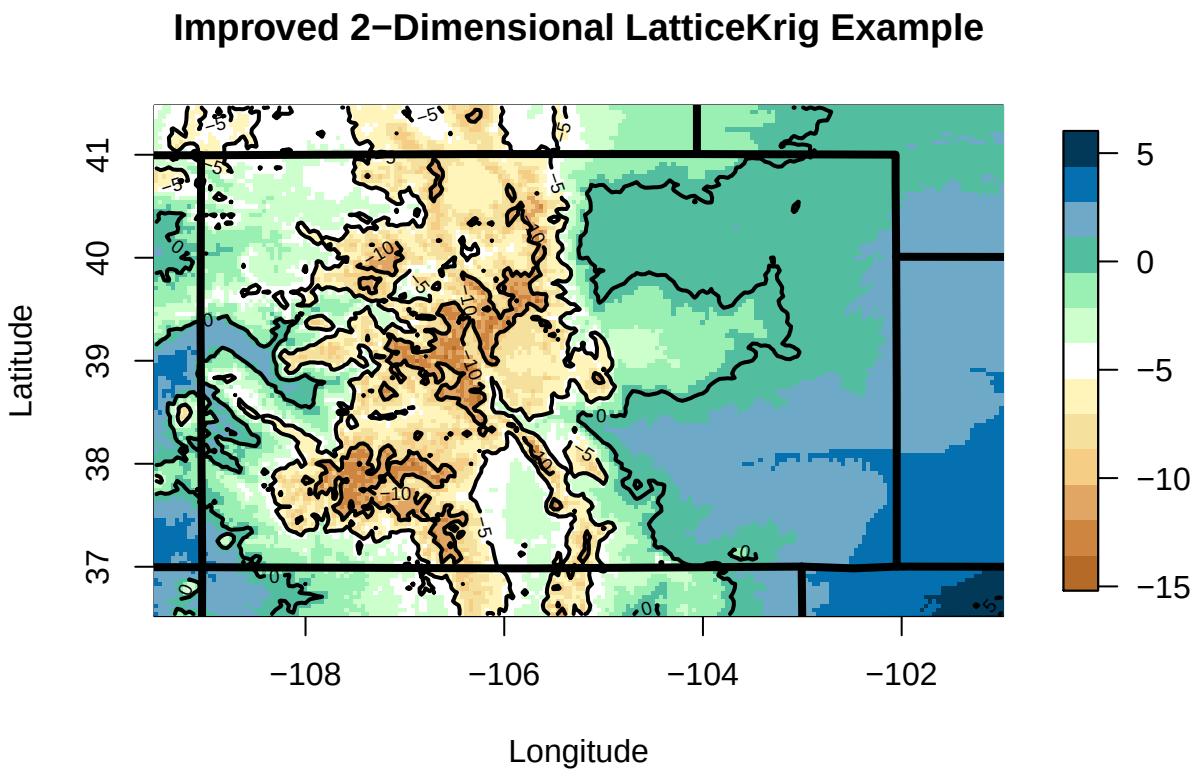
This plot is useful, but we can do better. We can see that the coldest temperatures are in the Rocky Mountains, which is not surprising. Thus, we might expect that we will get a more accurate fit by having `LatticeKrig` account for the elevation at each location as well. Another way we can improve the 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
```

```
# 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 2-Dimensional LatticeKrig Example",
        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. 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 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)

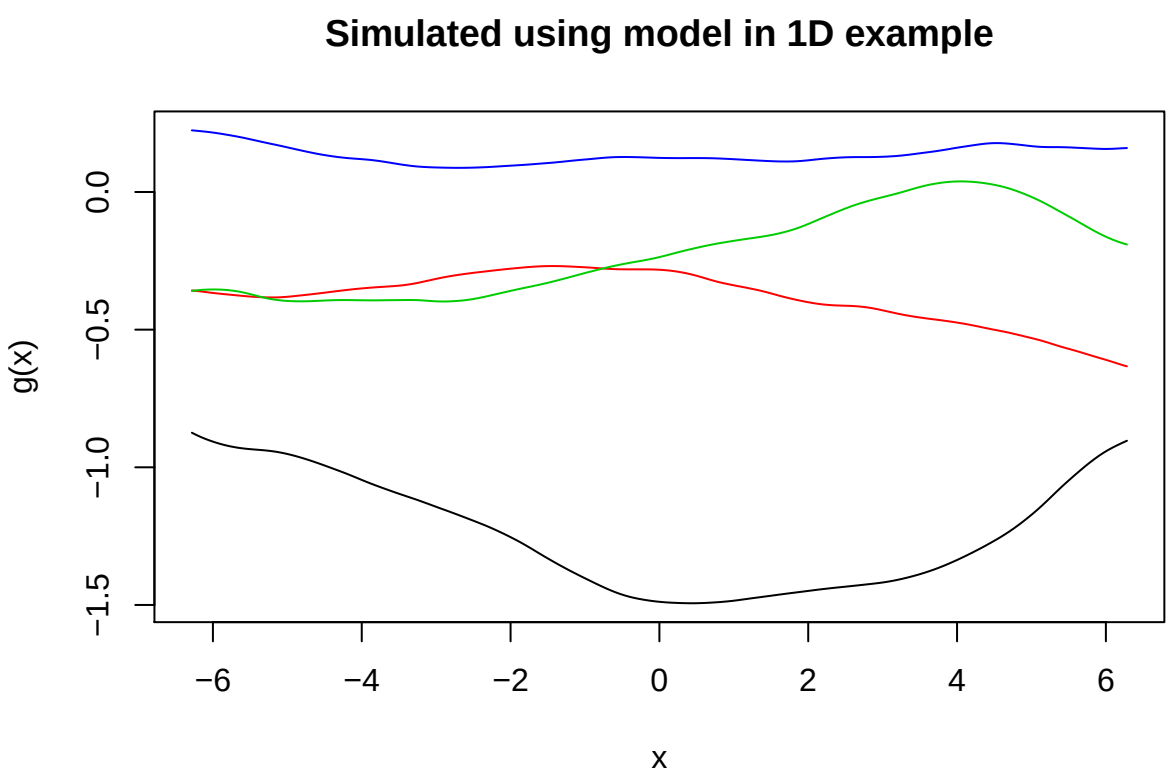
For `kFit1D` from Section 2.1 note that a listing of the full model is shown from.

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

```
## Classes for this object are:  LKinfo LKInterval
## The second class usually will indicate the geometry
##      e.g.  2-d rectangle is  LKRectangle
##
## Some details on spatial autoregression flags:
## stationary:
## first order (by level):
## isotropic:  TRUE
##
## Ranges of locations in raw scale:
## [1] -5.665279  5.489935
##
## Logical (collapseFixedEffect) if fixed effects will be pooled: FALSE
##
## Number of levels: 3
## delta scalings: 1.859202 0.9296012 0.4648006
## with an overlap parameter of  2.5
## alpha:  0.7619048 0.1904762 0.04761905
## based on smoothness nu =  1
##
## a.wght:  2.01 2.01 2.01
##
## Basis  type: Radial using  WendlandFunction  and Euclidean  distance.
## Basis functions will be normalized
##
## Total number of basis functions  75
##  Level Basis size mLevel
##      1         17     17
##      2         23     23
##      3         35     35
##
## Lambda value:  0.0001236536
```

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 using model in 1D example")
```



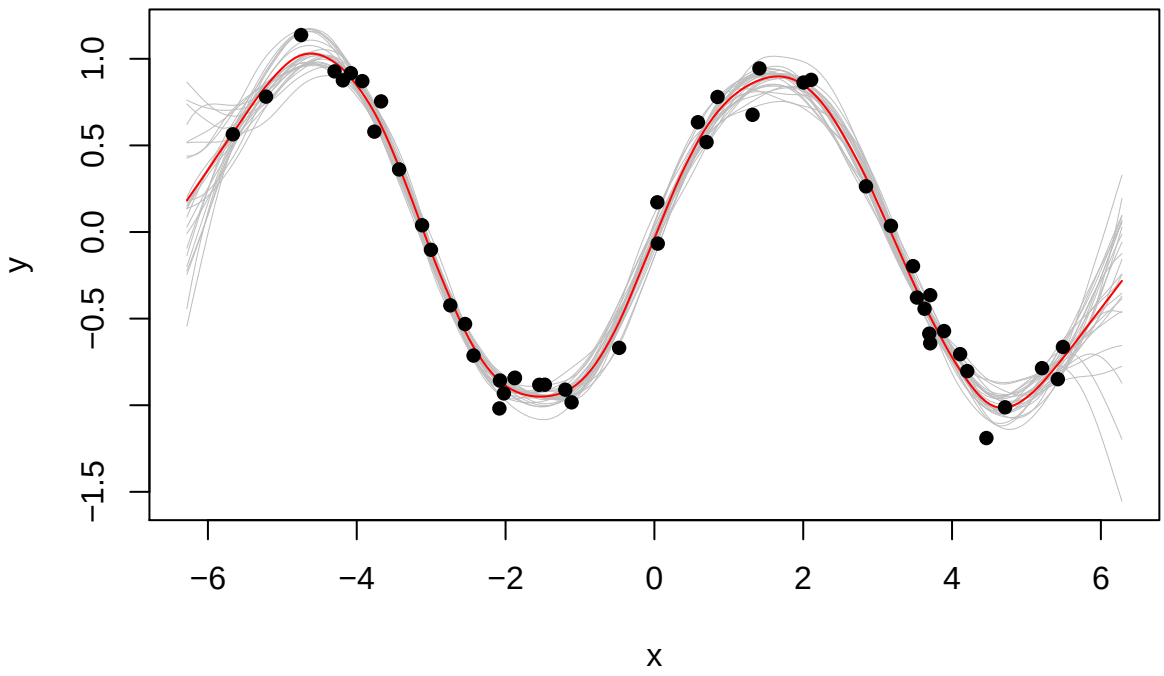
Note that in actually fitting the data a linear function is also included but since this is not a random component it is not part of the simulated process. Also the variance of the process is set to one.

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. The example below creates 25 draws from fitting the 1D example and to highlight the variability in these draws the plot is restricted to just a subset of the range of the data. 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$g.draw, type="l", lty=1, xlab="x", ylab="y",
         col="grey", lwd=.5)
lines(xGrid,predict( kFit1D, xGrid), col="red")
points( kFit1D$x,kFit1D$y, pch=16, col="black")
```



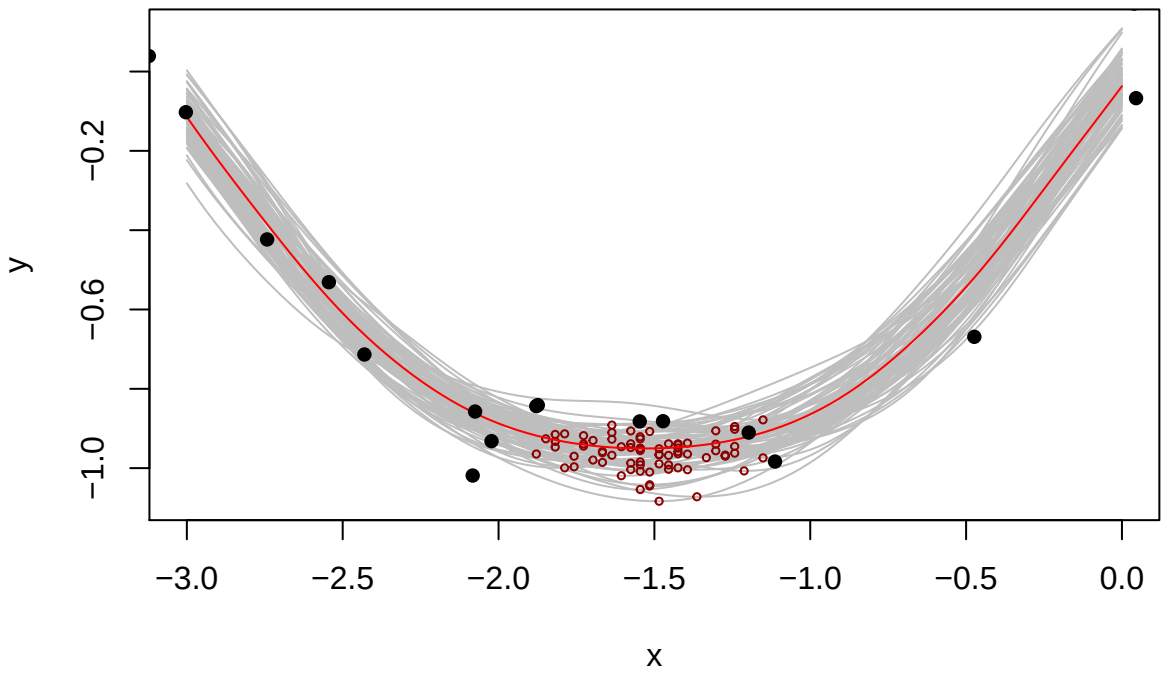
2.6 Extra Credit

Here is a final example illustrating the power of deteriming the unceratinty 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. 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. Moreover, it would be difficult to derive an analytic formula for this distribution.

```
xGrid2<- as.matrix( seq(-3,0,length.out=100) )
set.seed(333)
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")
```


y
−1.0
−0.6
−0.2
−3.0
−2.5
−2.0
−1.5
−1.0
−0.5
0.0
x

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`. For context, this is the printout of the `LKinfo` object created by `LatticeKrig` in the quick start guide's one-dimensional example.

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

```
## Classes for this object are:  LKinfo LKInterval
## The second class usually will indicate the geometry
##      e.g.  2-d rectangle is  LKRectangle
##
## Some details on spatial autoregression flags:
## stationary:
## first order (by level):
## isotropic:  TRUE
##
## Ranges of locations in raw scale:
## [1] -5.665279  5.489935
##
## Logical (collapseFixedEffect) if fixed effects will be pooled: FALSE
##
## Number of levels: 3
## delta scalings: 1.859202 0.9296012 0.4648006
## with an overlap parameter of  2.5
## alpha:  0.7619048 0.1904762 0.04761905
## based on smoothness nu =  1
##
## a.wght:  2.01 2.01 2.01
##
## Basis  type: Radial using  WendlandFunction  and Euclidean  distance.
## Basis functions will be normalized
##
## Total number of basis functions  75
##  Level Basis size mLevel
##      1         17     17
##      2         23     23
##      3         35     35
##
## Lambda value:  0.0001236536
```

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 will be different because there are 5 additional basis functions (this can be changed with the optional `NC.buffer` parameter) added outside the domain on the each end of longest side. For example, if the domain for the data locations is a rectangle whose length is double its width and `NC = 6`, the first level of basis functions will contain 16x13 basis functions (6x3 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 default geometry, the minimum value is two times the number of dimensions, and it is recommended to add a small fraction. 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 measurement error in the data. If not listed, `LatticeKrig` and `LKrig` will estimate it using generalized cross-validation.

- `LKGeometry`

Changing `LKGeometry` allows you to change the geometry used for kriging. 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, you may also need to change the `distance.type`. This is also covered in more depth in the next section.

- `NC.buffer`

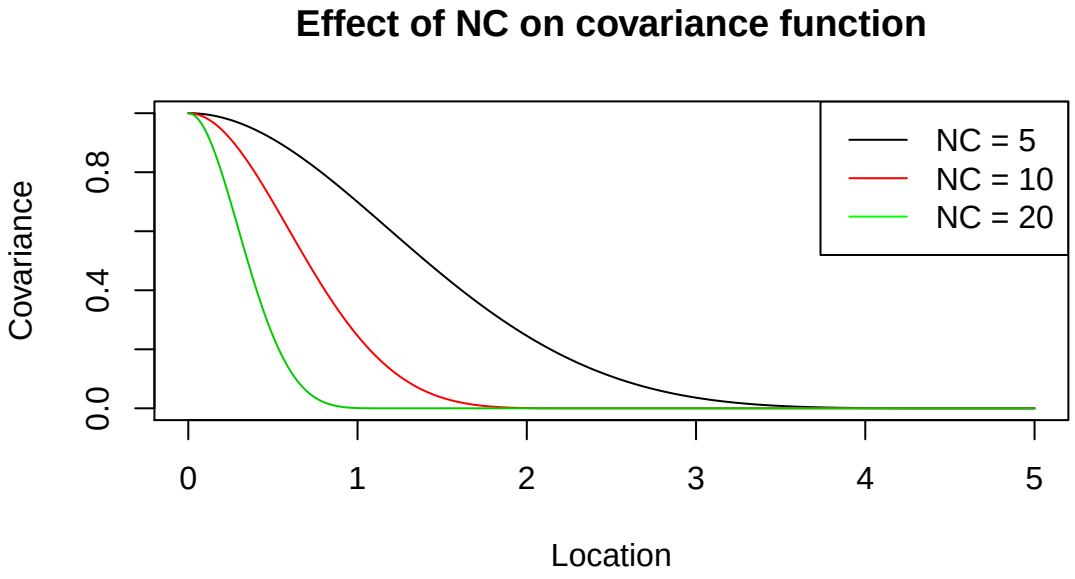
This parameter determines how many lattice points to add outside the range of the data in each direction. The effect of changing this parameter is relatively minor compared to the effect of changing `NC`, and it can only affect the prediction near the edges of the data.

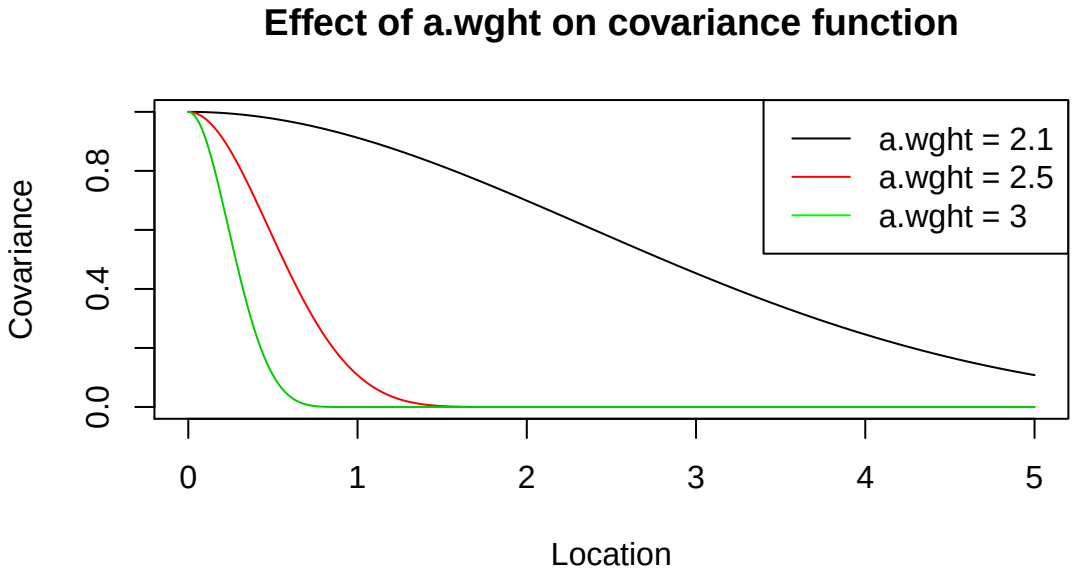
- `normalize`

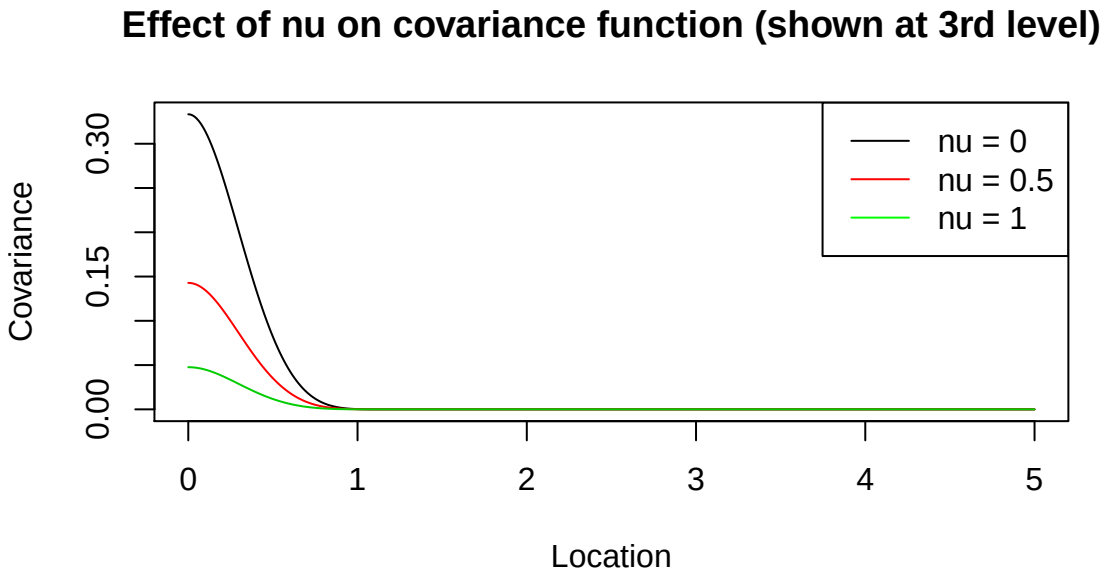
This parameter determines whether or not to normalize the basis functions after computing them, making the variance 1. This is set to `TRUE` by default, sacrificing some computing time to reduce edge artifacts created by the model that aren't present in the real data.

3.3 Effects on 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; recall that the covariance function is radially symmetric in higher dimensions.





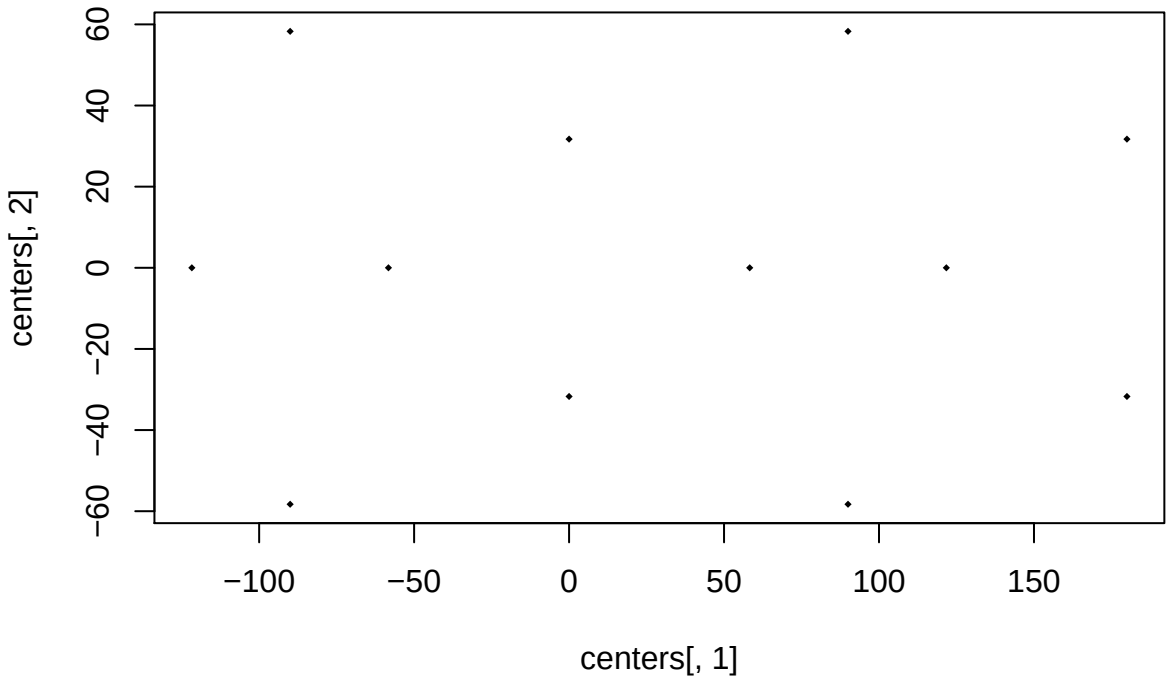

Effect of nu on covariance function (shown at 3rd level)
Covariance
0.00
0.15
0.30
0
1
2
3
4
5
Location
nu = 0
nu = 0.5
nu = 1

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 measurements for other geometries. For instance, this package can work with locations on a sphere, which is useful for locations of latitude and longitude on Earth. 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 dimensions in the given location data. However, if you aren't using `LKRectangle`, 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, which you can set 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 = 1`, where they are at the vertices of an icosohedron inscribed in the sphere; for more information, check the `LKSphere` help page.

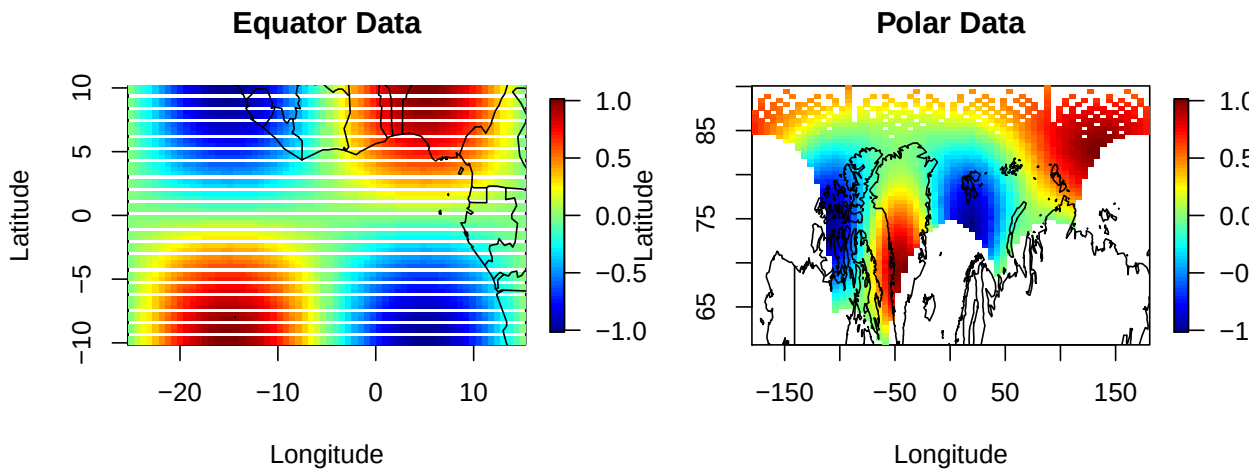


4.1 Working with spherical coordinates

For an example of fitting data taken on the globe using spherical geometry instead of rectangular, we will create some sample data at the equator, rotate it up to 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, 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)
surface(rectEqFit, main="Equator Surface Prediction \nUsing Rectangular Kriging",
        xlab="Longitude", ylab="Latitude")
#world(add=TRUE)
sqrt(sum(rectEqFit$residuals^2) / nrow(equatorLocations))
```

```
## [1] 0.0007707522
```

```
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)
surface(rectPoleFit, main="Polar Surface Prediction \nUsing Rectangular Kriging",
        xlab="Longitude", ylab="Latitude")
#world(add=TRUE)
sqrt(sum(rectPoleFit$residuals^2) / nrow(polarLocations))
```

```
## [1] 0.02332026
```

```
info1 <- LKrigSetup(equatorLocations, nlevel = 2, startingLevel = 6,
                    alpha = c(0.8, 0.2), a.wght = 1.01, LKGeometry = "LKSphere")
sphereEquatorFit <- LatticeKrig(equatorLocations, equatorValues, LKinfo = info1)
surface(sphereEquatorFit, main="Equator Surface Prediction \nUsing Spherical Kriging",
        xlab="Longitude", ylab="Latitude")
#world(add=TRUE)
sqrt(sum(sphereEquatorFit$residuals^2) / nrow(equatorLocations))
```

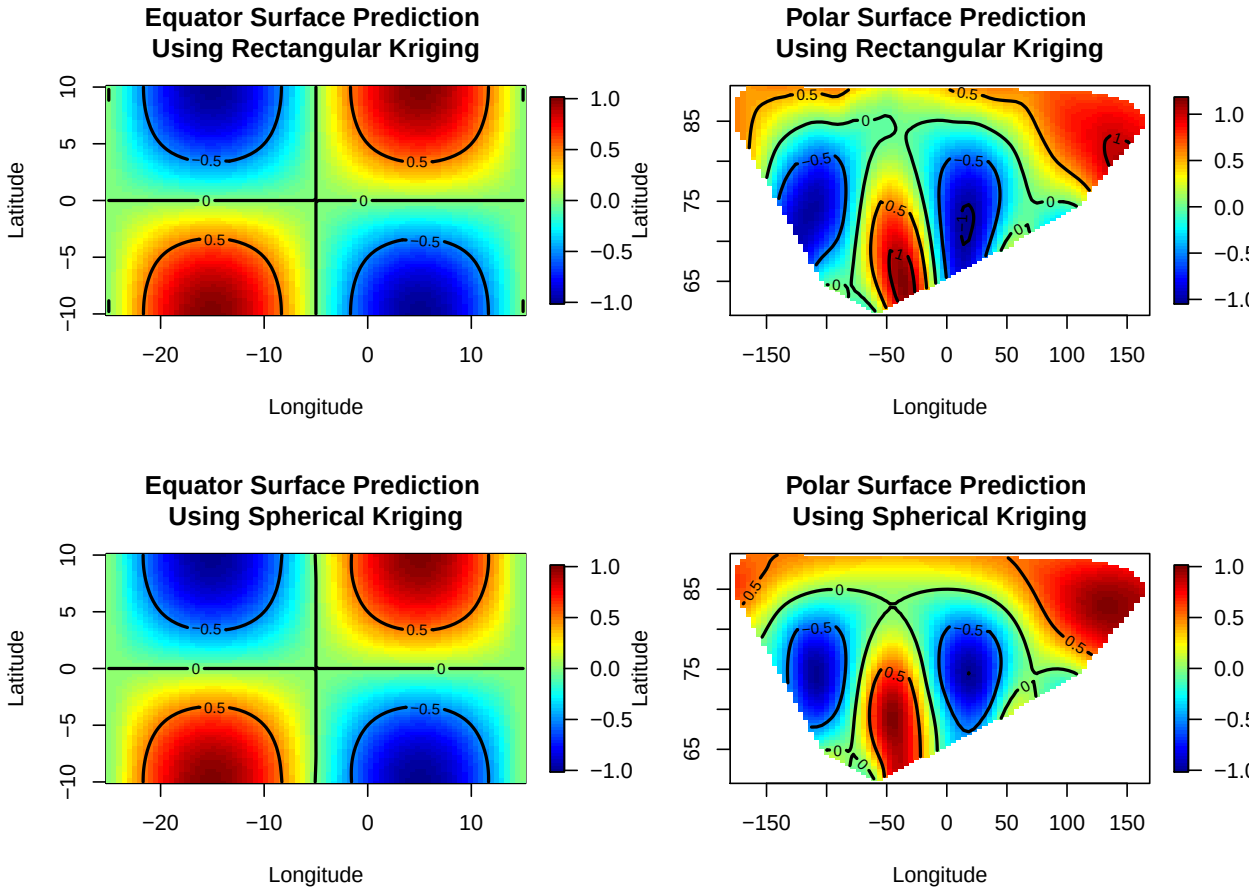
```
## [1] 0.00549062
```

```
info2 <- LKrigSetup(polarLocations, nlevel = 2, startingLevel = 6,
                    alpha = c(0.8, 0.2), a.wght = 1.01, LKGeometry = "LKSphere")
spherePolarFit <- LatticeKrig(polarLocations, polarValues, LKinfo = info2)
```

```
sqrt(sum(spherePolarFit$residuals^2) / nrow(polarLocations))
```

```
## [1] 0.001795302
```

```
surface(spherePolarFit, main="Polar Surface Prediction \nUsing Spherical Kriging",
        xlab="Longitude", ylab="Latitude")
```




```
#world(add=TRUE)
```

As we can see, the rectangular fit fails badly on the data that has been rotated up to the north pole, with approximately 15 times the root mean square error of the corresponding spherical model.

5 Using Sparse Matrices

One unique feature of LatticeKrig is the assumption that the covariance function and basis function have compact support, meaning they equal 0 everywhere outside a certain region. We use radially symmetric basis functions, so the region where the functions have nonzero values is a circle (or sphere in 3D or interval in 1D). This means that many of the pairs of basis functions or data locations will be too far apart to fit in the region, so the covariance between the two points — or the basis function from one point evaluated at the other point, since the basis function and covariance function are the same — will be 0. This leads to covariance matrices and basis matrices where the majority of the entries are 0, which is called a sparse matrix. Computing with sparse matrices can be much faster than the equivalent dense matrices, since the computer can save space by only tracking the location 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.

In the following code, we will time how long it takes to compute the Cholesky decomposition of sparse matrices 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.

```
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")
  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 secs
## Sparse Matrix:   Time difference of 0 secs
##
## Matrix size:  300
## Full Matrix: Time difference of 0.003989935 secs
## Sparse Matrix:   Time difference of 0 secs
##
## Matrix size:  1000
```

```
## Full Matrix: Time difference of 0.148437 secs
## Sparse Matrix:   Time difference of 0 secs
##
## Matrix size:  3000
## Full Matrix: Time difference of 4.233748 secs
## Sparse Matrix:   Time difference of 0.0009968281 secs
```

6 How this package works

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 and so much of 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 the ranges and 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 disptaching and the two following functions actually handle the two cases. Now to use these we create some objects and just call `makeGrid`.

```
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 makes some checks on the passed arguments and will fill in some with defaults if not specified. LatticeKrig provides a print method for this object class and that creates the summary of the model when this object is printed. Printing this 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. 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 what is in the component `LatticeInfo` will change reflecting different lattices based on the 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`

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 for the sequential levels, 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 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: it calls the functions to create the covariate matrix, basis function matrix, and precision matrix; runs a series of intermediate calculations; calls another function that calculates the estimates for $\mathbf{c}$ and $\mathbf{d}$; uses those coefficients to calculate the fitted values and residuals; calls a function that estimates the likelihood of the calculated fit; and finally estimates 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 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 evalatued 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 optimzation 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. One could call the LKrig function over a grid of parameters to explore the likelihood surface, however, 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 models 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 specification 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.

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 a 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 known as 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. The sample covariances of the ensemble will converge to the correct covariance matrix expressing the unceratinty in the estimate. Refer to the Quick Start for an example of the difference between unconditional and conditional simulation.

We note that like the unconditional simulation this code is depends on the LKinfo object in MyFit, 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 Errors

7.1 Could not find function [FunctionName]

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 Error in object$x %*% t(Vinv) : 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`.

7.7 Error in if (ncol(object$x) != 1) { : 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)), ...)`.

8 Frequently Asked Questions

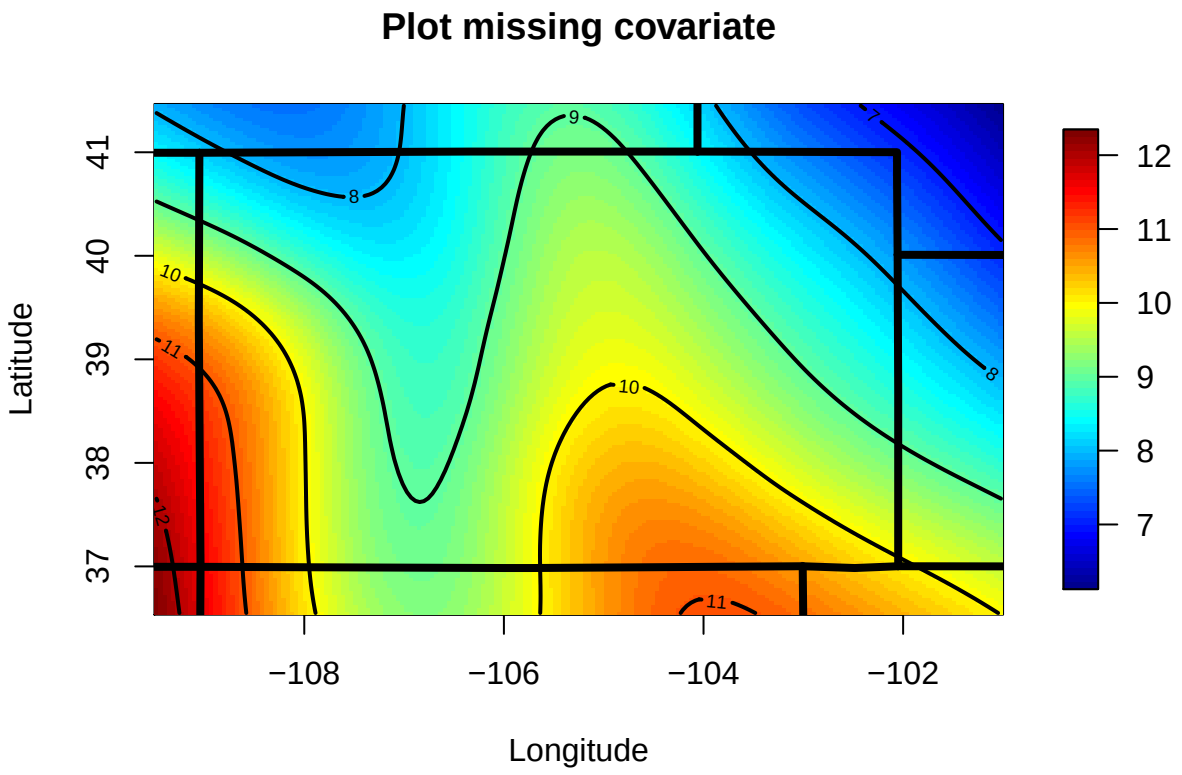
8.1 Does the order of the parameters matter?

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.

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

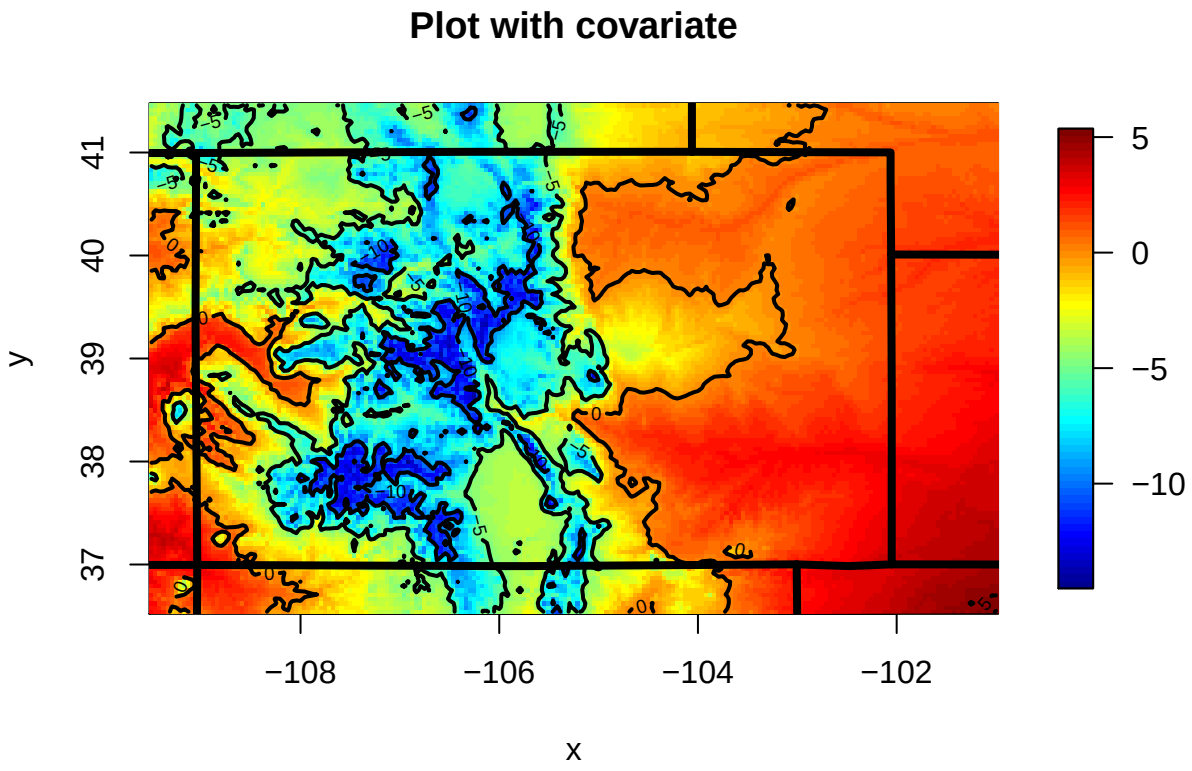
If your model includes covariates (the `Z` parameter of `LatticeKrig` and `LKrig`), your plot may not have included the effect of the covariate. The following code demonstrates this issue using the Colorado temperature data and kriging fit from the quick start guide, and how to fix the issue. Using the `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)
```



8.3 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.

9 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 $\mathbf{Z}_i$ 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 $\mathbf{y} = Z\mathbf{d} + \Phi\mathbf{c} + \mathbf{e}$. We can't predict measurement error, so instead we focus on predicting $\mathbf{f} = Z\mathbf{d} + \Phi\mathbf{c}$ at new locations. The matrix of covariates Z 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: $\mathbf{d} = (Z^T\Sigma^{-1}Z)^{-1}Z^T\Sigma^{-1}$. Estimating $\mathbf{c}$ is more involved. First, we partition Z and $\mathbf{y}$ into two parts: the parts corresponding to the known data, Z_1 and $\mathbf{y}_1$, and the parts corresponding to the data we want to predict, Z_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 $Z\mathbf{d}$ term: that is, $\mu_1 = Z_1\mathbf{d}$ and $\mu_2 = Z_2\mathbf{d}$. 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 $E[\mathbf{y}_2|\mathbf{y}_1] = Z_2\mathbf{d} + \Phi_2\mathbf{c}$, 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

$$Z_2\mathbf{d} + \Phi_2\mathbf{c} = Z_2\mathbf{d} + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1).$$

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:

$$\begin{aligned}
Z_2\mathbf{d} + \Phi_2\mathbf{c} &= Z_2\mathbf{d} + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1) \\
\Phi_2\mathbf{c} &= \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1) \\
\Phi_2\mathbf{c} &= \Phi_2\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1) \\
\mathbf{c} &= \Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1)
\end{aligned}$$

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 $\hat{\mathbf{c}} = P\Phi^T\Sigma_{11}^{-1}(\mathbf{y} - Z\mathbf{d})$.

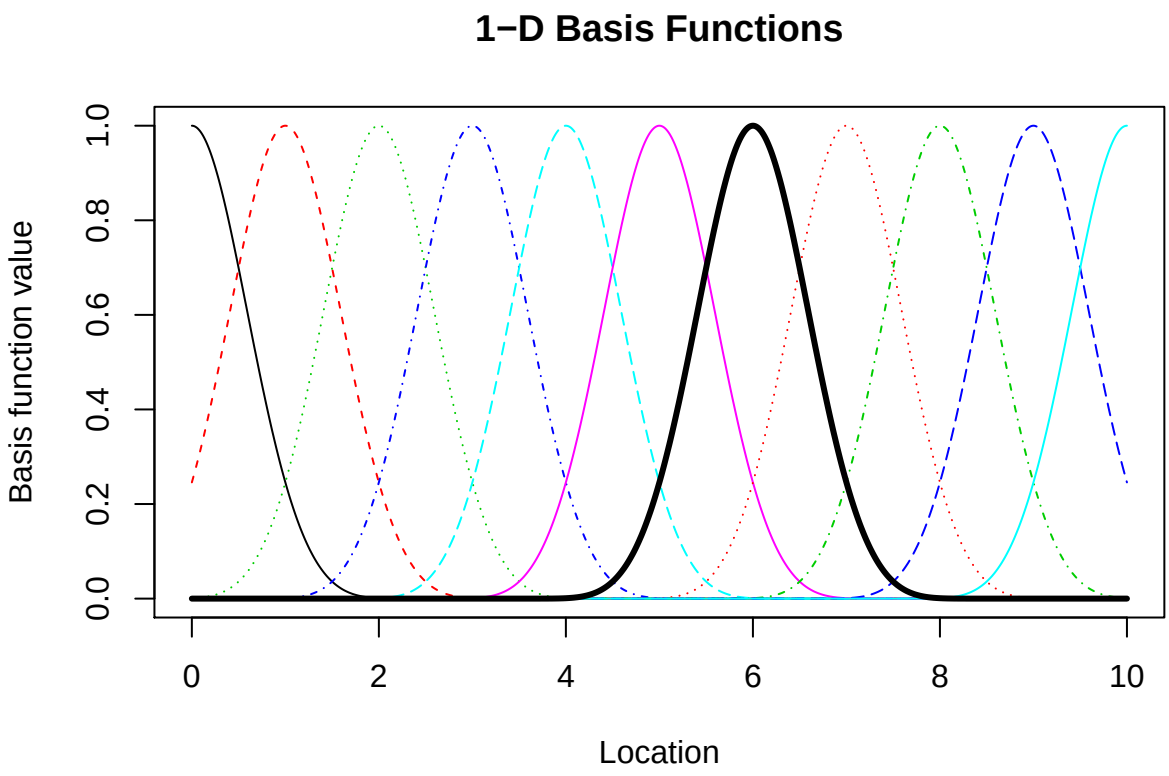
9.1 Sparse Matrix Algorithms

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.

10 Appendix B: Comparison with kriging 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.

11 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.

11.1 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
basis <- 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 <- basis(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, lambd
```

```
krigFit <- LKrig(x, y, LKinfo = info)

#compare kriging prediction with calculated prediction
xGrid <- seq(0,1,length = 200)
krigPredictions <- predict(krigFit, xGrid)
PhiPredict <- basis(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
```

11.2 Second example: One level with normalization

In this example, we normalize `Phi` so that the basis functions have covariance 1 at each data point. 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 <- basis(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, lambd
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
```

11.3 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
basis <- function(d) {
  return(1/3 * (1-d)^6 * (35*d^2 + 18*d + 3) * (d < 1))
}
```

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 <- basis(rdist(x, L1) / (overlap*delta)) * sqrt(alpha[1])
Phi2 <- basis(rdist(x, L2) / (overlap*delta/2)) * sqrt(alpha[2])
Phi3 <- basis(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
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
```

11.4 Using the kriging equations directly

Recall the standard kriging equations for $\hat{\mathbf{c}}$ and $\hat{\mathbf{d}}$ in Appendix A:

$$\hat{\mathbf{d}} = (Z^T\Sigma^{-1}Z)^{-1}Z^T\Sigma^{-1}$$
$$\hat{\mathbf{c}} = P\Phi^T\Sigma_{11}^{-1}(\mathbf{y} - Z\mathbf{d})$$

In this section, we will compute the estimates directly using these equations to show that the computations in LatticeKrig match them. For brevity, we will only consider the case with one level and no normalization; adjustments for more levels and normalization can be made in the same way as in the previous section.

```
data(KrigingExampleData)
info <- LKrigSetup(as.matrix(c(0,1)), NC = 6, NC.buffer = 5, nlevel = 1, a.wght = 3, alpha = 1, lambda =
krigFit <- LKrig(x, y, LKinfo = info)
nc <- 6
ncBuffer <- 5
lambda = 0.05
delta <- 1/(nc-1)
latInside <- seq(from=0, to=1, by=delta)
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)
overlap <- 2.5

cov <- function(d) {
  s <- d/(overlap*delta)
  return(1/3 * (1-d)^6 * (35*d^2 + 18*d + 3) * (d < 1))
}
Sigma <- cov(rdist(x, x)) + lambda*diag(1, length(x))
SigmaInv <- solve(Sigma)
Phi <- cov(rdist(x, lattice))
```

```
P <- cov(rdist(lattice, lattice))
ones <- rep(1, length(x))
Z <- cbind(ones, x)
dHat <- solve(t(Z) %*% SigmaInv %*% Z) %*% t(Z) %*% SigmaInv
cHat <- P %*% t(Phi) %*% SigmaInv %*% (y - Z %*% dHat)
test.for.zero(dHat, krigFit$d.coef)
```

```
## FAILED test value =  110.2513  at tolerance  1e-08
```

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

```
## FAILED test value =  2433.011  at tolerance  1e-08
```