LatticeKrig Vignette

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Contents

1 Introduction

In this vignette, we will briefly explain what kriging is, explore the functions in the LatticeKrig package, and show examples of how they can be used to solve problems.

1.1 What is Kriging?

Kriging (named for South African satistician Danie Krige) is a method for making predictions from a data set. It is designed to be used on spatial data – that is, our data contains the observed variable and the location it was observed at, and pairs of observations taken close together have similar values. As such, it can be applied to a variety of physical data sets, from geological data to atmospheric data.

The goal of kriging is to create a model, based on data from some locations, that can accurately predict the observed variable at any location inside the data given.

1.2 The LatticeKrig Model

In the LatticeKrig package, we model the given data as the sum of a linear polynomial in the locations (and covariates, if provided) and a spatial process with mean 0. We fit the linear polynomial using generalized least squares, so the linear polynomial will be as close as possible to all of the data. To approximate the spatial process, we then fit a collection of radial 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 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.

1.3 Glossary of Important Functions

- `LatticeKrig`: Calls LKrig, passing in default values and estimates for the needed parameters.
- `LKrig`: Fits a kriging estimate to the given data.
- `LKInfo`: Creates an object to store the parameters to use for a `LatticeKrig` / `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

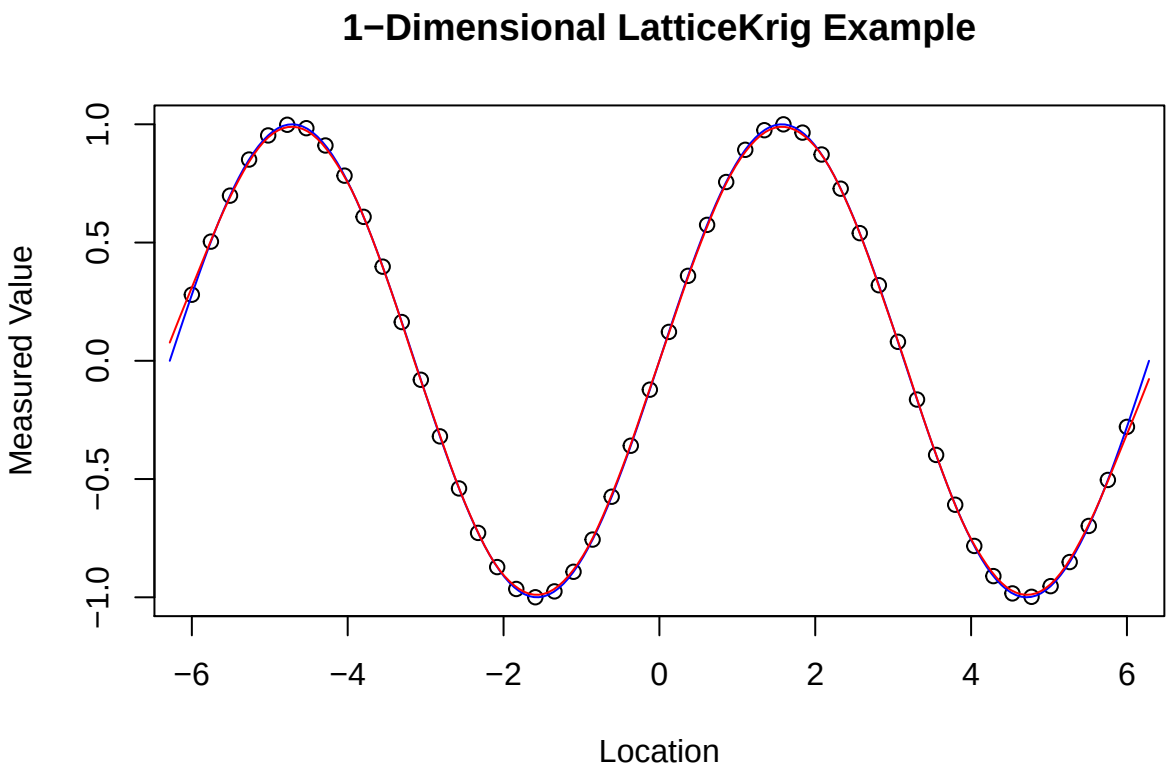
In this section, we will lay out the bare essentials of the package to make the central features as easily accessible as possible. To fit a surface and interpolate data using `LatticeKrig`, the only required arguments are the measurement locations (formatted in a matrix where each row is one location) and measurement values. Calling the `LatticeKrig` function and passing in the locations and values will produce an `LKrig` object that contains all the information needed to calculate the model at any location. For a simple, 1-dimensional example, we will take our locations to be 50 equally spaced points on the interval $[-6, 6]$, and our variable measurements to be the values of $\sin(x)$ at these locations.

```
locations <- seq(-6,6, len=50)
observations <- sin(locations)
kFit <- LatticeKrig(locations, observations)
kFit
```

```
## Call:
## LatticeKrig(x = locations, y = observations)
##
##
##  Number of Observations:                      50
##  Number of parameters in the fixed component 2
##   Effective degrees of freedom (EDF)         13.68
##     Standard Error of EDF estimate:          0.9584
##  MLE sigma                                   0.06153
##  MLE rho                                     30.62
##  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     2.0
##      2             23     1.0
##      3             35     0.5
##
## Nonzero entries in Ridge regression matrix 814
```

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)
plot(locations, observations, main="1-Dimensional LatticeKrig Example",
     xlab="Location", ylab="Measured Value")
lines(xGrid, sin(xGrid), col='blue')
lines(xGrid, predict(kFit, xGrid), col='red')
```

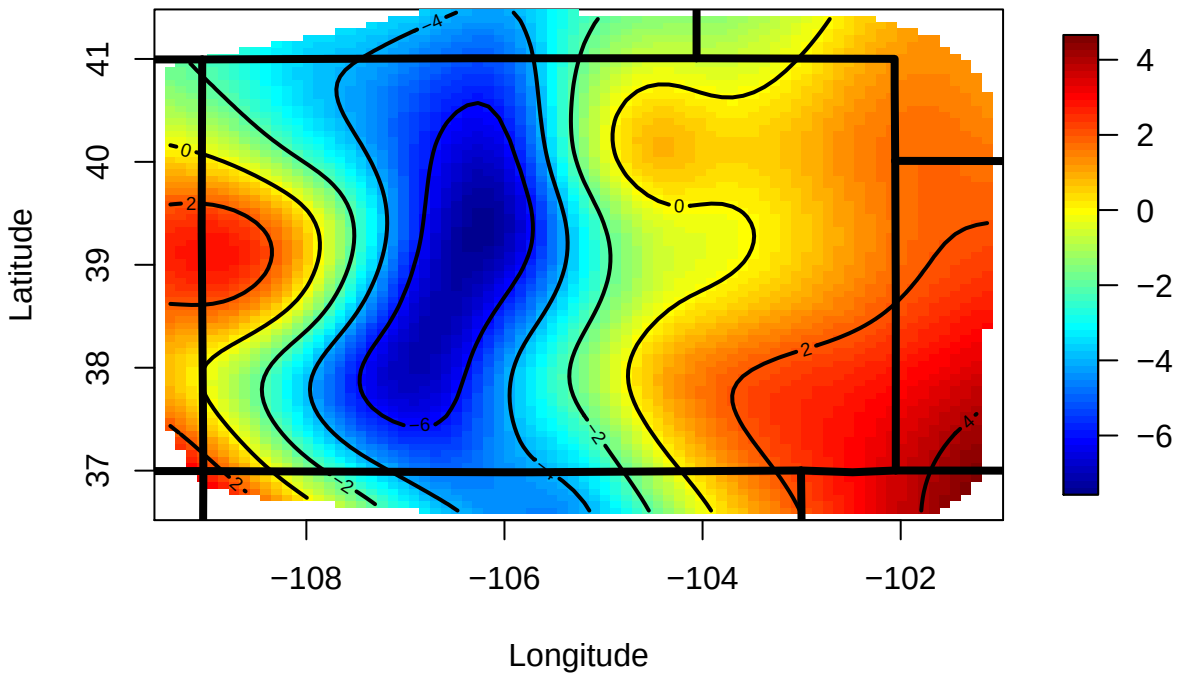


We can see that `LatticeKrig` takes in the data points (shown above in black) and produces a prediction over the whole interval (in red) that matches the true function (in blue) rather closely. For another, more practical example, we will predict the average spring temperature for locations throughout 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.

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

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

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

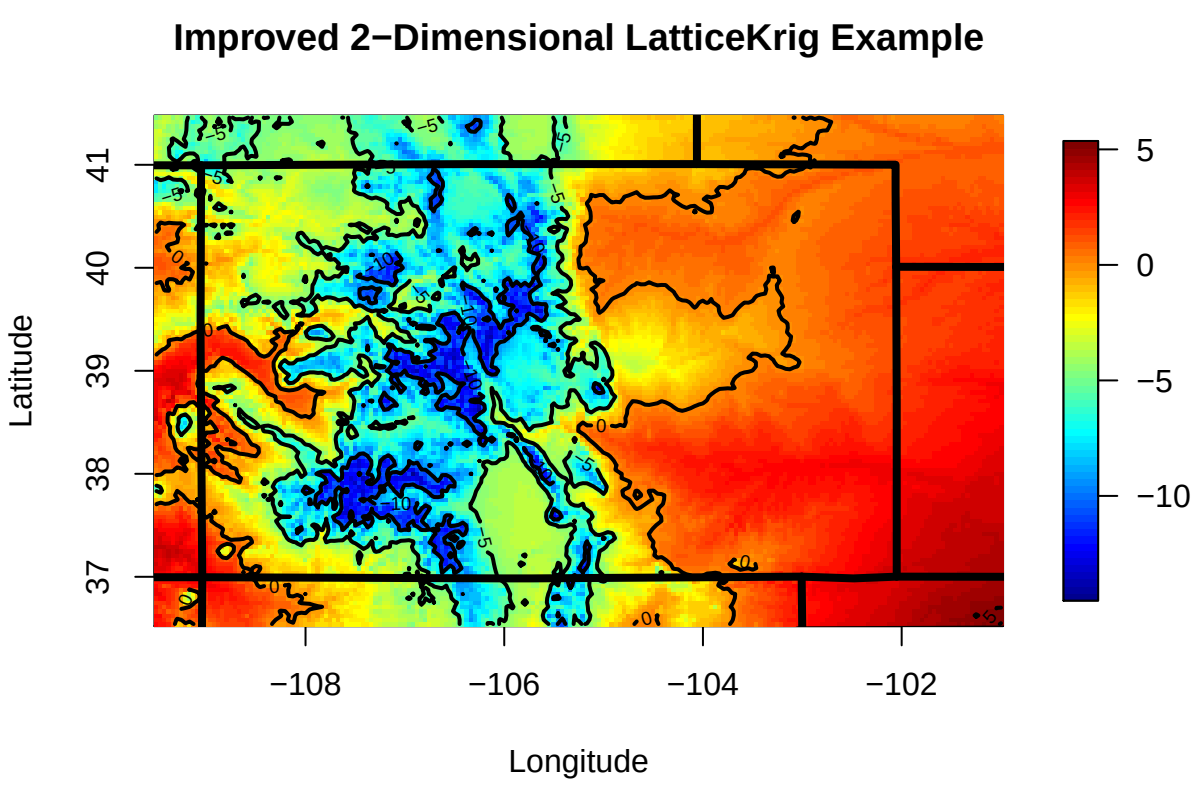


This plot is nice, but we can do better. We can see that the coldest temperatures are in the Rocky Mountains, which is unsurprising. Thus, we might expect that we will get a more accurate fit by having `LatticeKrig` account for the elevation at each location as well. Another way we can improve the plot is by increasing its resolution - the current plot is somewhat pixelated. We can tell the `surface` function to evaluate the surface at more points by using the `nx` and `ny` arguments, which will take longer to compute but produces a nicer looking, more detailed plot. Finally, we can also have `surface` extend the computation 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 `LatticeKrig` fitting method isn't designed to extrapolate and so the expected error increases dramatically when predicting outside of the given data. However, extending the plot to the corners will make it look nicer.

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

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

```
prediction <- predictSurface(kFit, 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")
US(add=TRUE, col='black', lwd=4)
```


Improved 2−Dimensional LatticeKrig Example
Latitude
41
40
39
38
37
−108
−106
−104
−102
Longitude
5
0
−5
−10

3 `LatticeKrig` Optional Arguments

The only required arguments for the `LatticeKrig` function are the set of locations and variable observations. However, `LatticeKrig` also allows for a huge range of optional arguments to tweak the model that `LatticeKrig` uses. 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.

3.1 `Z`

The optional parameter Z is a matrix of covariates (variables aside from location) to include in the model. Each column of this matrix must contain the value of one of the covariates at each data location, so the number of rows in Z must match the number of rows in the required parameter x, the set of locations. For an example, see the last two plots in the Quick Start section.

3.2 `nlevel`

The optional parameter `nlevel` is an integer that determines the number of different lattice sizes to compute the basis function coefficients on. Each different lattice size is computed independently, and the resulting layers are each scaled by the values in the parameter `alpha` (provided in the LKInfo or automatically computed) the before being added together.

3.3 `alpha`

The optional parameter `alpha` is a vector of length `nlevel` holds the weights that scale the basis functions on each different lattice size. Since each level is calculated independently, the sum of the weights in `alpha` should be 1 to make sure the model fits correctly.

3.4 `X`

The optional parameter X (different from the required parameter x) is used for solving linear inverse problems; X is the sparse matrix that transforms the coefficients of the basis to the observations. The optional parameter U must also be specified.

3.5 `U`

The optional parameter U is used for solving linear inverse problems; U is the matrix that transforms the coefficients of the fixed part of the model to the observations.

3.6 `LKinfo`

The optional parameter `LKinfo` holds many other parameter values, expanded on in the next section.

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 on a sphere, interpreting the given locations as latitude and longitude on Earth. There are also other options for non-Euclidean geometries: a cylinder, which uses 3 dimensional cylindrical coordinates, and a ring, which takes 2 dimensional polar coordinates. You can change the geometry used by passing it into the `LKGeometry` parameter of an `LKinfo` object. These are the names that `LKinfo` recognizes:

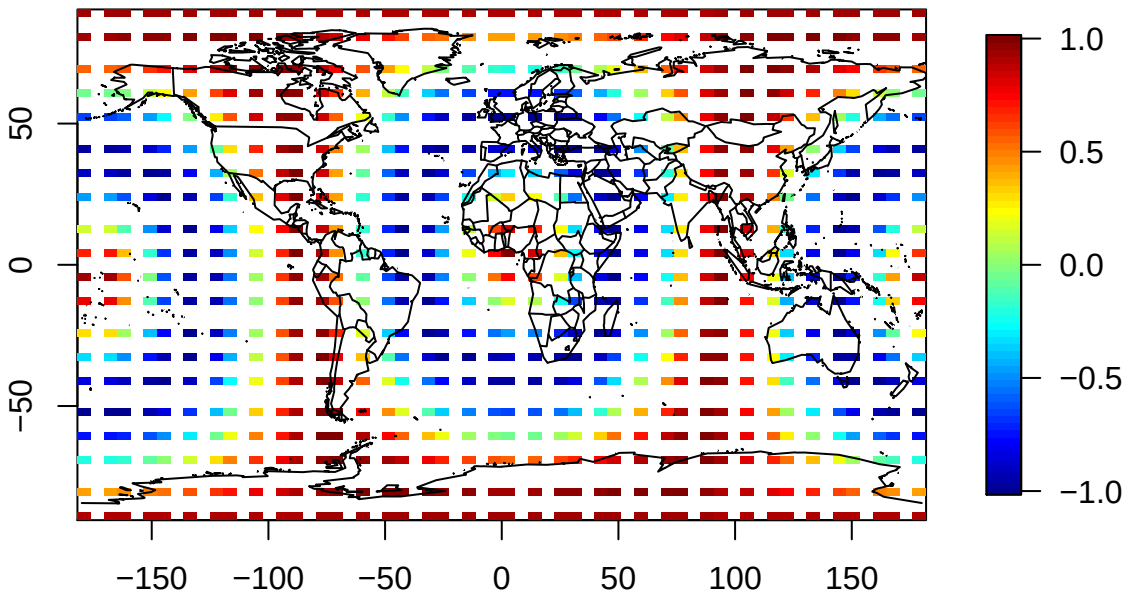
- `LKInterval`: 1 dimensional Euclidean space
- `LKRectangle`: 2 dimensional Euclidean space
- `LKBox`: 3 dimensional Euclidean space
- `LKSphere`: 2 dimensional spherical coordinates (longitude and latitude, with fixed radius)
- `LKCylinder`: 3 dimensional spherical coordinates
- `LKRing`: 2 dimensional polar coordinates

By default, `LKinfo` will use either `LKInterval`, `LKRectangle`, or `LKBox`, depending on the number of dimensions in the given location data. When using the `LKSphere` geometry, there are also different ways of measuring distance, which you can set using the `distance.type` parameter of the `LKinfo` object - you can use `GreatCircle`, which measures the shortest distance over the surface of the sphere, or you can use `Chordal` to measure the shortest straight-line distance, going under the surface of the sphere. You need to specify which one to use or the default (`Euclidean`) will be used, which can lead to a badly-conditioned system.

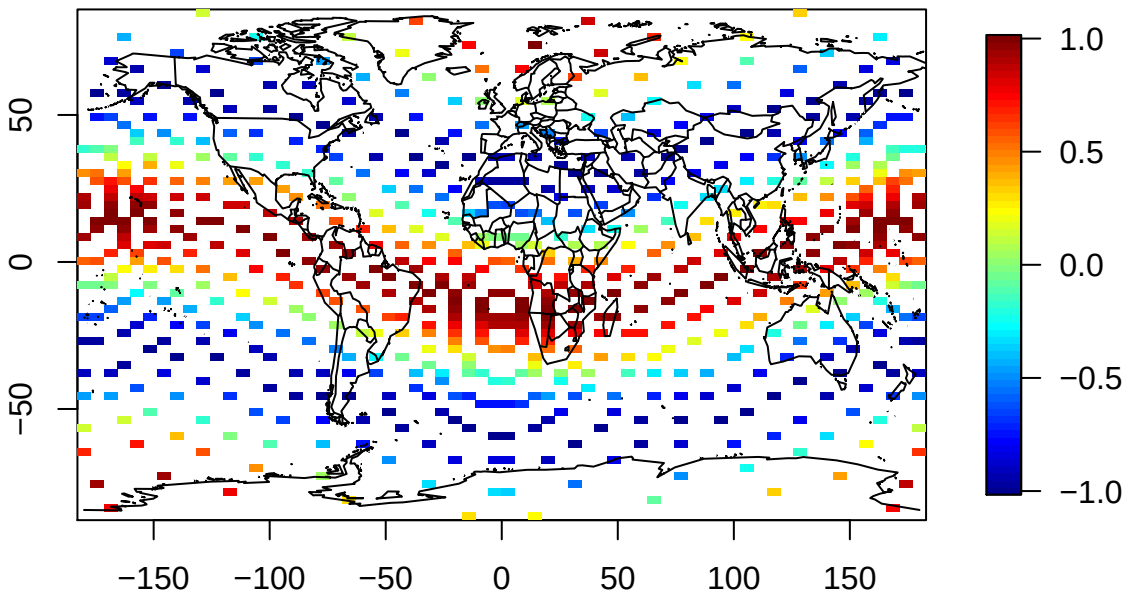
4.1 Working with spherical coordinates

For an example of fitting data taken on the globe using spherical geometry, we create a sample data set over the whole globe and run the kriging with the default (rectangular) geometry and the spherical geometry. Note that R expects the coordinates to be listed as (longitude, latitude) in degrees, with longitude on the interval [-180, 180] and latitude on the interval [-90, 90], with negative numbers corresponding to western longitudes and southern latitudes.

```
n = 40
grid <- list(x = seq(-179,179,len=n), y = seq(-89, 89, len=n/2));
dataLocations <- make.surface.grid(grid)
dataValues <- cos(4*acos(directionCosines(dataLocations) %*% rbind(sqrt(0.98), 0.1, 0.1)))
#image.plot(as.surface(dataLocations, dataValues))
quilt.plot(dataLocations, dataValues)
world(add=TRUE)
```

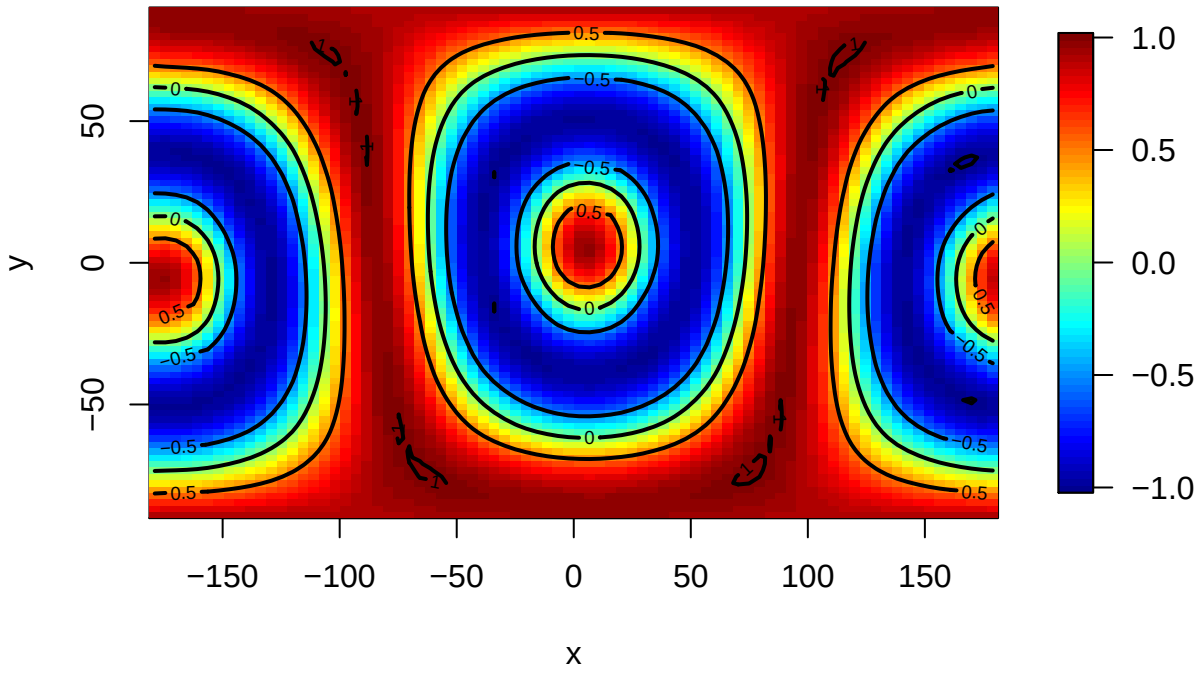



```
#rotating the locations up 85 degrees to the north pole
theta = 70 * (pi/180)
cosineGrid <- directionCosines(dataLocations)
rotationMatrix <- cbind(c(cos(theta), 0, sin(theta)), c(0,1,0), c(-sin(theta), 0, cos(theta)))
newCosineGrid <- t(rotationMatrix %*% t(cosineGrid))
newLocations <- toSphere(newCosineGrid)
#newValues <- cos(4*acos(cosineGrid %*% rotationMatrix %*% #c(sqrt(0.98), 0.1, 0.1)))
#image.plot(as.surface(dataLocations, newValues))
quilt.plot(newLocations, dataValues)
world(add=TRUE)
```

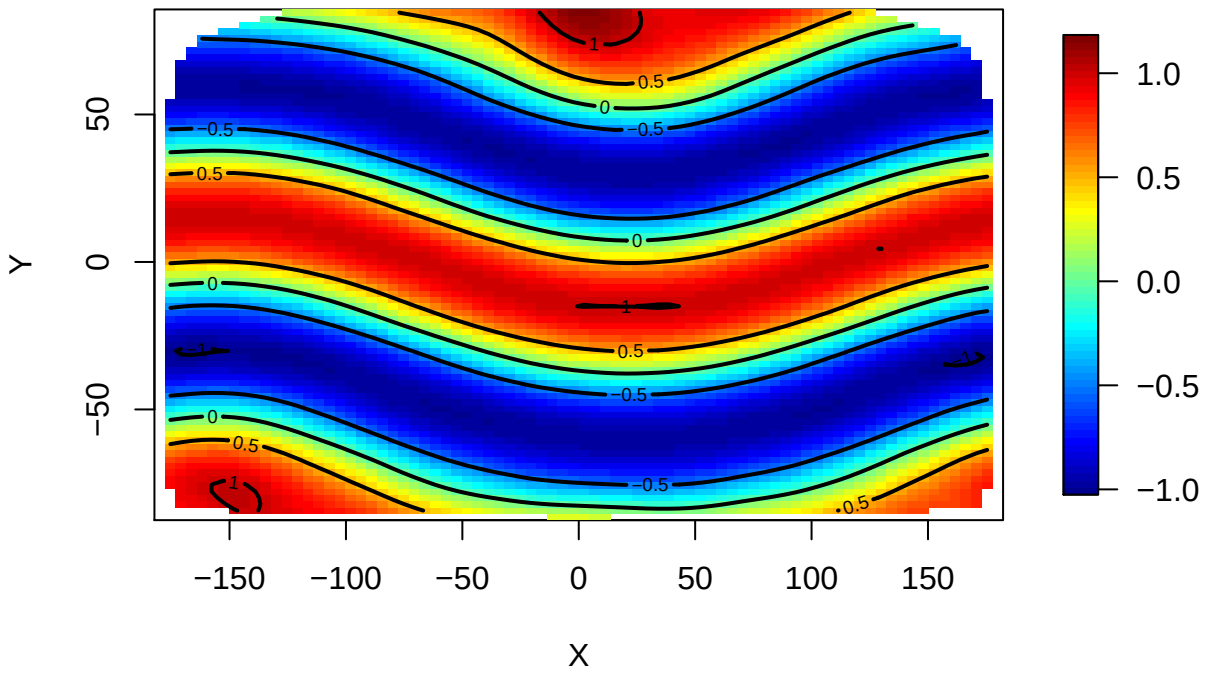


Now, we will use `LatticeKrig` to approximate the surface in both rectangular and spherical geometries.

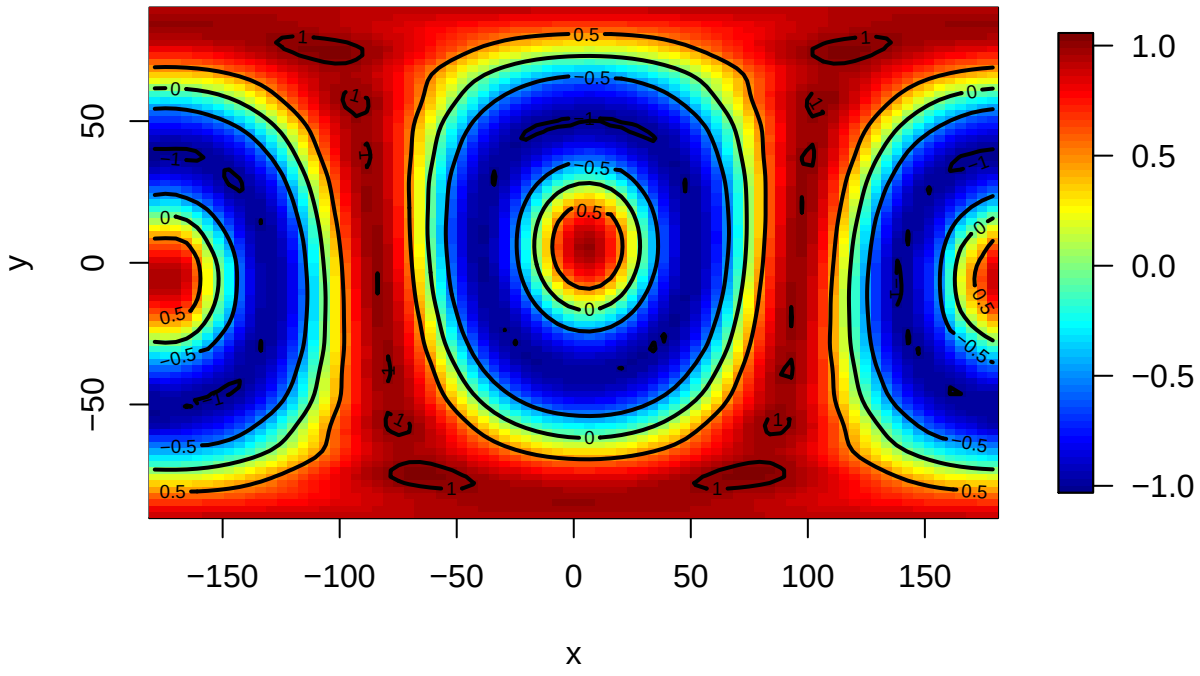
```
kFit <- LatticeKrig(dataLocations, dataValues)
surface(kFit)
```



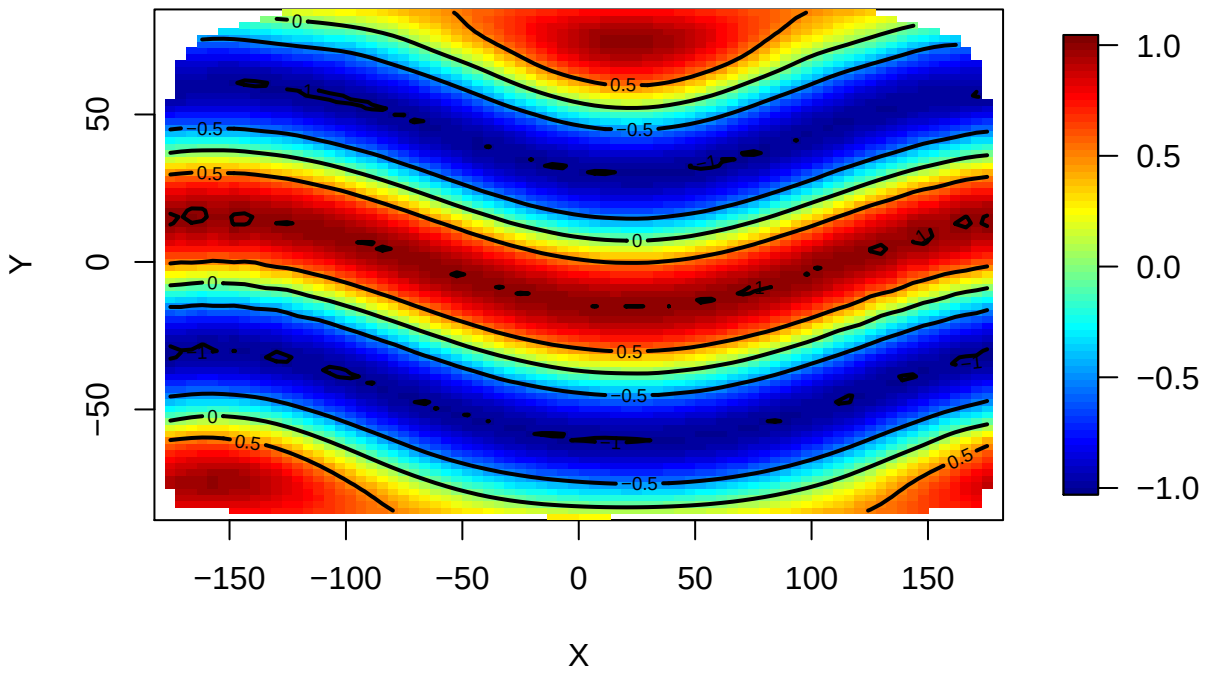

```
kFit <- LatticeKrig(newLocations, dataValues)
surface(kFit)
```




```
info <- LKrigSetup(dataLocations, nlevel = 2, NC = 3, alpha = c(0.8, 0.2), a.wght = 6.01, LKGeometry =
kFit <- LatticeKrig(dataLocations, dataValues, LKinfo=info)
surface(kFit)
```




```
info <- LKrigSetup(newLocations, nlevel = 2, NC = 3, alpha = c(0.8, 0.2), a.wght = 6.01, LKGeometry = "
kFit <- LatticeKrig(newLocations, dataValues, LKinfo=info)
surface(kFit)
```




```
#sum(kFit$residuals^2)
```

5 Frequently Asked Questions

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

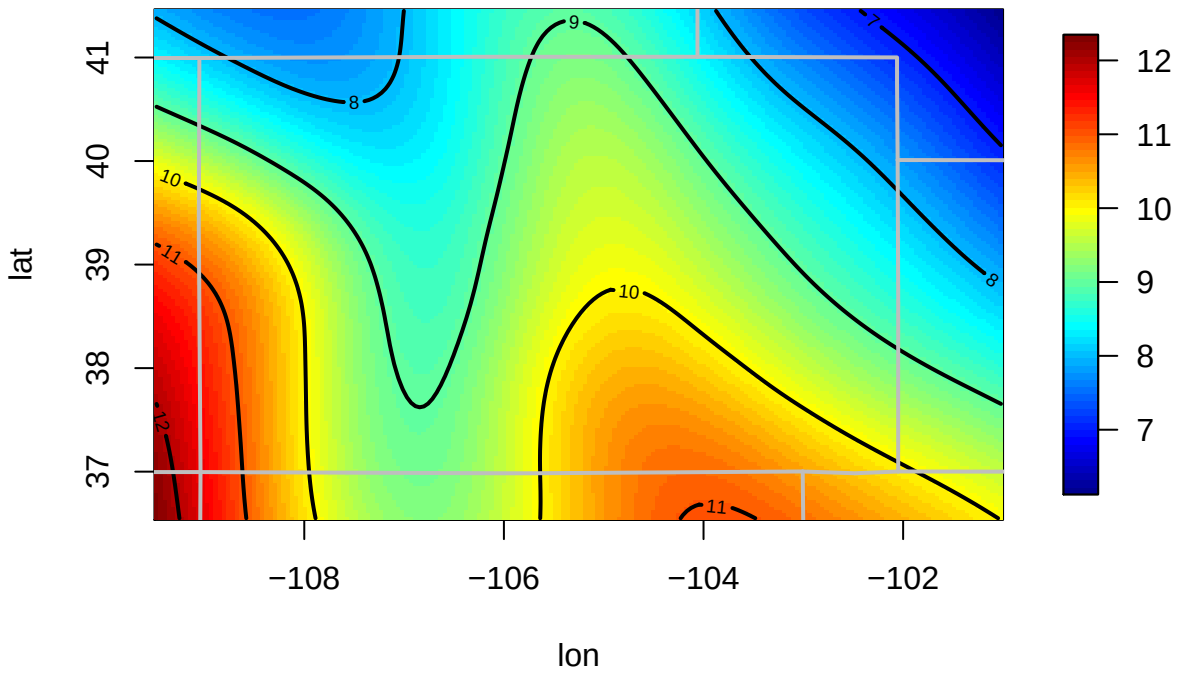
If your model includes covariates (the `Z` parameter of `LatticeKrig` and `LKrig`), your plot may not have included the effect of the covariate. The following code demonstrates this issue using the Colorado temperature data and how to fix it; first, we will set up the model.

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

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

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.

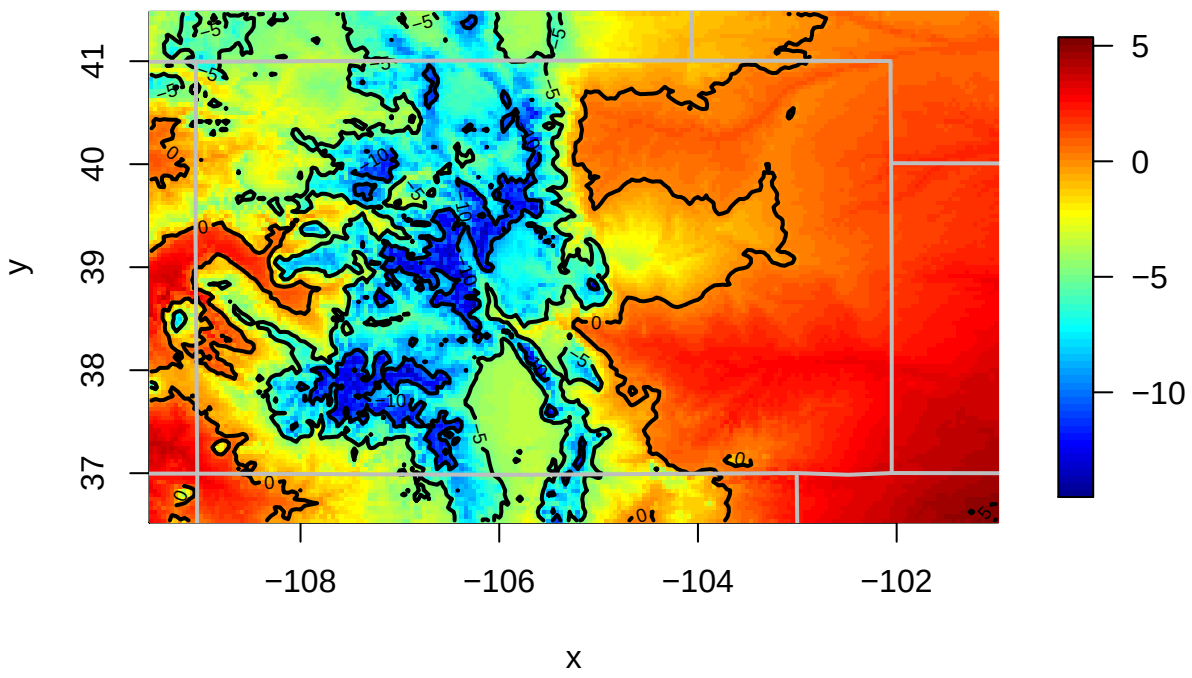
```
surface(kFit, nx = 200, ny = 150, extrap = TRUE)
US(add=TRUE, col='gray', lwd=2)
```



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(kFit, grid.list = CO.Grid,
                  ZGrid = CO.elevGrid, nx = 200, ny = 150, extrap = TRUE)
```

```
surface(prediction)
US(add=TRUE, col='gray', lwd=2)
```



5.2 Why aren't the settings in my LKrigSetup object aren't 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.

6 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 matrix Z 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

$$\mathbf{y} = Z\mathbf{d} + \epsilon$$

where $\epsilon \sim MN(\mathbf{0}, \Sigma)$ for some covariance matrix Σ. We can then make assumptions to determine the form of Σ: Assuming the process is stationary, σ_{ij} will only depend on the vector $\mathbf{s}_i - \mathbf{s}_j$; assuming the process is isotropic, σ_{ij} will only depend on the scalar $||\mathbf{s}_i - \mathbf{s}_j||$, which also means that Σ will be symmetric. This then allows us to establish a covariance function, c, such that $\sigma_{ij} = c(||\mathbf{s}_i - \mathbf{s}_j||)$. The covariance function describes how strongly correlated observations at varying distances are; as such, we would expect that c has a global maximum at 0. 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 $\epsilon = \Phi\mathbf{c} + \mathbf{e}$, 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 each radial basis function is the same except for a shift in location; $\mathbf{c}$ is the vector of coefficents that each basis function is weighted by; and $\mathbf{e}$ is the vector of measurement errors, distributed $N(0, \sigma^2 I)$. 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 $Z\mathbf{d} + \Phi\mathbf{c}$ 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 $\hat{\mathbf{c}} = P\Phi^T\Sigma_{11}^{-1}(\mathbf{y} - Z\mathbf{d})$.