Advanced Machine Learning
LAB 3: Reinforcement Learning

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Contents

Question 1: GP Regression **2**
Question 1-1: 2
The exponential kernel method: 2
Now we can set the parameters: 2
Posterior Gaussian Process Function 3
Question 1-2: 3
Question1-3: 4
Question1-4: 5
Question1-5: 9

Question 2: **13**
Question2-1: 13
Question2-2: 14
Question2-3: 15
Question2-4: 16

Question2-5: **17**

Question 3: **19**
Question3-1: 19
Question3-2: 22
Question3-3: 22

Appendix **23**

Question 1: GP Regression

Implementing GP Regression. This first exercise will have you writing your own code for the Gaussian process regression model:

$y = f(x) + \epsilon$
with $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$
and $f \sim \mathcal{GP}(0, k(x, x'))$

You must implement Algorithm 2.1 on page 19 of Rasmussen and Willams' book. The algorithm uses the Cholesky decomposition (chol in R) to attain numerical stability. Note that L in the algorithm is a lower triangular matrix, whereas the R function returns an upper triangular matrix. So, you need to transpose the output of the R function. In the algorithm, the notation A /bb means the vector x that solves the equation A x = b (see p. xvii in the book). This is implemented in R with the help of the function solve.

Question 1-1:

Write your own code for simulating from the posterior distribution of f using the squared exponential kernel. The function (name it posteriorGP) should return a vector with the posterior mean and variance of f , both evaluated at a set of x-values X_*. You can assume that the prior mean of f is zero for all x. The function should have the following inputs:

- X: Vector of training inputs.
- y: Vector of training targets/outputs.
- *XStar*: Vector of inputs where the posterior distribution is evaluated, i.e. X_* .
- *sigmaNoise*: Noise standard deviation σ_n .
- k: Covariance function or kernel. That is, the kernel should be a separate function

The exponential kernel method:

```
#The squared exponential function
SquaredExpKernel <- function(x1,x2,sigmaF=1,l=0.3){
  n1 <- length(x1)
  n2 <- length(x2)
  K <- matrix(NA,n1,n2)
  for (i in 1:n2){
    K[,i] <- sigmaF^2*exp(-0.5*( (x1-x2[i])/l)^2 )
  }
  return(K)
}
```

Now we can set the parameters:

```
sigmaF = 1
l = 0.3
sigmaNoise = 0.1
xGrid <- seq(-1,1,length=20)
nSim = 1
```

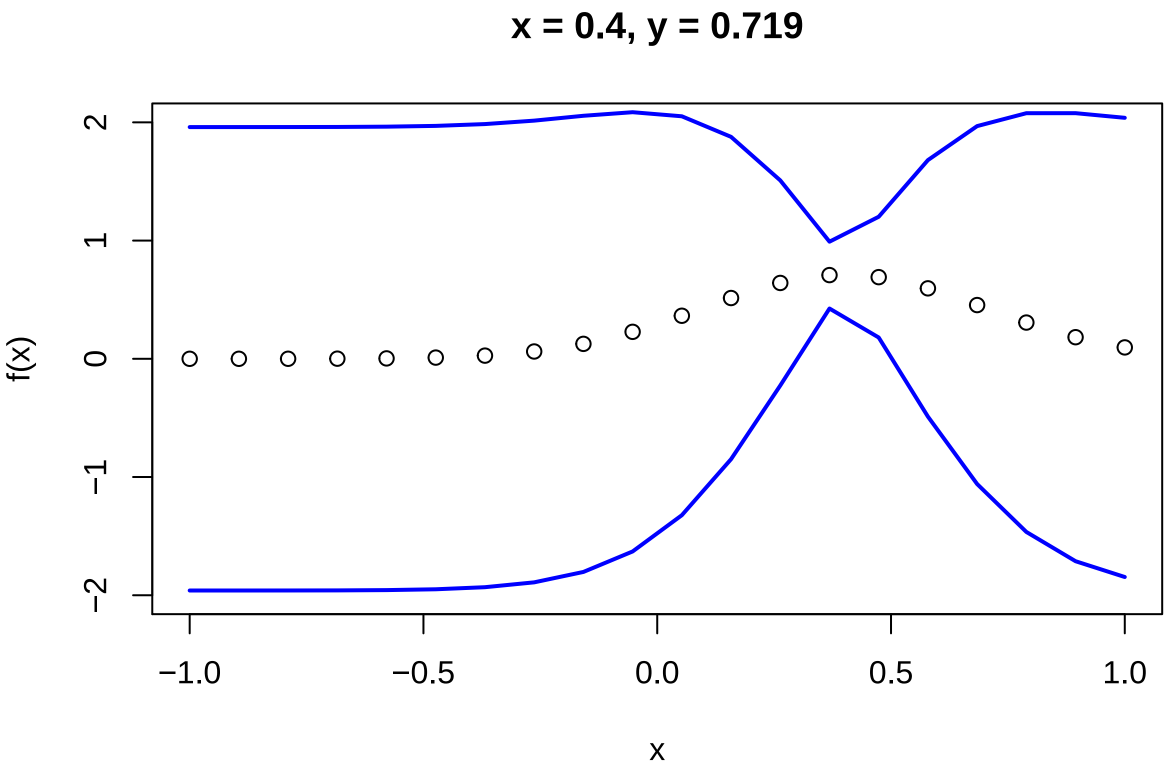
Posterior Gaussian Process Function

```
#Question1:  The posterior function ##########################################################
posteriorGP = function(X, y, XStar, sigmaNoise, k){
  #The algorithm
  K = k(X, X)
  n = length(X)

  L = chol(K + sigmaNoise^2*diag(n))
  alpha = solve(t(L),solve(L,y))

  if (length(XStar)==1){
    KStar = XStar
  }
  else{
    KStar = k(X,XStar)
  }

  FStar = t(KStar)*alpha
  v = solve(L,KStar)
  VFStar = k(XStar, XStar)-t(v)%*%v
  logP = -0.5*t(y)%*%alpha - sum(log(diag(L))) - (n/2)*log(2*pi)

  return(list('mean'=FStar, 'variance'= VFStar, 'logMargLik' = logP))
}
```

Question 1-2:

Evaluating the function on *(x,y) = (0.4,0.719)*

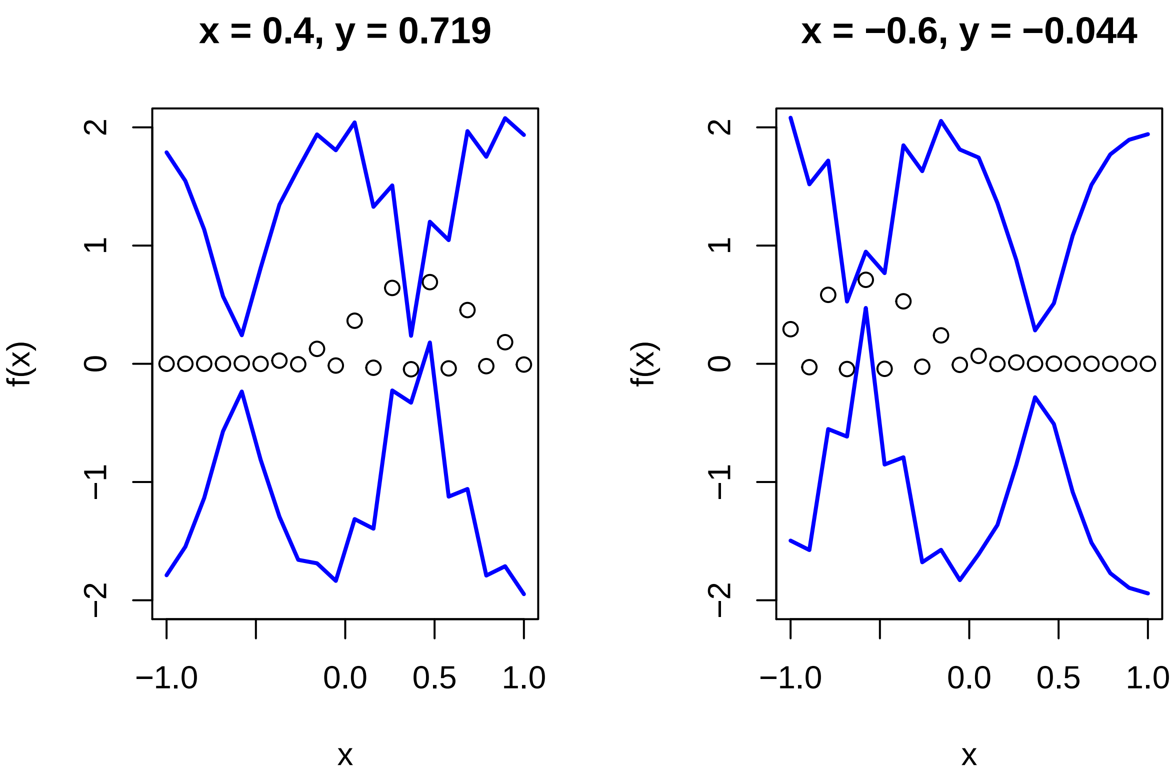
```
#Question2: evaluating on (0.4,0.719)############################################
x = 0.4
y = 0.719
posteriorValue = posteriorGP(X = x,
                             y = y,
                             XStar = xGrid,
                             sigmaNoise = sigmaNoise,
                             k = SquaredExpKernel)
postMean = posteriorValue$mean
postVar = posteriorValue$variance

#Plotting the posterior mean
plotMean = function(mean,var, title){
  plot(xGrid, mean, type="p", ylab="f(x)", xlab="x", ylim = c(-2,2), main = title)

  #Plotting confidence band
  lines(xGrid, mean - 1.96*sqrt(diag(var)), col = "blue", lwd = 2)
  lines(xGrid, mean + 1.96*sqrt(diag(var)), col = "blue", lwd = 2)
}
par(mfrow = c(1,1))
plotMean(postMean,postVar, title = 'x = 0.4, y = 0.719')
```



Question1-3:

Updating the posterior with observation (-0.6, -0.044)

```
x = c(0.4,-0.6)
y = c(0.719,-0.044)

posteriorValue2 = posteriorGP(X = x,
                              y = y,
                              XStar = xGrid,
                              sigmaNoise = sigmaNoise,
                              k = SquaredExpKernel)
postMean2 = posteriorValue2$mean
postVar2 = posteriorValue2$variance

par(mfrow = c(1,2))
plotMean(postMean2[,1], postVar2, title = 'x = 0.4, y = 0.719')
plotMean(postMean2[,2], postVar2, title = 'x = -0.6, y = -0.044')
```



Question1-4:

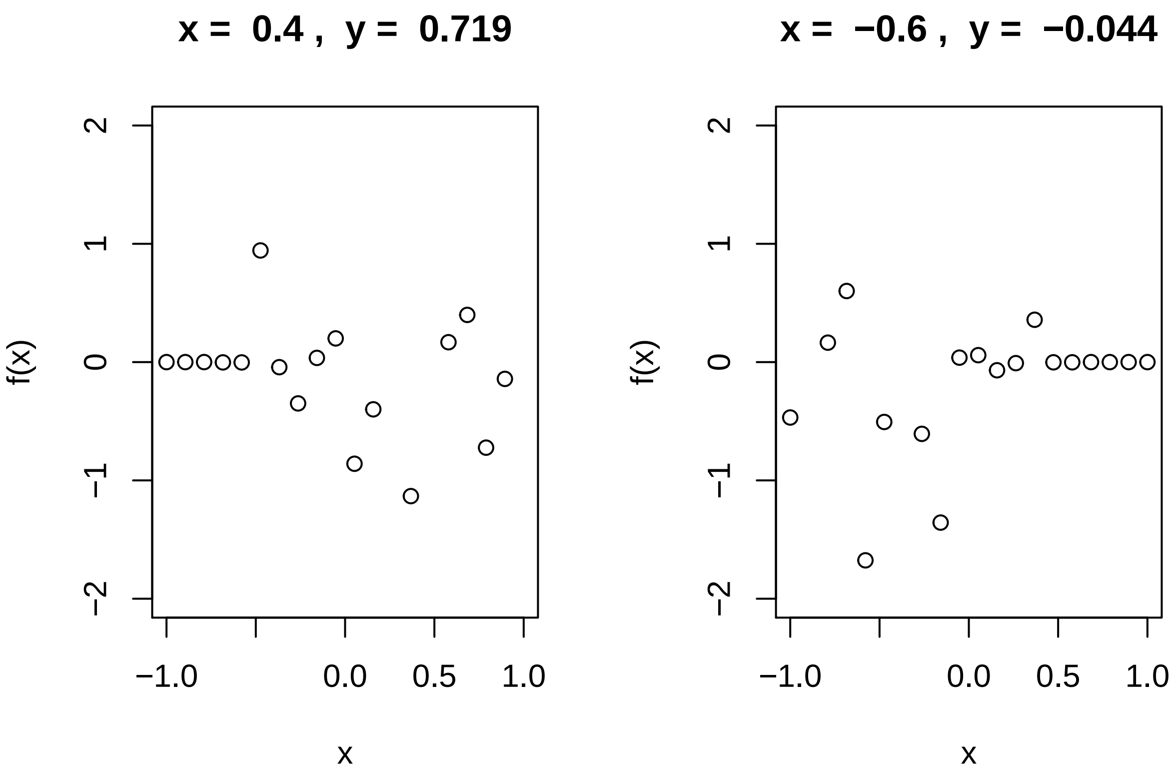
Compute the posterior distribution of f using all the five data points in the table below (note that the two previous observations are included in the table). Plot the posterior mean of f over the interval $x \in [-1, 1]$. Plot also 95 % probability (pointwise) bands for *f*.

The posterior with all five observations plus the previous two observations:

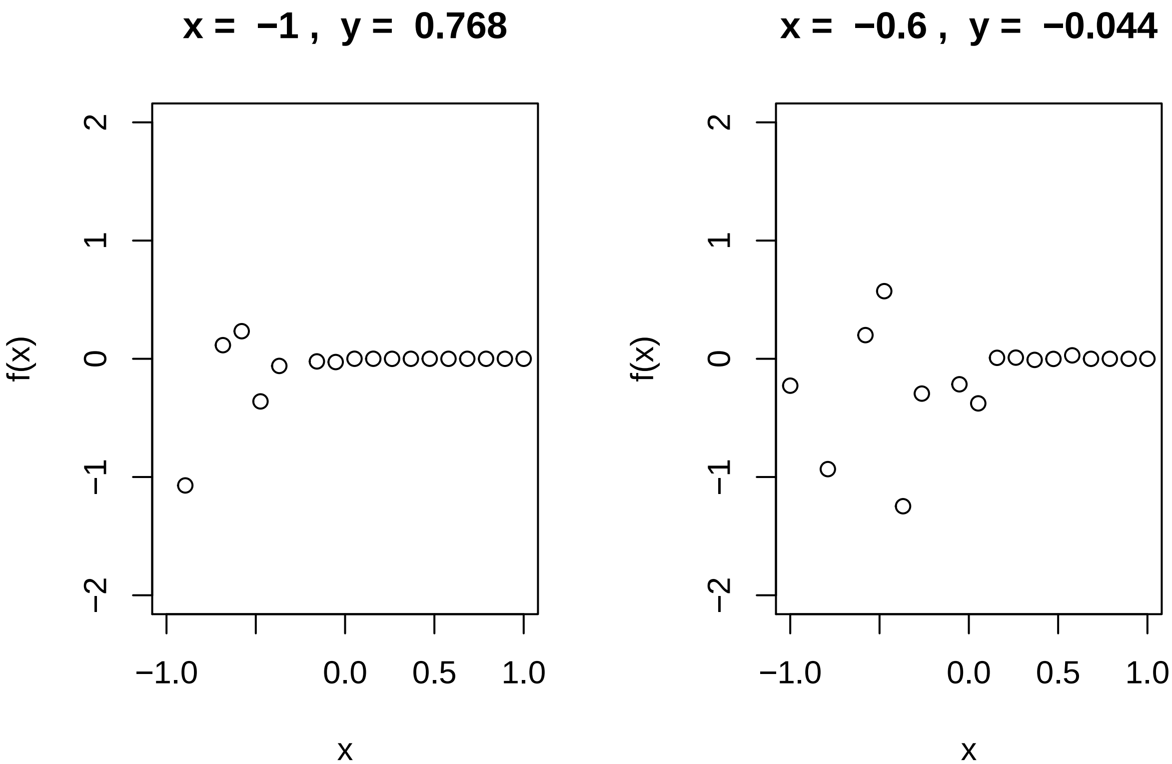
```
#Question4: The posterior with five observations################################
x = c(0.4, -0.6, -1.0, -0.6, -0.2, 0.4, 0.8)
y = c(0.719, -0.044, 0.768, -0.044, -0.940, 0.719, -0.664)

posteriorValue3 = posteriorGP(X = x,
                              y = y,
                              XStar = xGrid,
                              sigmaNoise = sigmaNoise,
                              k = SquaredExpKernel)
postMean3 = posteriorValue3$mean
postVar3 = posteriorValue3$variance

par(mfrow=c(1,2))
for (i in 1:length(x)){
  plotMean(postMean3[,i],postVar3, title = paste('x = ',x[i], ',  y = ',y[i]))
}
```

```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```

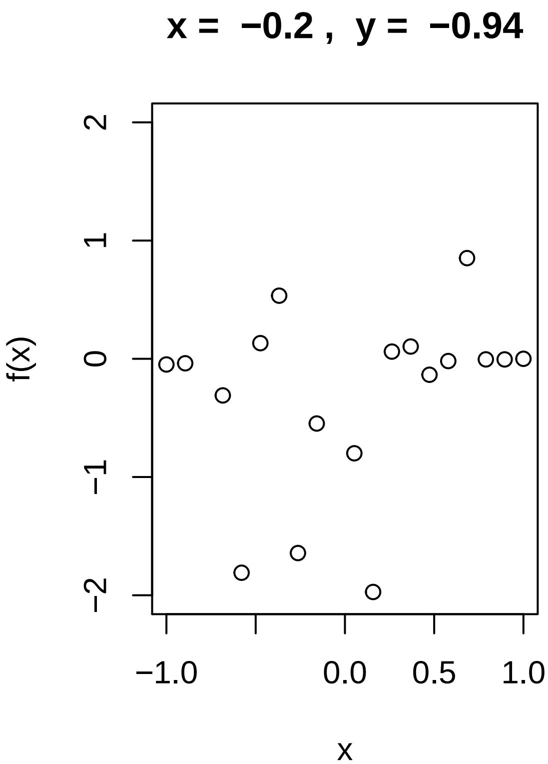
```
## Warning in sqrt(diag(var)): NaNs produced
```

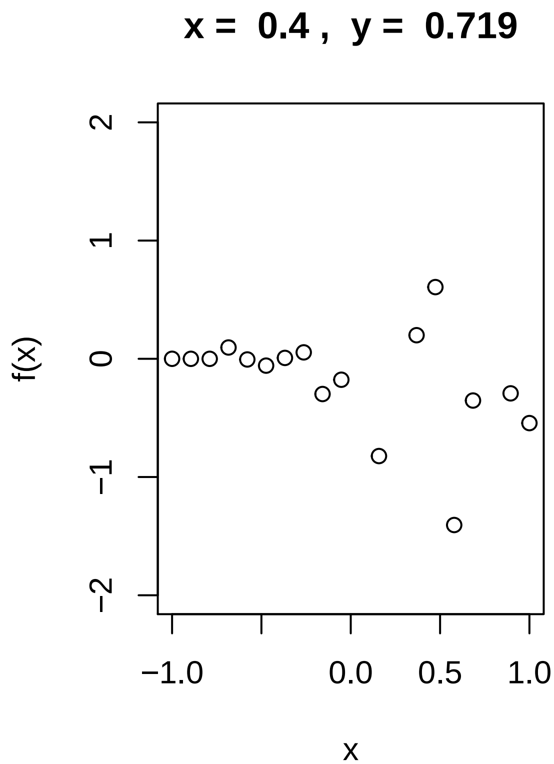



```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```

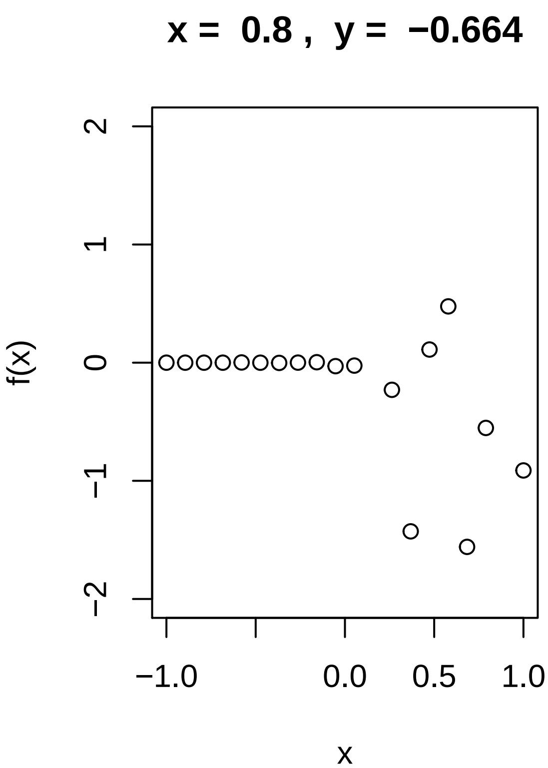



```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```






```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```

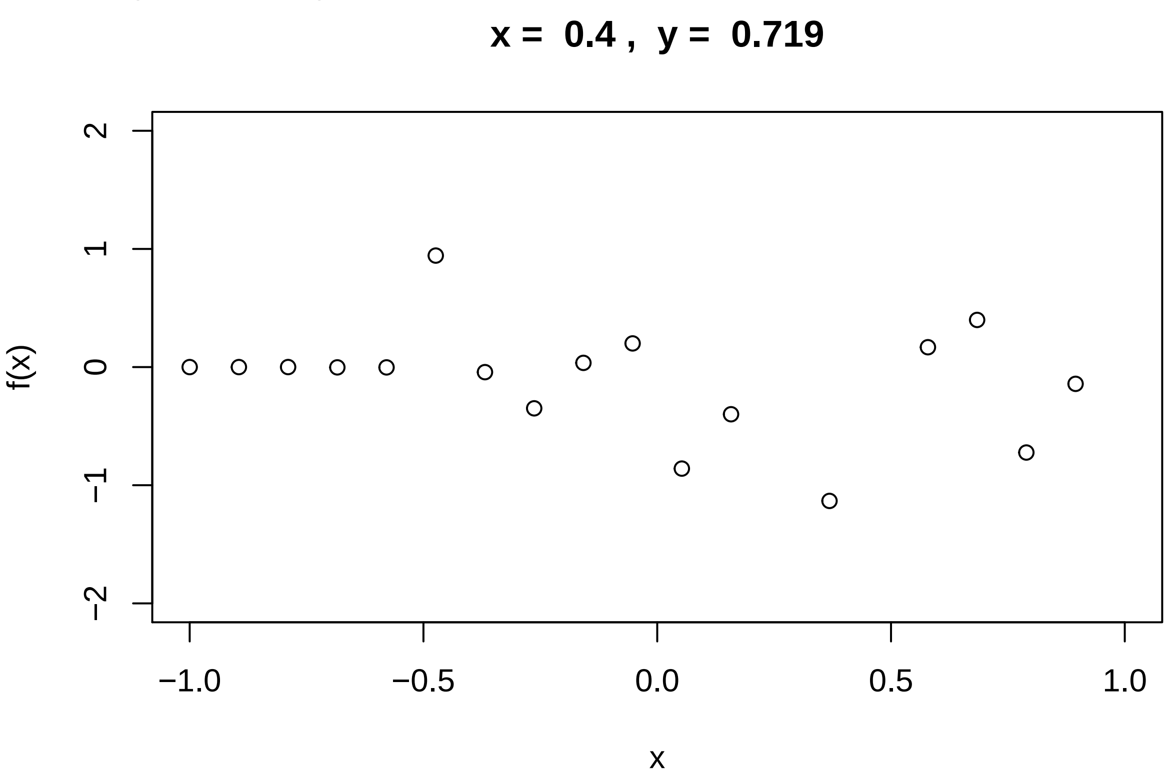


Question1-5:

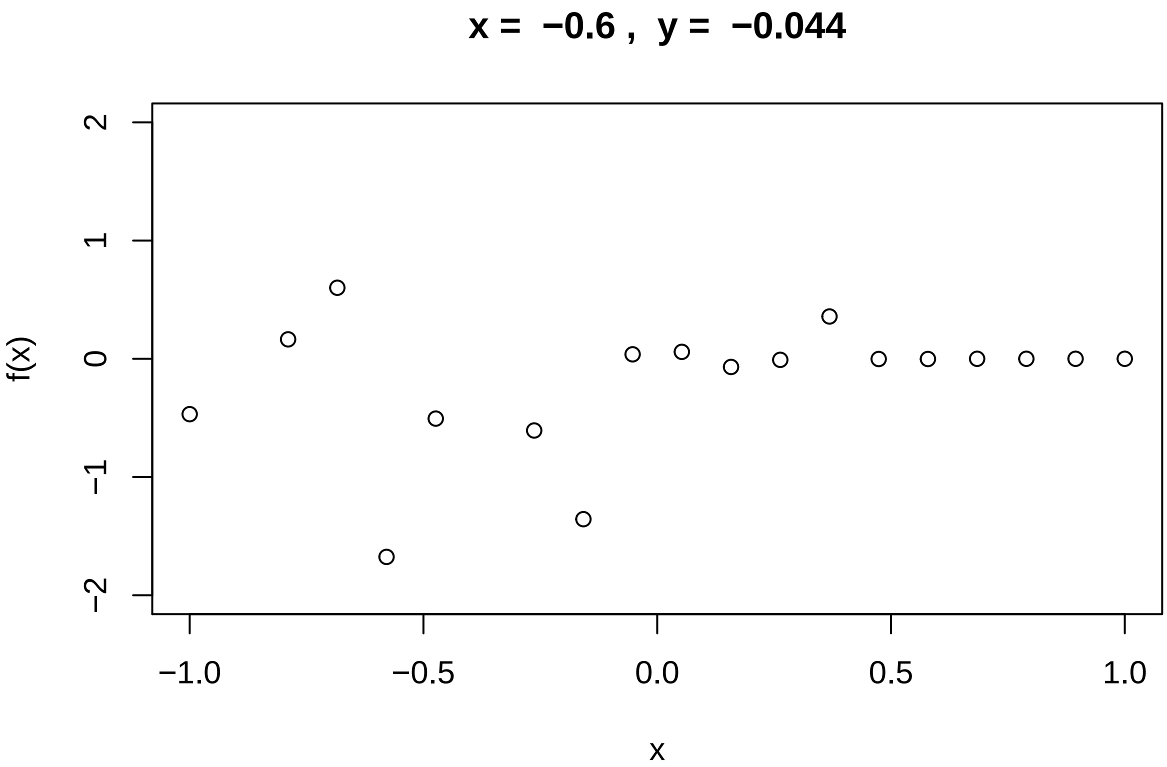
Repeating with different hyperparameters:

```
#Question5: Repeating with different hyperparameters.

sigmaF = 1
L = 1
posteriorValue4 = posteriorGP(X = x,
                              y = y,
                              XStar = xGrid,
                              sigmaNoise = sigmaNoise,
                              k = SquaredExpKernel)
postMean4 = posteriorValue4$mean
postVar4 = posteriorValue4$variance

for (i in 1:length(x)){
  plotMean(postMean4[,i],postVar4, title = paste('x = ',x[i], ',  y = ',y[i]))
}
```

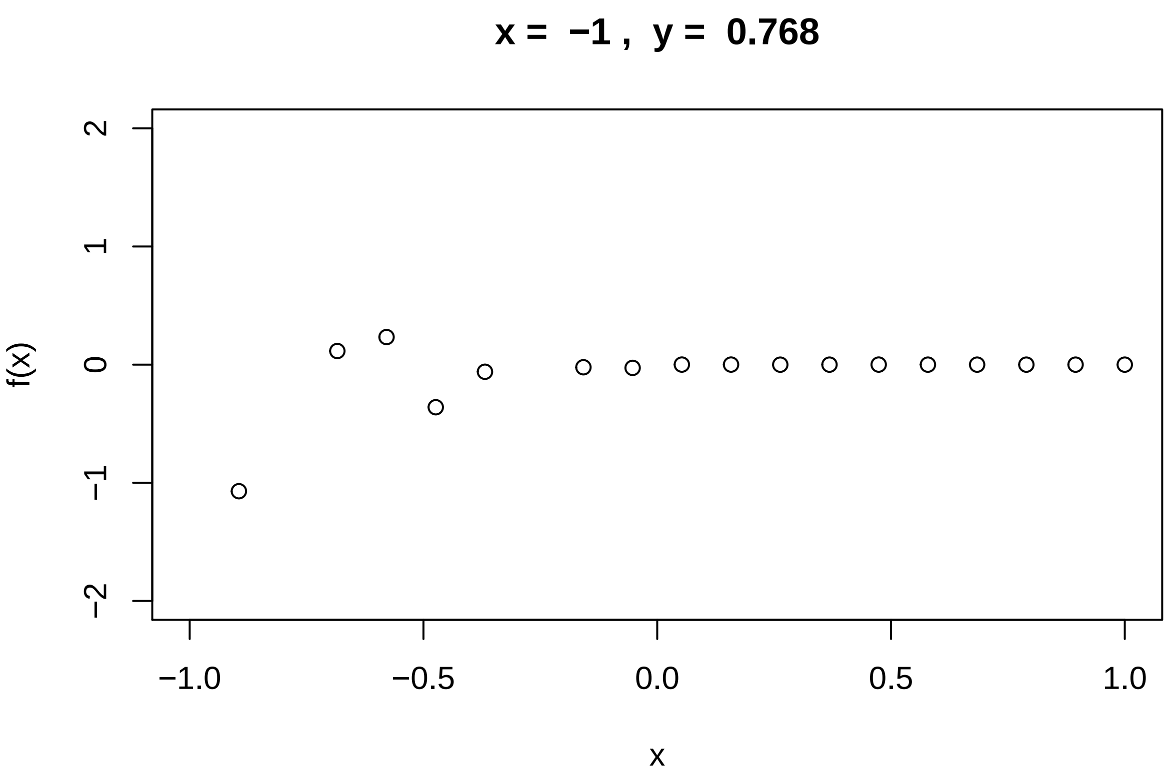
```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```




```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```

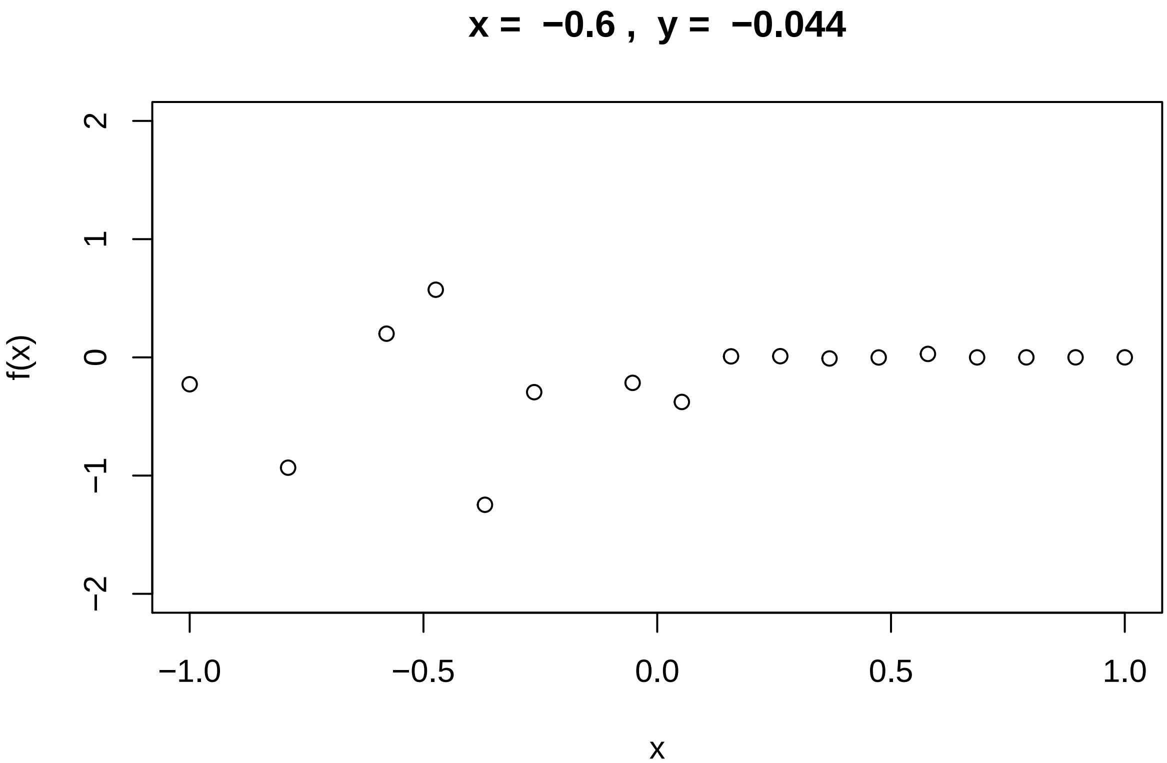



```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```



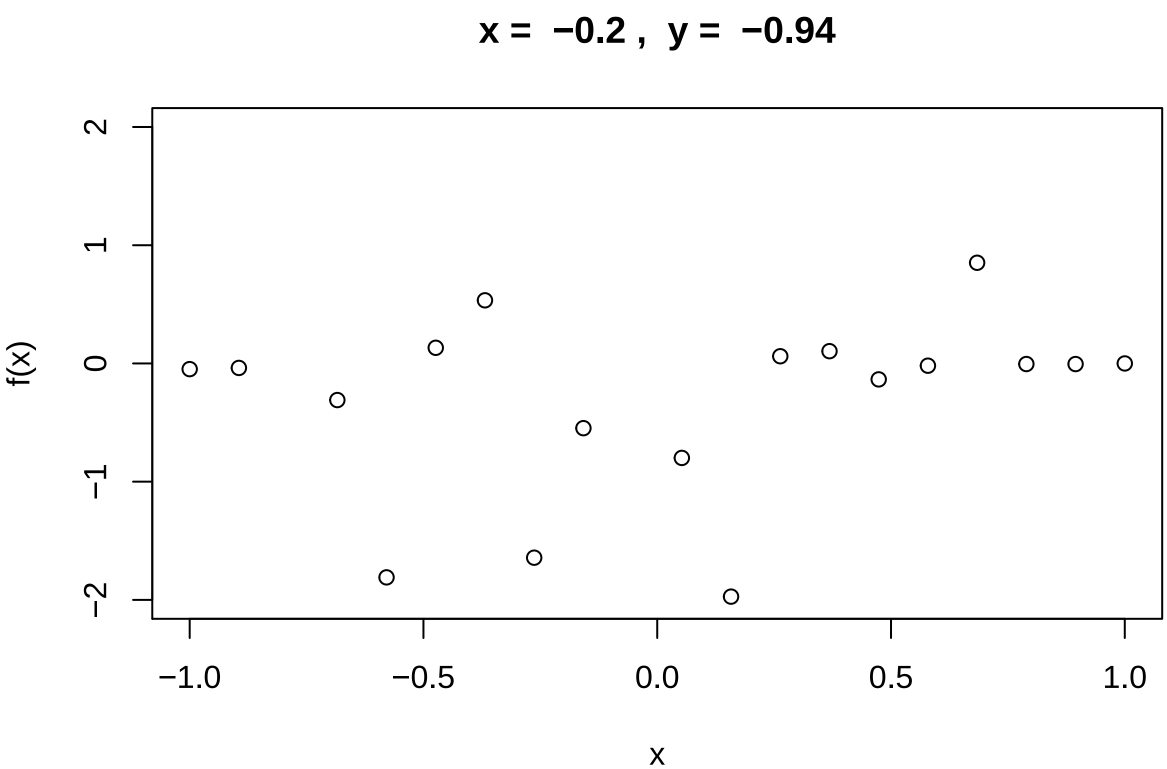

```
## Warning in sqrt(diag(var)): NaNs produced
```

```
## Warning in sqrt(diag(var)): NaNs produced
```

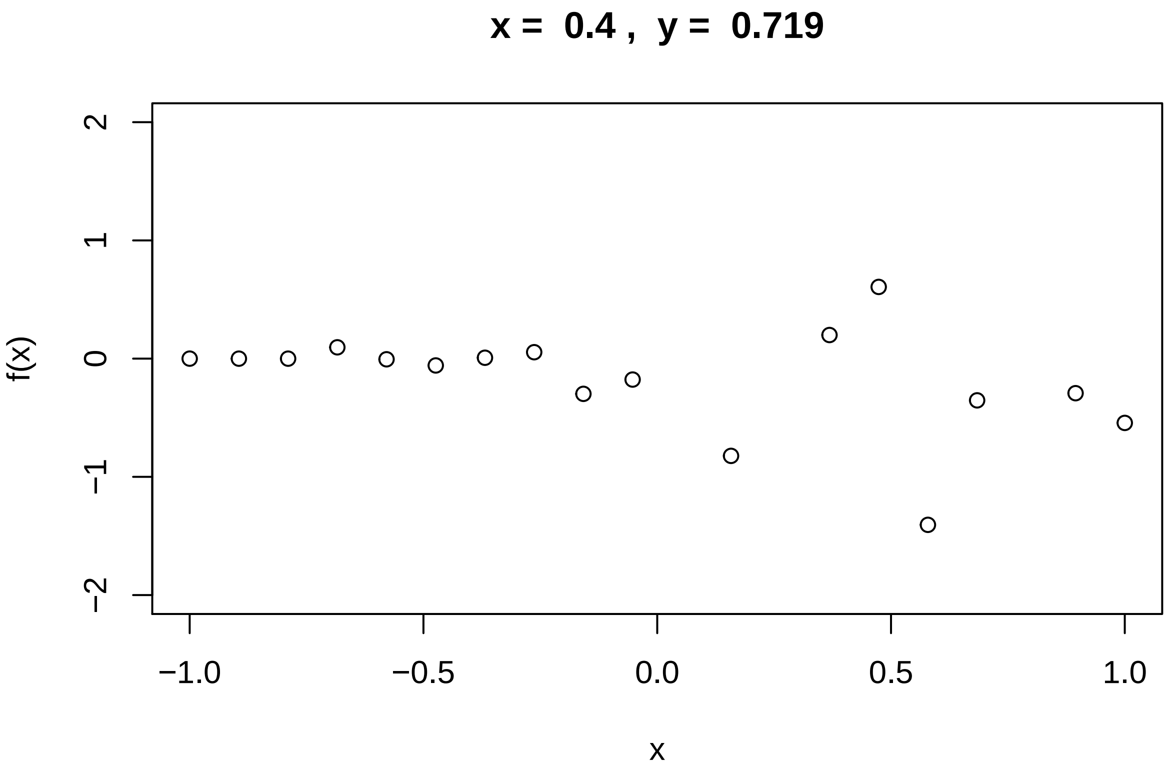



```
## Warning in sqrt(diag(var)): NaNs produced
```

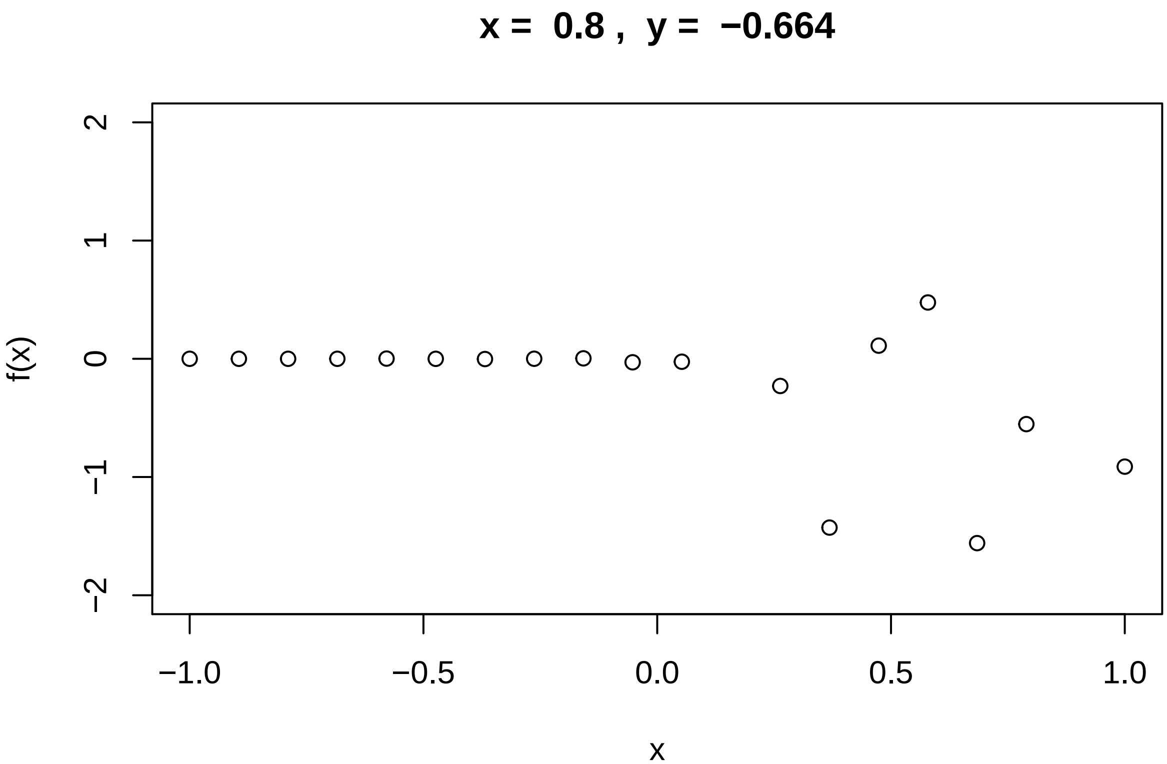
```
## Warning in sqrt(diag(var)): NaNs produced
```



```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```




```
## Warning in sqrt(diag(var)): NaNs produced

## Warning in sqrt(diag(var)): NaNs produced
```



Question 2:

GP Regression with kernlab:

In this exercise, you will work with the daily mean temperature in Stockholm (Tullinge) during the period January 1, 2010 - December 31, 2015. We have removed the leap year day February 29, 2012 to make things simpler.
Create the variable time which records the day number since the start of the dataset (i.e., time= 1, 2, . . ., $365 \times 6 = 2190$). Also, create the variable day that records the day number since the start of each year (i.e., day= 1, 2, . . ., 365, 1, 2, . . ., 365). Estimating a GP on 2190 observations can take some time on slower computers, so let us subsample the data and use only every fifth observation. This means that your time and day variables are now time= 1, 6, 11, . . ., 2186 and day= 1, 6, 11, . . ., 361, 1, 6, 11, . . ., 361.

```
#Takinng every fifth observation

time = seq(from = 1, to = length(time), by = 5)
day = day[time]
scaledTime = (time-mean(time))/sd(time)
```

Question2-1:

Defining and evaluating square exponential kernel function

```
Matern32 <- function(sigmaf = 1, ell = 1)
{
  rval <- function(x, y = NULL) {
    r = sqrt(crossprod(x-y));
    return(sigmaf^2*(1+sqrt(3)*r/ell)*exp(-sqrt(3)*r/ell))
  }
  class(rval) <- "kernel"
```

```r
  return(rval)
}

#Evaluating the function
MaternFunc = Matern32(sigmaf = 20, ell = 0.2) # MaternFunc is a kernel FUNCTION
MaternFunc(1,2)
```

```
##           [,1]
## [1,] 0.6698044
```

```r
#Computing the covarance matrix K
X = c(1,3,4)
Xstar = c(2,3,4)

K <- kernelMatrix(kernel = MaternFunc, x = X, y = Xstar)
```

The covariance matrix for 1, 3, 4 and 2, 3, 4 is:

```
## An object of class "kernelMatrix"
##              [,1]         [,2]         [,3]
## [1,] 0.6698044031 2.201894e-04 5.620987e-08
## [2,] 0.6698044031 4.000000e+02 6.698044e-01
## [3,] 0.0002201894 6.698044e-01 4.000000e+02
```

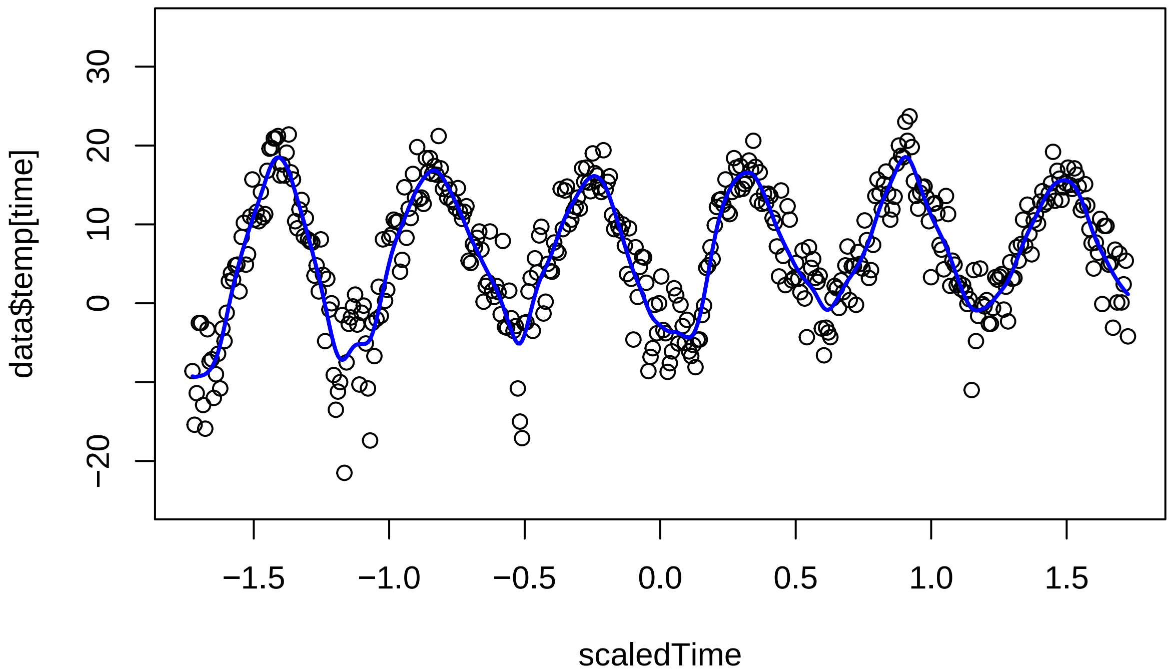
Question2-2:

The model is:
$\sqcup emp = f(time) + \epsilon$ with $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$ and $f \sim \mathcal{GP}(0, k(time, time'))$

```r
#Letting sigma noise equal to residual variance of a quadratic regression fit using lm
modelData = data.frame(data$temp[time], scaledTime)
colnames(modelData) = c('temp', 'time')
polyFit <- lm(temp ~ time + I(time^2) + I(time^3), data = modelData)
sigmaNoise = sd(polyFit$residuals)
cat('sigmaNoise is: ',sigmaNoise)
```

```
## sigmaNoise is:  8.142339
```

```r
plot(scaledTime,data$temp[time], ylim = c(-25,35))

# Fit the GP with Square expontial kernel

MaternFunc = Matern32(sigmaf = 20, ell = 0.2)
GPfit <- gausspr(scaledTime, data$temp[time],
                 kernel = MaternFunc,
                 kpar = list(sigmaf = 20, ell = 0.2),
                 var = sigmaNoise^2)
meanPred <- predict(GPfit, scaledTime)
lines(scaledTime, meanPred, col="blue", lwd = 2)
```

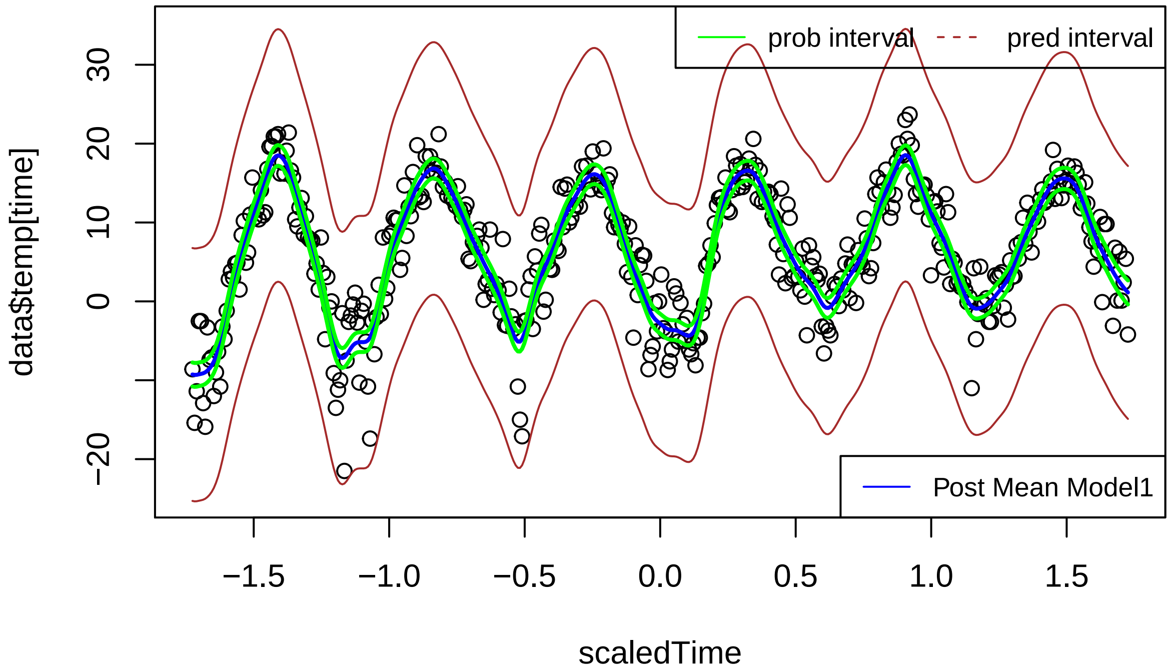


Question2-3:

kernlab can compute the posterior variance of f , but it seems to be a bug in the code. So, do your own computations for the posterior variance of f and plot the 95 % probability (pointwise) bands for f . Superimpose these bands on the figure with the posterior mean that you obtained in (2)

```
ell <- 0.5
SEkernel <- rbfdot(sigma = 1/(2*ell^2))

x<-scaledTime
xs<-scaledTime # XStar
n <- length(x)
Kss <- kernelMatrix(kernel = SEkernel, x = xs, y = xs)
Kxx <- kernelMatrix(kernel = SEkernel, x = x, y = x)
Kxs <- kernelMatrix(kernel = SEkernel, x = x, y = xs)
Covf = Kss-t(Kxs)%*%solve(Kxx + sigmaNoise^2*diag(n), Kxs) # Covariance matrix of fStar

# Probability intervals for fStar
plot(scaledTime,data$temp[time], ylim = c(-25,35))
lines(scaledTime, meanPred, col="blue", lwd = 2)

lines(xs, meanPred - 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)
lines(xs, meanPred + 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)

# Prediction intervals for yStar
lines(xs, meanPred - 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")
lines(xs, meanPred + 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")

legend("bottomright",
       legend = c('Post Mean Model1'),
       col = c( 'blue'),
       lty=1:2,
       cex=0.8)
```

```r
legend("topright",
       legend = c('prob interval',
                  'pred interval'),
       col = c('green', 'brown'),
       lty=1:2,
       cex=0.8,
       horiz = TRUE)
```



Question2-4:

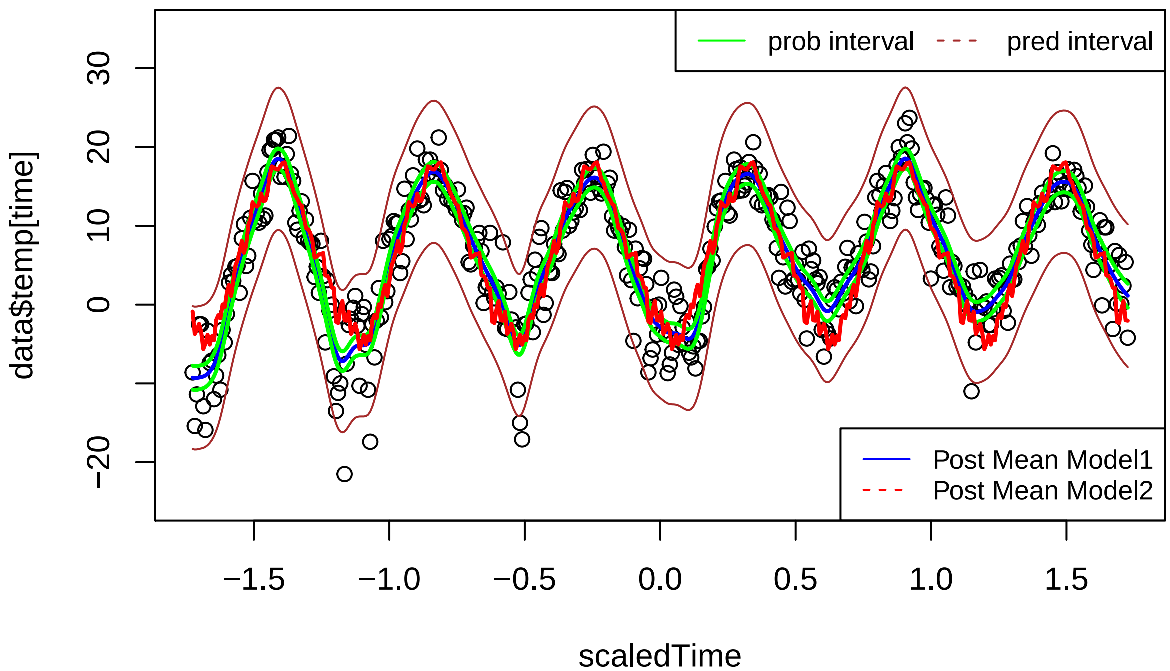
The model is:
$\sqcup emp = f(day) + \epsilon$ with $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$ and $f \sim \mathcal{GP}(0, k(day, day'))$

```r
#Letting sigma noise equal to residual variance of a quadratic regression fit using lm
modelData = data.frame(data$temp[time], day)
colnames(modelData) = c('temp', 'day')
polyFit <- lm(temp ~ day + I(day^2) + I(day^3), data = modelData)
sigmaNoise = sd(polyFit$residuals)
sigmaNoise
```

```
## [1] 4.558032
```

```r
# Fit the GP with built in Square expontial kernel (called rbfdot in kernlab)

MaternFunc = Matern32(sigmaf = 20, ell = 0.2)
GPfit <- gausspr(day,
                 data$temp[time],
                 kernel = MaternFunc,
                 kpar = list(sigmaf = 20, ell = 0.2),
                 var = sigmaNoise^2)
meanPred2 <- predict(GPfit, day)

plot(scaledTime,data$temp[time], ylim = c(-25,35))
```

```r
lines(scaledTime, meanPred, col="blue", lwd = 2)
# Probability intervals for fStar
lines(xs, meanPred - 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)
lines(xs, meanPred + 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)

# Prediction intervals for yStar
lines(xs, meanPred - 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")
lines(xs, meanPred + 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")
lines(scaledTime, meanPred2, col="red", lwd = 2)
legend("bottomright",
       legend = c('Post Mean Model1',
                  'Post Mean Model2'),
       col = c( 'blue', 'red'),
       lty=1:2,
       cex=0.8)
legend("topright",
       legend = c('prob interval',
                  'pred interval'),
       col = c('green', 'brown'),
       lty=1:2,
       cex=0.8,
       horiz = TRUE)
```




```r
#The first model has a smoother posterior mean than the second model, the second model seems not smooth
```

Question2-5:

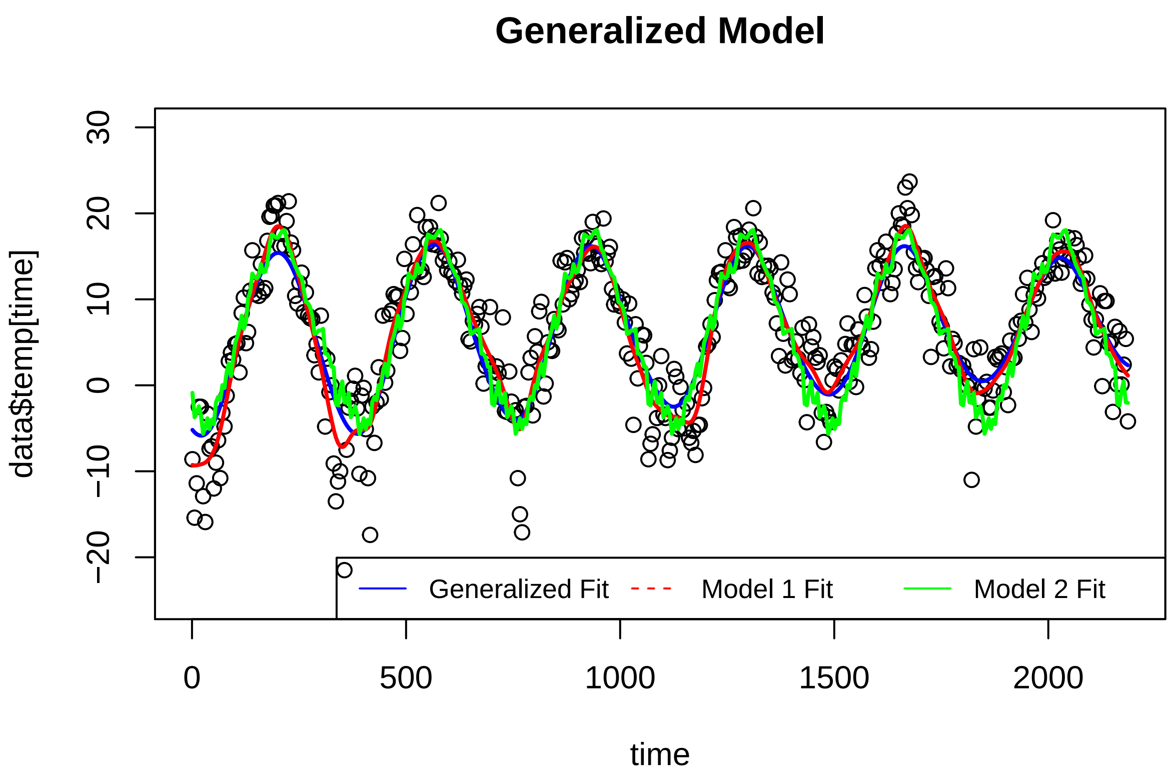
Implement a generalization of the periodic kernel

$$k(x, x') = \sigma_f^2 exp \frac{-2\int in^2(\pi|x-x'|/d)}{l_1^2} * exp - \frac{1}{2}\frac{|x-x'|^2}{l_2^2}$$

```r
GPKernel = function(l1,l2, sigmaF, d){

  rval <- function(x1, x2 = NULL) {
    return(sigmaF^2 * exp(-(2*(sin(pi*abs(x1-x2)/d))^2)/l1^2)*(exp(-0.5*abs(x1-x2)^2)/l2^2))
  }
  class(rval) <- "kernel"
  return(rval)

}

l1 = 1
l2 = 10
sigmaF = 20
d = 365/sd(time)

GPKernelFun = GPKernel(l1,l2,sigmaF, d)
GPKernelFun(1,2)
```

```
## [1] 0.8074298
```

```r
#Fitting the generlaized model
GPfit <- gausspr(scaledTime, data$temp[time],
                 kernel = GPKernelFun,
                 kpar = list(sigmaF = sigmaF, l1 = l1, l2 = l2, d=d),
                 var = sigmaNoise^2)
meanPred3 <- predict(GPfit, scaledTime)
plot(time,data$temp[time], ylim = c(-25,30), main = 'Generalized Model')
lines(time, meanPred3, col="blue", lwd = 2)
lines(time, meanPred, col="red", lwd = 2)
lines(time, meanPred2, col="green", lwd = 2)
legend("bottomright",
       legend = c('Generalized Fit',
                  'Model 1 Fit',
                  'Model 2 Fit'),
       col = c('blue', 'red', 'green'),
       lty=1:2,
       cex=0.8,
       horiz = TRUE)
```



From the plot, it can be seen that model 1 fits the data more accurately than model 2 with the generalized kernel. The second model also does a good job in fitting the data, however, it's not smooth.

Question 3:

GP Classification with kernlab

Question3-1:

Use the R package *kernlab* to fit a Gaussian process classification model for fraud on the training data. Use the default kernel and hyperparameters. Start using only the covariates *varWave* and *skewWave* in the model. Plot contours of the prediction probabilities over a suitable grid of values for varWave and skewWave. Overlay the training data for fraud = 1 (as blue points) and fraud = 0 (as red points). You can reuse code from the file *KernLabDemo.R* available on the course website. Compute the confusion matrix for the classifier and its accuracy.

```
data = read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/banknoteFraud.
names(data) = c("varWave","skewWave","kurtWave","entropyWave","fraud")
data[,5] = as.factor(data[,5])

#Dividing the data into training and testing
set.seed(111)
SelectTraining = sample(1:dim(data)[1],
                        size = 1000,
                        replace = FALSE)
trainingData = data[SelectTraining,]
testingData = data[-SelectTraining,]

GPfitFraud <- gausspr(fraud ~  varWave + skewWave, data=trainingData)
```

```
## Using automatic sigma estimation (sigest) for RBF or laplace kernel
```

```r
GPfitFraud
```

```
## Gaussian Processes object of class "gausspr"
## Problem type: classification
##
## Gaussian Radial Basis kernel function.
##  Hyperparameter : sigma =  1.2043047635594
##
## Number of training instances learned : 1000
## Train error : 0.068
```

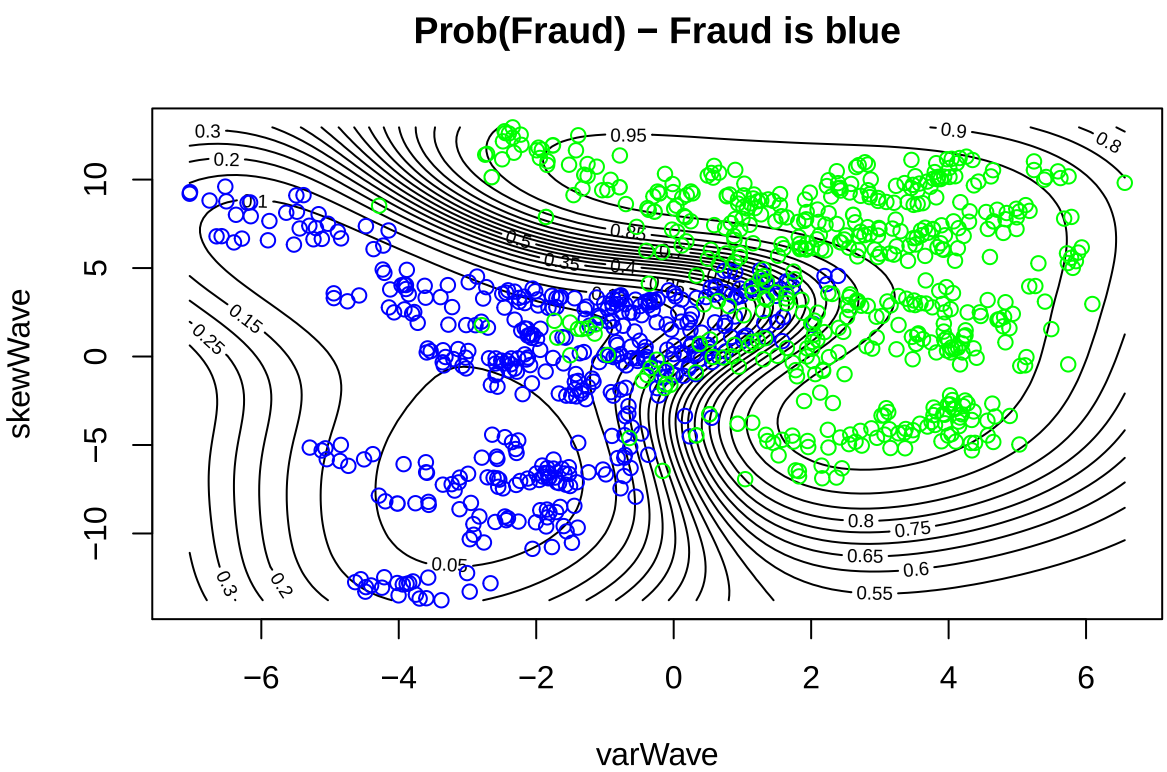
```r
# predict on the training set
trainPredict = predict(GPfitFraud,trainingData[,1:2])
confusionMatrix = table(trainPredict, trainingData[,5])
trainAccuracy = sum(diag(confusionMatrix))/sum(confusionMatrix)
trainAccuracy
```

```
## [1] 0.932
```

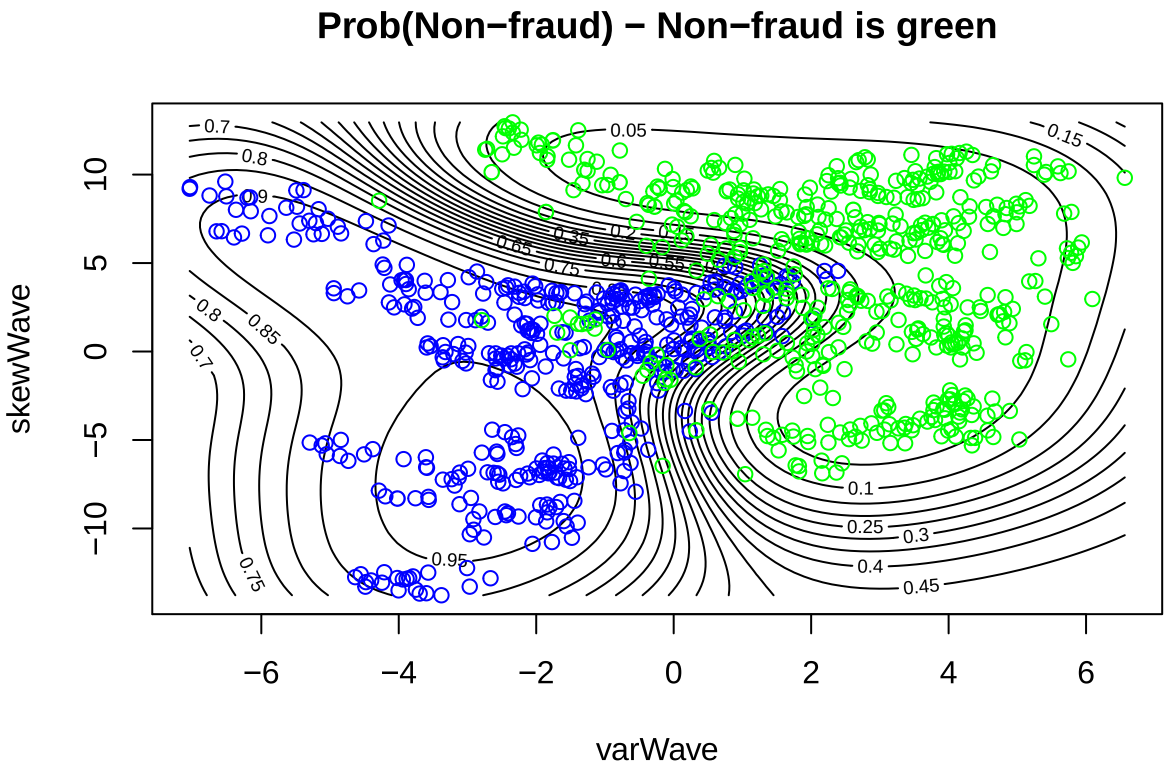
```r
cat('The training accuracy for the training data is: ', trainAccuracy)
```

```
## The training accuracy for the training data is:  0.932
```

```r
#Plotting class probabilities
# class probabilities
probPreds <- predict(GPfitFraud, trainingData[,1:2], type="probabilities")
x1 <- seq(min(trainingData[,1]),max(trainingData[,1]),length=100)
x2 <- seq(min(trainingData[,2]),max(trainingData[,2]),length=100)
gridPoints <- meshgrid(x1, x2)
gridPoints <- cbind(c(gridPoints$x), c(gridPoints$y))

gridPoints <- data.frame(gridPoints)
names(gridPoints) <- names(trainingData)[1:2]
probPreds <- predict(GPfitFraud, gridPoints, type="probabilities")

# Plotting for Prob(Fraud)
contour(x1,x2,matrix(probPreds[,1],100,byrow = TRUE),
        20,
        xlab = "varWave",
        ylab = "skewWave",
        main = 'Prob(Fraud) - Fraud is blue')
points(trainingData[trainingData[,5]==1,1],trainingData[trainingData[,5]==1,2],col="blue")
points(trainingData[trainingData[,5]==0,1],trainingData[trainingData[,5]==0,2],col="green")
```




```r
# Plotting for Prob(Non-fraud)
contour(x1,x2,matrix(probPreds[,2],100,byrow = TRUE),
        20,
        xlab = "varWave",
        ylab = "skewWave",
        main = 'Prob(Non-fraud) - Non-fraud is green')
points(trainingData[trainingData[,5]==1,1],trainingData[trainingData[,5]==1,2],col="blue")
points(trainingData[trainingData[,5]==0,1],trainingData[trainingData[,5]==0,2],col="green")
```



Question3-2:

Using the estimated model from (1), make predictions for the test set. Compute the accuracy.

```
testPredict = predict(GPfitFraud,testingData[,1:2])
confusionMatrix = table(testPredict, testingData[,5])
testAccuracy = sum(diag(confusionMatrix))/sum(confusionMatrix)
cat('The accuracy for the testing data is: ', testAccuracy)
```

```
## The accuracy for the testing data is:  0.9354839
```

Question3-3:

Train a model using all four covariates. Make predictions on the test set and compare the accuracy to the model with only two covariates.

```
GPfitFraudAll <- gausspr(fraud ~  varWave + skewWave + kurtWave + entropyWave, data=trainingData)
```

```
## Using automatic sigma estimation (sigest) for RBF or laplace kernel
```

```
GPfitFraudAll
```

```
## Gaussian Processes object of class "gausspr"
## Problem type: classification
##
## Gaussian Radial Basis kernel function.
##  Hyperparameter : sigma =  0.399933221120042
##
## Number of training instances learned : 1000
## Train error : 0.004
```

```
testAllPredict = predict(GPfitFraudAll,testingData[,1:4])
confusionMatrixAll = table(testAllPredict, testingData[,5])
testAllAccuracy = sum(diag(confusionMatrixAll))/sum(confusionMatrixAll)
cat('The test data accuracy when fitting the model with all the data is: ',testAllAccuracy)
```

```
## The test data accuracy when fitting the model with all the data is:  0.9973118
```

When fitting the model with all the data the accuracy increases up to 99 percent # References
Course Documents
https://stackoverflow.com/

Appendix

```
RNGversion('3.5.1')
knitr::opts_chunk$set(echo = TRUE)
library(kernlab)
library(AtmRay)
library(mvtnorm)
set.seed(111)
#The squared exponential function
SquaredExpKernel <- function(x1,x2,sigmaF=1,l=0.3){
  n1 <- length(x1)
  n2 <- length(x2)
  K <- matrix(NA,n1,n2)
  for (i in 1:n2){
    K[,i] <- sigmaF^2*exp(-0.5*( (x1-x2[i])/l)^2 )
  }
  return(K)
}
sigmaF = 1
l = 0.3
sigmaNoise = 0.1
xGrid <- seq(-1,1,length=20)
nSim = 1


#Question1:  The posterior function ########################################################
posteriorGP = function(X, y, XStar, sigmaNoise, k){
  #The algorithm
  K = k(X, X)
  n = length(X)

  L = chol(K + sigmaNoise^2*diag(n))
  alpha = solve(t(L),solve(L,y))

  if (length(XStar)==1){
    KStar = XStar
  }
  else{
    KStar = k(X,XStar)
  }

  FStar = t(KStar)*alpha
```

```r
  v = solve(L,KStar)
  VFStar = k(XStar, XStar)-t(v)%*%v
  logP = -0.5*t(y)%*%alpha - sum(log(diag(L))) - (n/2)*log(2*pi)

  return(list('mean'=FStar, 'variance'= VFStar, 'logMargLik' = logP))
}


#Question2: evaluating on (0.4,0.719)############################################
x = 0.4
y = 0.719
posteriorValue = posteriorGP(X = x,
                             y = y,
                             XStar = xGrid,
                             sigmaNoise = sigmaNoise,
                             k = SquaredExpKernel)
postMean = posteriorValue$mean
postVar = posteriorValue$variance

#Plotting the posterior mean
plotMean = function(mean,var, title){
  plot(xGrid, mean, type="p", ylab="f(x)", xlab="x", ylim = c(-2,2), main = title)

  #Plotting confidence band
  lines(xGrid, mean - 1.96*sqrt(diag(var)), col = "blue", lwd = 2)
  lines(xGrid, mean + 1.96*sqrt(diag(var)), col = "blue", lwd = 2)
}
par(mfrow = c(1,1))
plotMean(postMean,postVar, title = 'x = 0.4, y = 0.719')
x = c(0.4,-0.6)
y = c(0.719,-0.044)

posteriorValue2 = posteriorGP(X = x,
                              y = y,
                              XStar = xGrid,
                              sigmaNoise = sigmaNoise,
                              k = SquaredExpKernel)
postMean2 = posteriorValue2$mean
postVar2 = posteriorValue2$variance

par(mfrow = c(1,2))
plotMean(postMean2[,1], postVar2, title = 'x = 0.4, y = 0.719')
plotMean(postMean2[,2], postVar2, title = 'x = -0.6, y = -0.044')


#Question4: The posterior with five observations################################
x = c(0.4, -0.6, -1.0, -0.6, -0.2, 0.4, 0.8)
y = c(0.719, -0.044, 0.768, -0.044, -0.940, 0.719, -0.664)

posteriorValue3 = posteriorGP(X = x,
                              y = y,
                              XStar = xGrid,
                              sigmaNoise = sigmaNoise,
```

```
                              k = SquaredExpKernel)
postMean3 = posteriorValue3$mean
postVar3 = posteriorValue3$variance

par(mfrow=c(1,2))
for (i in 1:length(x)){
  plotMean(postMean3[,i],postVar3, title = paste('x = ',x[i], ',  y = ',y[i]))
}

#Question5: Repeating with different hyperparameters.

sigmaF = 1
L = 1
posteriorValue4 = posteriorGP(X = x,
                              y = y,
                              XStar = xGrid,
                              sigmaNoise = sigmaNoise,
                              k = SquaredExpKernel)
postMean4 = posteriorValue4$mean
postVar4 = posteriorValue4$variance

for (i in 1:length(x)){
  plotMean(postMean4[,i],postVar4, title = paste('x = ',x[i], ',  y = ',y[i]))
}

data = read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/TempTullinge.cs

date = data$date
time = c(1:dim(data)[1])
temp = data$temp
day = rep(c(1:365), length(time)/365)

#Takinng every fifth observation

time = seq(from = 1, to = length(time), by = 5)
day = day[time]
scaledTime = (time-mean(time))/sd(time)
Matern32 <- function(sigmaf = 1, ell = 1)
{
  rval <- function(x, y = NULL) {
    r = sqrt(crossprod(x-y));
    return(sigmaf^2*(1+sqrt(3)*r/ell)*exp(-sqrt(3)*r/ell))
  }
  class(rval) <- "kernel"
  return(rval)
}

#Evaluating the function
MaternFunc = Matern32(sigmaf = 20, ell = 0.2) # MaternFunc is a kernel FUNCTION
MaternFunc(1,2)

#Computing the covarance matrix K
X = c(1,3,4)
```

```r
Xstar = c(2,3,4)

K <- kernelMatrix(kernel = MaternFunc, x = X, y = Xstar)
K
#Letting sigma noise equal to residual variance of a quadratic regression fit using lm
modelData = data.frame(data$temp[time], scaledTime)
colnames(modelData) = c('temp', 'time')
polyFit <- lm(temp ~ time + I(time^2) + I(time^3), data = modelData)
sigmaNoise = sd(polyFit$residuals)
cat('sigmaNoise is: ',sigmaNoise)

plot(scaledTime,data$temp[time], ylim = c(-25,35))

# Fit the GP with Square expontial kernel

MaternFunc = Matern32(sigmaf = 20, ell = 0.2)
GPfit <- gausspr(scaledTime, data$temp[time],
                 kernel = MaternFunc,
                 kpar = list(sigmaf = 20, ell = 0.2),
                 var = sigmaNoise^2)
meanPred <- predict(GPfit, scaledTime)
lines(scaledTime, meanPred, col="blue", lwd = 2)


ell <- 0.5
SEkernel <- rbfdot(sigma = 1/(2*ell^2))

x<-scaledTime
xs<-scaledTime # XStar
n <- length(x)
Kss <- kernelMatrix(kernel = SEkernel, x = xs, y = xs)
Kxx <- kernelMatrix(kernel = SEkernel, x = x, y = x)
Kxs <- kernelMatrix(kernel = SEkernel, x = x, y = xs)
Covf = Kss-t(Kxs)%*%solve(Kxx + sigmaNoise^2*diag(n), Kxs) # Covariance matrix of fStar

# Probability intervals for fStar
plot(scaledTime,data$temp[time], ylim = c(-25,35))
lines(scaledTime, meanPred, col="blue", lwd = 2)

lines(xs, meanPred - 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)
lines(xs, meanPred + 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)

# Prediction intervals for yStar
lines(xs, meanPred - 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")
lines(xs, meanPred + 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")

legend("bottomright",
       legend = c('Post Mean Model1'),
       col = c( 'blue'),
       lty=1:2,
       cex=0.8)
legend("topright",
       legend = c('prob interval',
```

```
                'pred interval'),
       col = c('green', 'brown'),
       lty=1:2,
       cex=0.8,
       horiz = TRUE)

#Letting sigma noise equal to residual variance of a quadratic regression fit using lm
modelData = data.frame(data$temp[time], day)
colnames(modelData) = c('temp', 'day')
polyFit <- lm(temp ~ day + I(day^2) + I(day^3), data = modelData)
sigmaNoise = sd(polyFit$residuals)
sigmaNoise

# Fit the GP with built in Square expontial kernel (called rbfdot in kernlab)

MaternFunc = Matern32(sigmaf = 20, ell = 0.2)
GPfit <- gausspr(day,
                 data$temp[time],
                 kernel = MaternFunc,
                 kpar = list(sigmaf = 20, ell = 0.2),
                 var = sigmaNoise^2)
meanPred2 <- predict(GPfit, day)

plot(scaledTime,data$temp[time], ylim = c(-25,35))
lines(scaledTime, meanPred, col="blue", lwd = 2)
# Probability intervals for fStar
lines(xs, meanPred - 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)
lines(xs, meanPred + 1.96*sqrt(diag(Covf)), col = "green", lwd = 2)

# Prediction intervals for yStar
lines(xs, meanPred - 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")
lines(xs, meanPred + 1.96*sqrt((diag(Covf) + sigmaNoise^2)), col = "brown")
lines(scaledTime, meanPred2, col="red", lwd = 2)
legend("bottomright",
       legend = c('Post Mean Model1',
                'Post Mean Model2'),
       col = c( 'blue', 'red'),
       lty=1:2,
       cex=0.8)
legend("topright",
       legend = c('prob interval',
                'pred interval'),
       col = c('green', 'brown'),
       lty=1:2,
       cex=0.8,
       horiz = TRUE)



#The first model has a smoother posterior mean than the second model, the second model seems not smooth


GPKernel = function(l1,l2, sigmaF, d){
```

```
  rval <- function(x1, x2 = NULL) {
    return(sigmaF^2 * exp(-(2*(sin(pi*abs(x1-x2)/d))^2)/l1^2)*(exp(-0.5*abs(x1-x2)^2)/l2^2))
  }
  class(rval) <- "kernel"
  return(rval)

}

l1 = 1
l2 = 10
sigmaF = 20
d = 365/sd(time)

GPKernelFun = GPKernel(l1,l2,sigmaF, d)
GPKernelFun(1,2)

#Fitting the generlaized model
GPfit <- gausspr(scaledTime, data$temp[time],
                 kernel = GPKernelFun,
                 kpar = list(sigmaF = sigmaF, l1 = l1, l2 = l2, d=d),
                 var = sigmaNoise^2)
meanPred3 <- predict(GPfit, scaledTime)
plot(time,data$temp[time], ylim = c(-25,30), main = 'Generalized Model')
lines(time, meanPred3, col="blue", lwd = 2)
lines(time, meanPred, col="red", lwd = 2)
lines(time, meanPred2, col="green", lwd = 2)
legend("bottomright",
       legend = c('Generalized Fit',
                  'Model 1 Fit',
                  'Model 2 Fit'),
       col = c('blue', 'red', 'green'),
       lty=1:2,
       cex=0.8,
       horiz = TRUE)


data = read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/banknoteFraud.
names(data) = c("varWave","skewWave","kurtWave","entropyWave","fraud")
data[,5] = as.factor(data[,5])

#Dividing the data into training and testing
set.seed(111)
SelectTraining = sample(1:dim(data)[1],
                        size = 1000,
                        replace = FALSE)
trainingData = data[SelectTraining,]
testingData = data[-SelectTraining,]

GPfitFraud <- gausspr(fraud ~  varWave + skewWave, data=trainingData)
GPfitFraud

# predict on the training set
trainPredict = predict(GPfitFraud,trainingData[,1:2])
```

```r
confusionMatrix = table(trainPredict, trainingData[,5])
trainAccuracy = sum(diag(confusionMatrix))/sum(confusionMatrix)
trainAccuracy

cat('The training accuracy for the training data is: ', trainAccuracy)

#Plotting class probabilities
# class probabilities
probPreds <- predict(GPfitFraud, trainingData[,1:2], type="probabilities")
x1 <- seq(min(trainingData[,1]),max(trainingData[,1]),length=100)
x2 <- seq(min(trainingData[,2]),max(trainingData[,2]),length=100)
gridPoints <- meshgrid(x1, x2)
gridPoints <- cbind(c(gridPoints$x), c(gridPoints$y))

gridPoints <- data.frame(gridPoints)
names(gridPoints) <- names(trainingData)[1:2]
probPreds <- predict(GPfitFraud, gridPoints, type="probabilities")

# Plotting for Prob(Fraud)
contour(x1,x2,matrix(probPreds[,1],100,byrow = TRUE),
        20,
        xlab = "varWave",
        ylab = "skewWave",
        main = 'Prob(Fraud) - Fraud is blue')
points(trainingData[trainingData[,5]==1,1],trainingData[trainingData[,5]==1,2],col="blue")
points(trainingData[trainingData[,5]==0,1],trainingData[trainingData[,5]==0,2],col="green")

# Plotting for Prob(Non-fraud)
contour(x1,x2,matrix(probPreds[,2],100,byrow = TRUE),
        20,
        xlab = "varWave",
        ylab = "skewWave",
        main = 'Prob(Non-fraud) - Non-fraud is green')
points(trainingData[trainingData[,5]==1,1],trainingData[trainingData[,5]==1,2],col="blue")
points(trainingData[trainingData[,5]==0,1],trainingData[trainingData[,5]==0,2],col="green")

testPredict = predict(GPfitFraud,testingData[,1:2])
confusionMatrix = table(testPredict, testingData[,5])
testAccuracy = sum(diag(confusionMatrix))/sum(confusionMatrix)
cat('The accuracy for the testing data is: ', testAccuracy)


GPfitFraudAll <- gausspr(fraud ~  varWave + skewWave + kurtWave + entropyWave, data=trainingData)
GPfitFraudAll

testAllPredict = predict(GPfitFraudAll,testingData[,1:4])
confusionMatrixAll = table(testAllPredict, testingData[,5])
testAllAccuracy = sum(diag(confusionMatrixAll))/sum(confusionMatrixAll)
cat('The test data accuracy when fitting the model with all the data is: ',testAllAccuracy)
```