

# Report

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## #1. Implementing GP Regression

### 1.1

```
# Covariance function
SquaredExpKernel <- function(x1,x2,sigmaF=1,l=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)
}

posteriorGP = function(X , y , XStar, sigmaNoise , sigmaF , l){
  #Inputs
  #X: Vector of training inputs.
  #y: Vector of training targets/outputs.
  #XStar: Vector of inputs where the posterior distribution is evaluated
  #sigmaNoise: Noise standard deviation

  #k: Covariance function or kernel. #SquaredExpKernel
  k = SquaredExpKernel(x1 = X, x2 = X , sigmaF = sigmaF , l = l)

  L_upper = chol(k + (sigmaNoise * diag(length(diag(k))))))

  #since as per documentation of chol function, it returns upper triangle,
  #we have to take transpose of it

  L = t(L_upper)

  #now in order to calculate alpha we have alpha = L.Transpose / (L/y)
  #now using Ax = b => x = b/A so to find L/y solution we can use solve function

  L_by_y = solve(L , y)

  #now trans(x.trans) = x so we can use L_Upper directly
  alpha = solve(L_upper , L_by_y)
```

```

K_Star = SquaredExpKernel(x1 = X, x2 = XStar , sigmaF = sigmaF , l = 1)

#predicted mean
f.Star = t(K_Star) %*% alpha

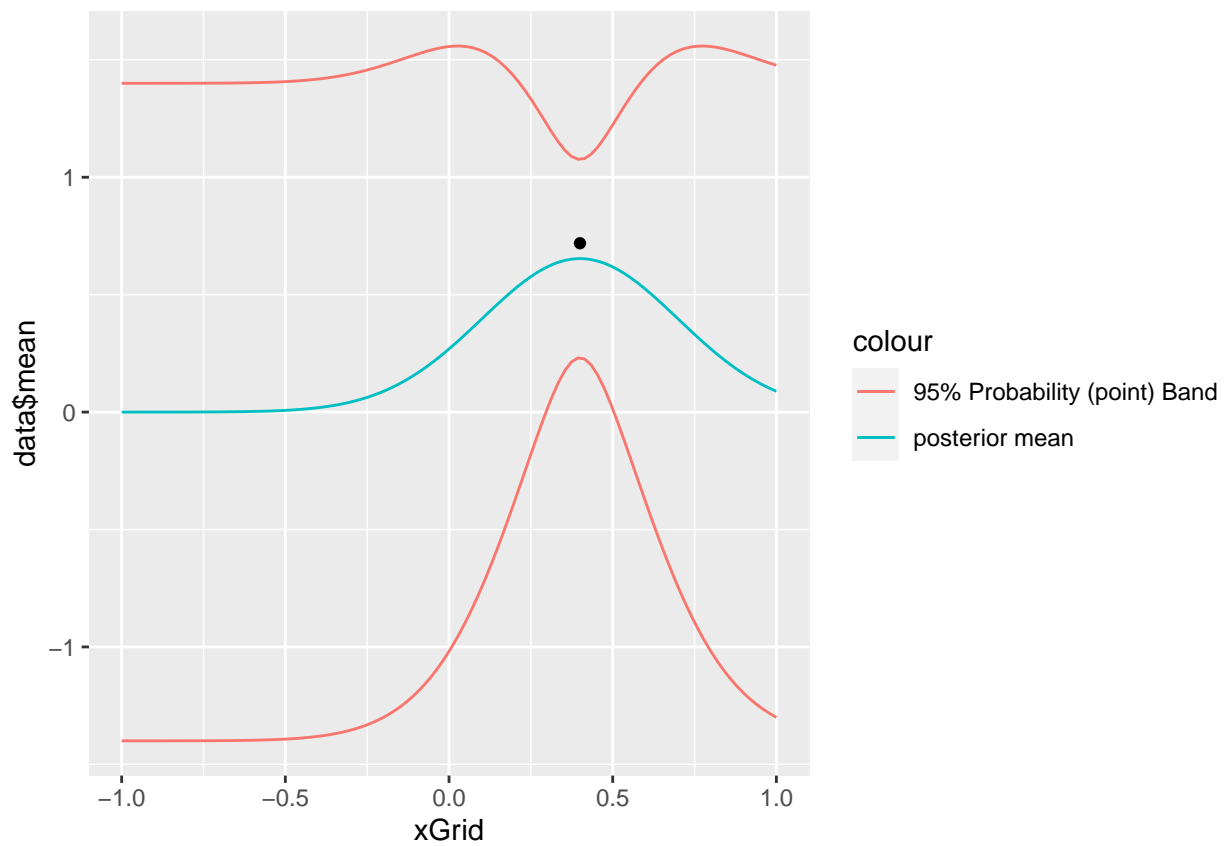
v = solve(L , K_Star)
#predicted Variance
V_f.Star = SquaredExpKernel(x1 = XStar, x2 = XStar ,
                             sigmaF = sigmaF , l = 1) - (t(v) %*% v)

#taking diagonol elements of covariance matrix for variance in ii
V_f.Star = diag(V_f.Star)
#log marginal likelihood
#logMargLikeli = -(0.5 * t(y) %*% alpha) -

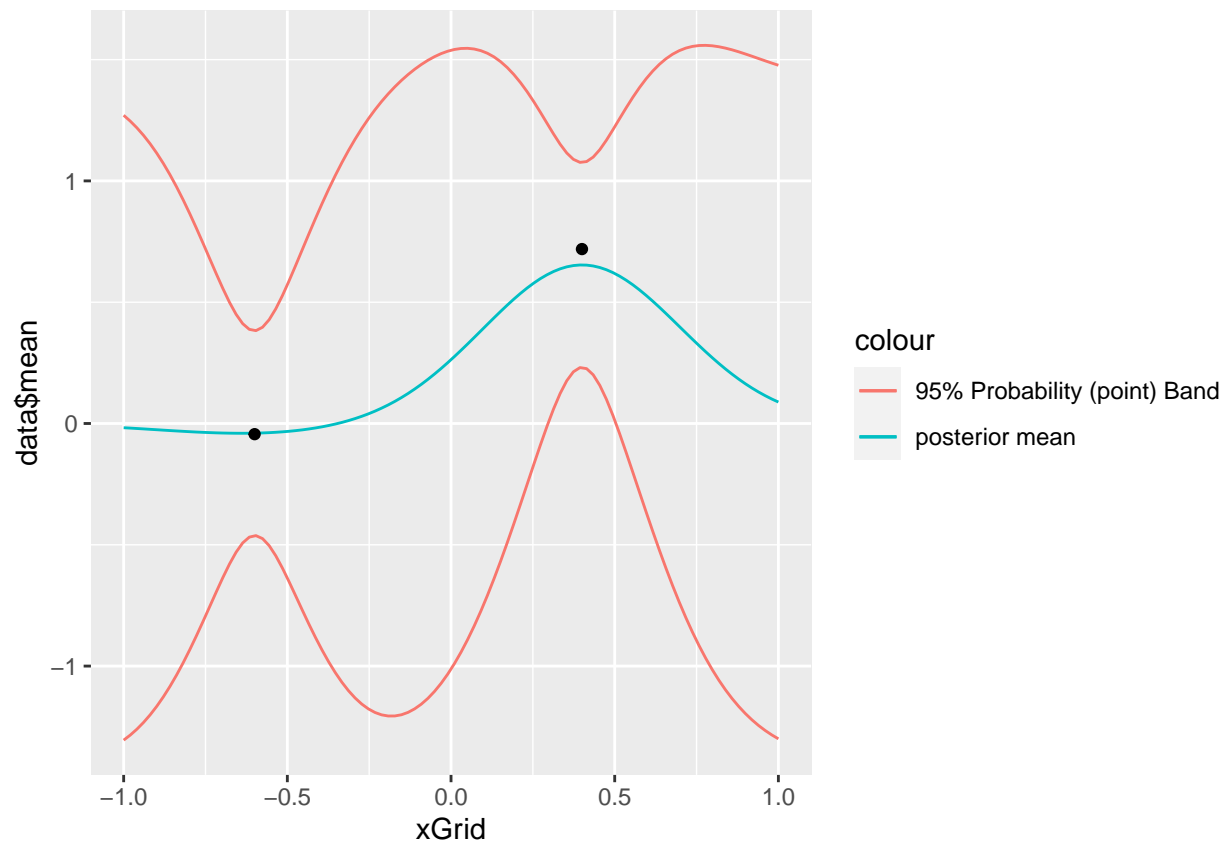
return(list("mean" = f.Star , "Variance" = V_f.Star))
}#posteriorDist

```

1.2



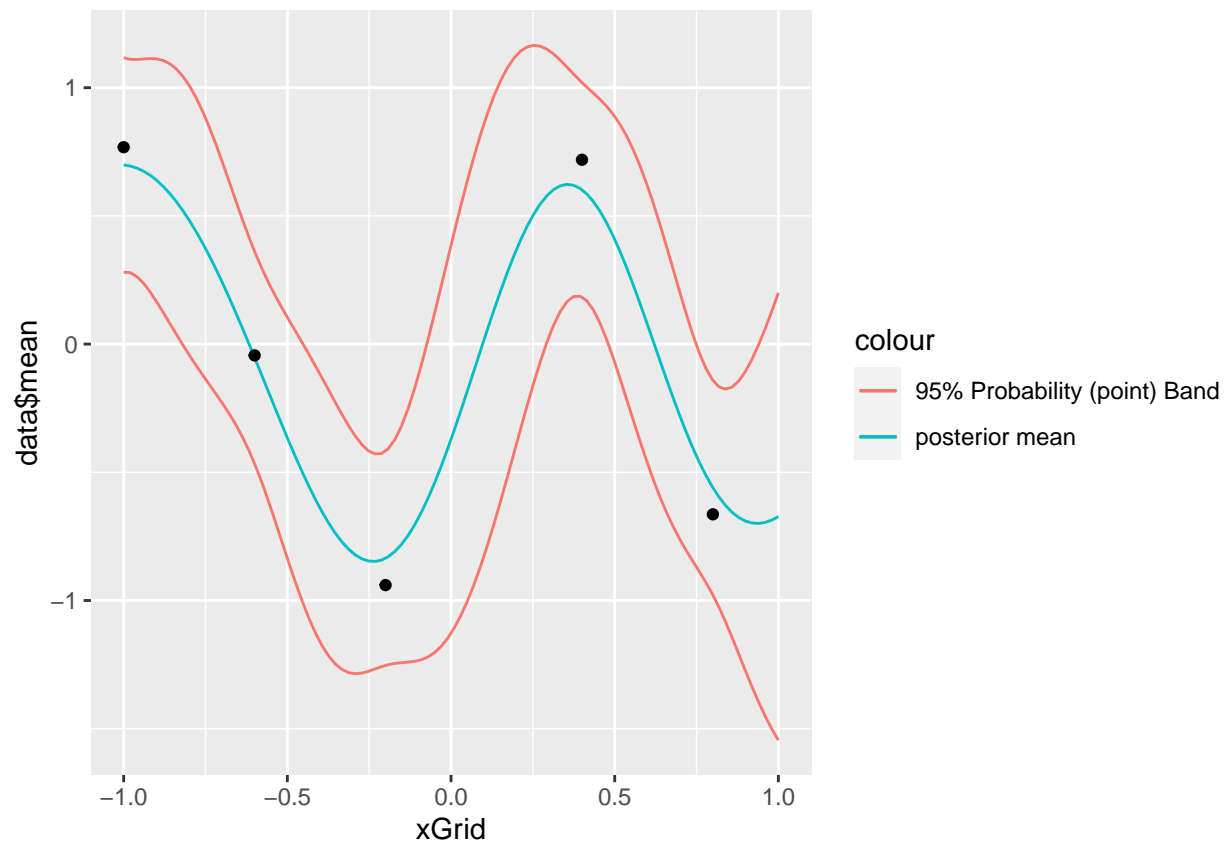
1.3



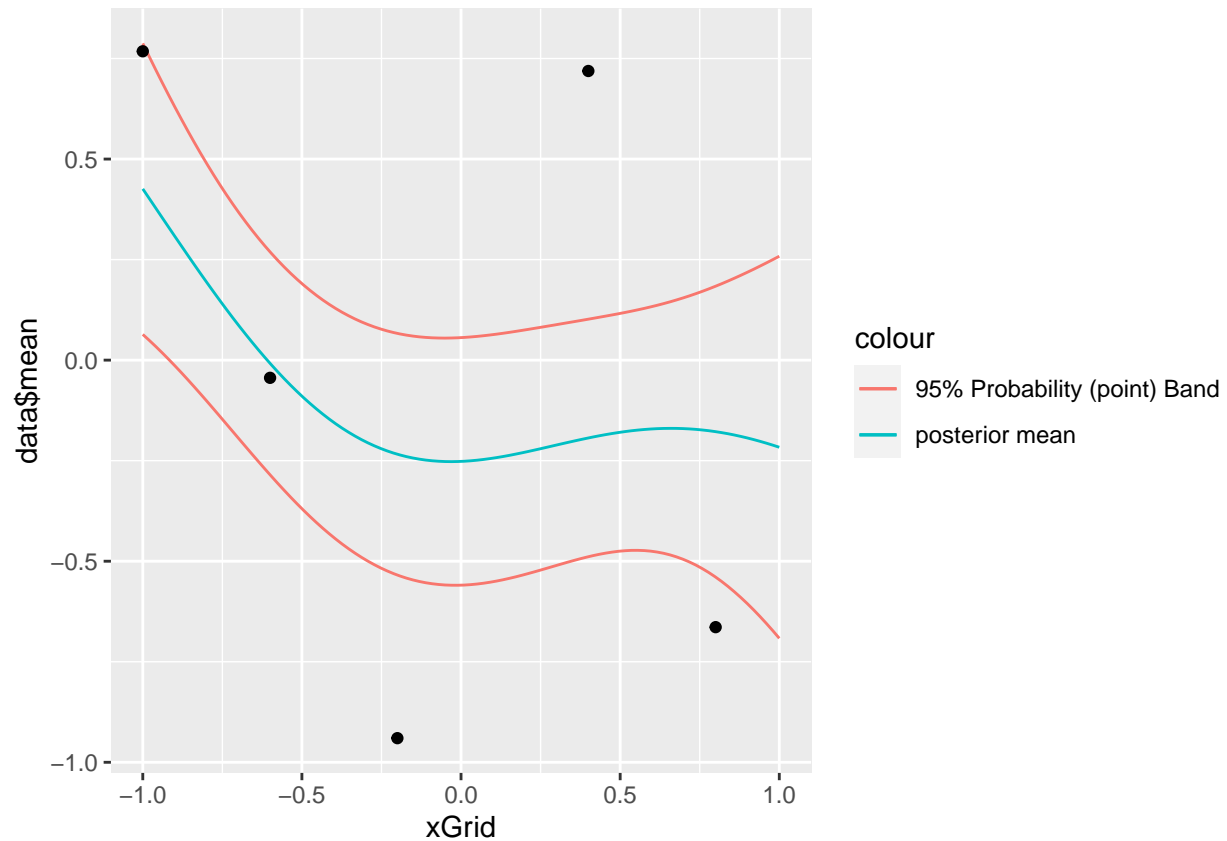
1.4

## Table of data points

##	[,1]	[,2]	[,3]	[,4]	[,5]
## x	-1.000	-0.600	-0.20	0.400	0.800
## y	0.768	-0.044	-0.94	0.719	-0.664



1.5



## #2. GP Regression with kernlab

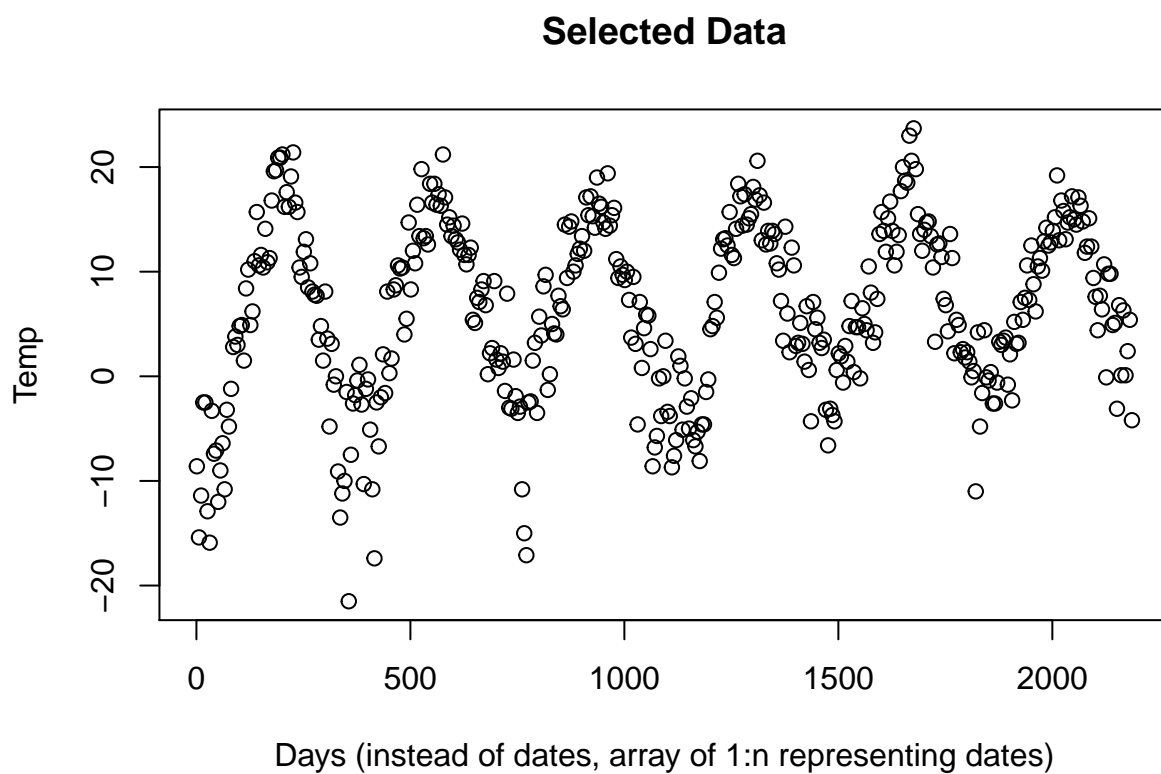
### 2.1

```
library(kernlab)
library(AtmRay)
#import data

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

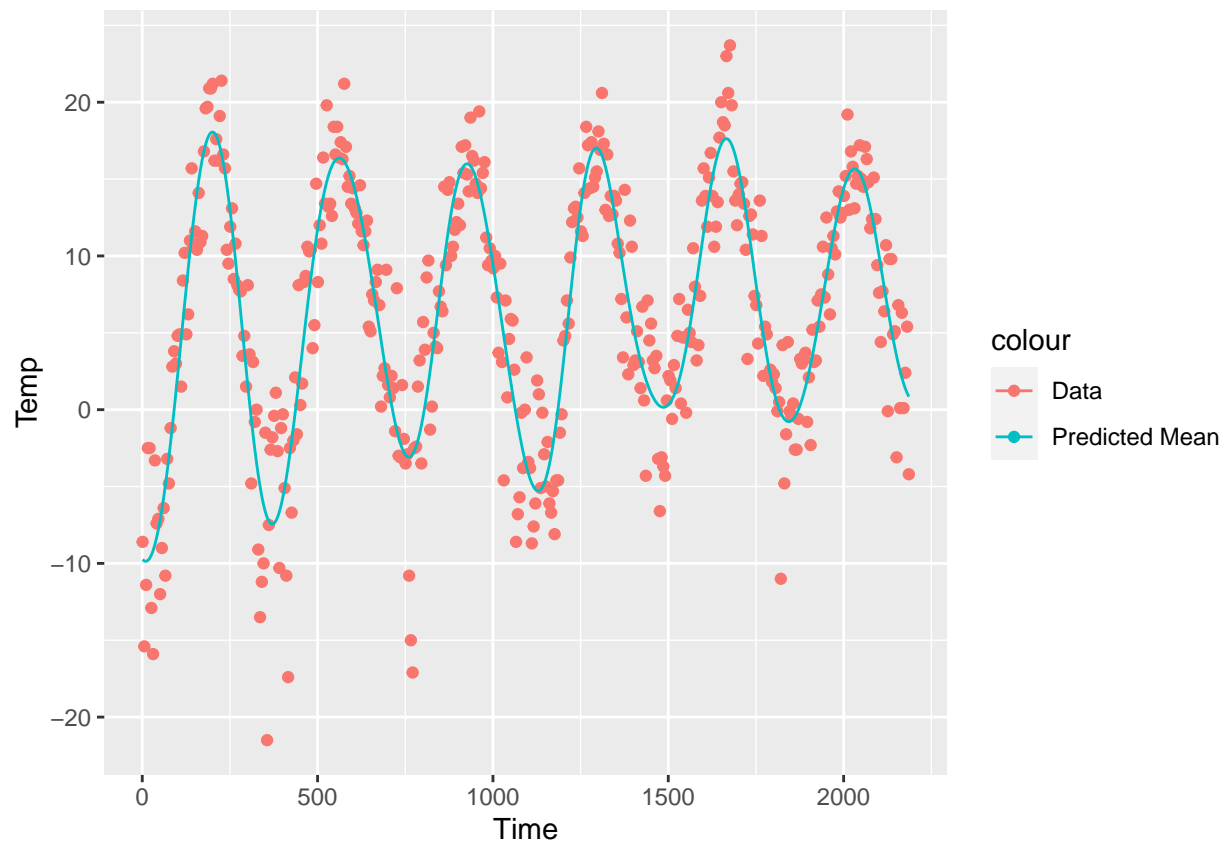
#create vector for time and date
#as per task comments
# Estimating a GP on 2190 observations can take some time on slower computers, so let us subsample the
# only every fifth observation. This means that your time and day variables are now time= 1, 6, 11, . . .
# day = 1, 6, 11, . . . , 361, 1, 6, 11, . . . , 361.
n = length(data$date)
time = seq(1, n, by = 5)
#leap year consideration is not catered for simplicity reasons
data.Day = rep(seq(1, 365, by = 5), times = (n/365))
data.Temp = data$temp[time]

plot(time, data.Temp, xlab = "Days (instead of dates, array of 1:n representing dates)",
      ylab = "Temp", main = "Selected Data",
      )
```

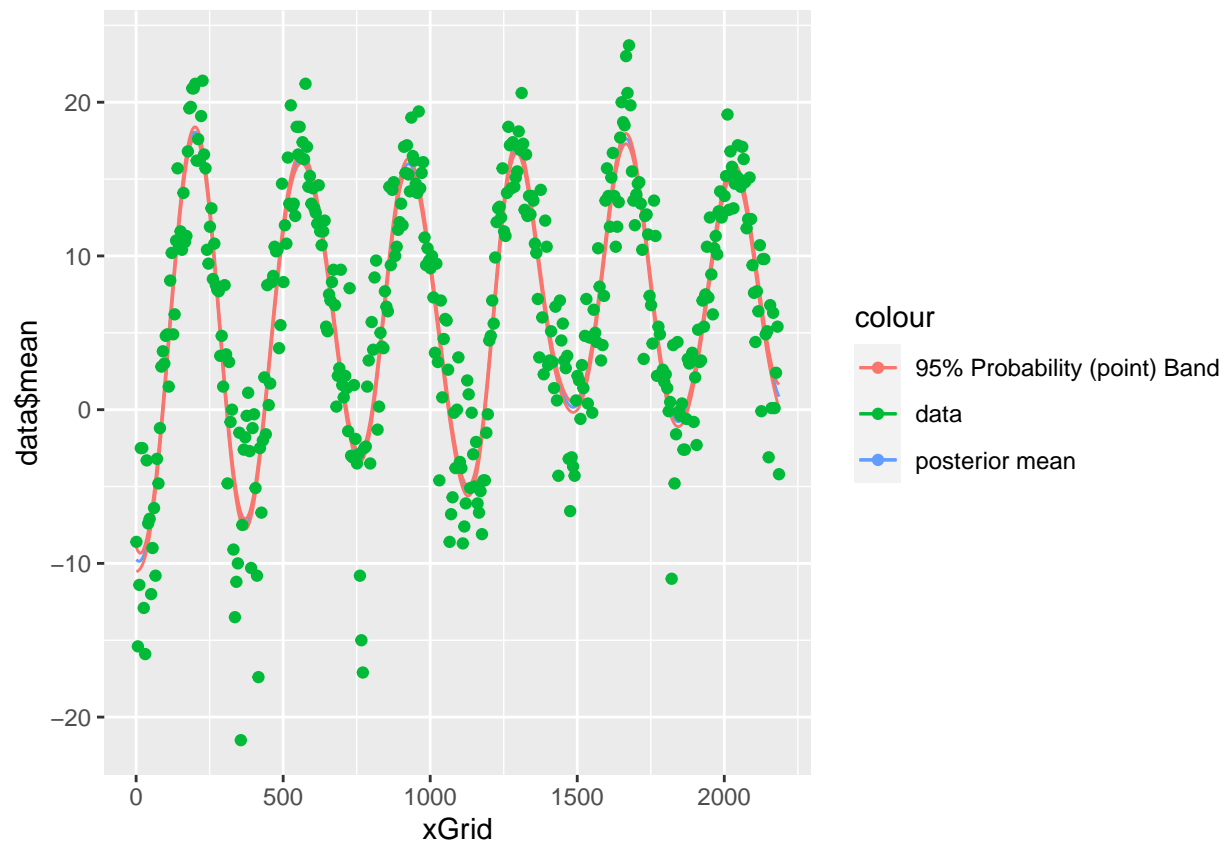


```
## Computed CoVariance Matrix is :  
  
## An object of class "kernelMatrix"  
##      [,1]      [,2]      [,3]  
## [1,] 0.6065307 0.1353353 0.0111090  
## [2,] 0.6065307 1.0000000 0.6065307  
## [3,] 0.1353353 0.6065307 1.0000000
```

2.2

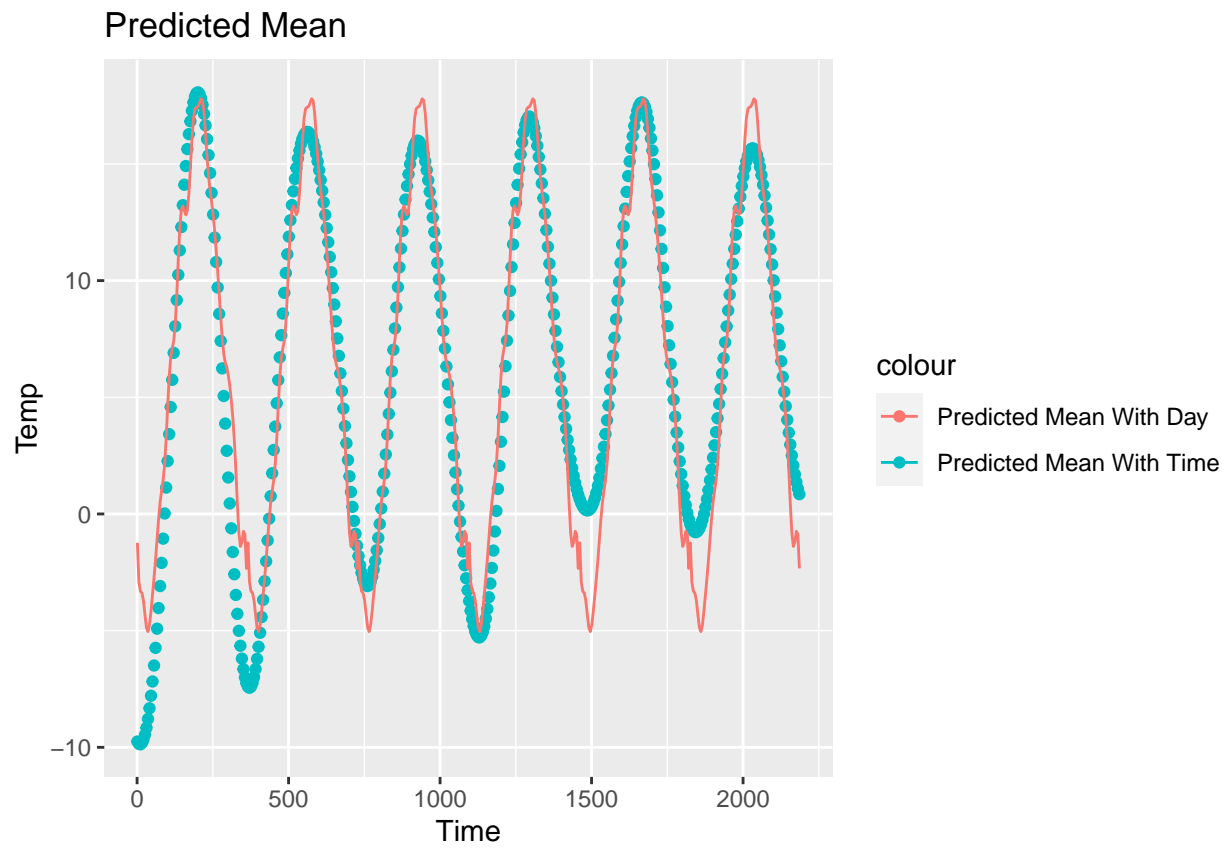


2.3

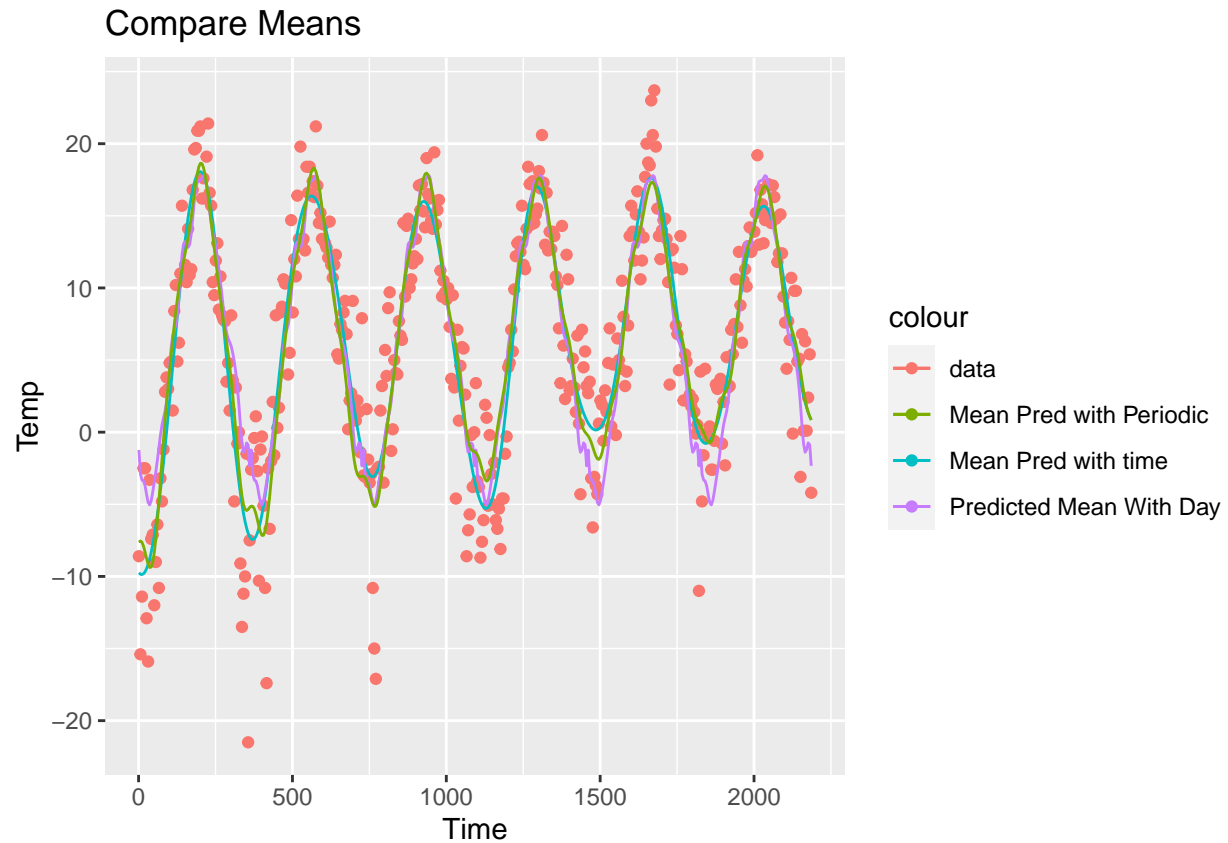


1.4





1.5



With mean value predicted with day values we can see that it is repeating in cycle which could be understood in terms of repeating value of days in band of 1 to 365 while mean predicted by Time is very smooth but it does not follow shift in data mass which is accurately captured in mean calculated by periodic kernel.

## GP Classification with kernlab

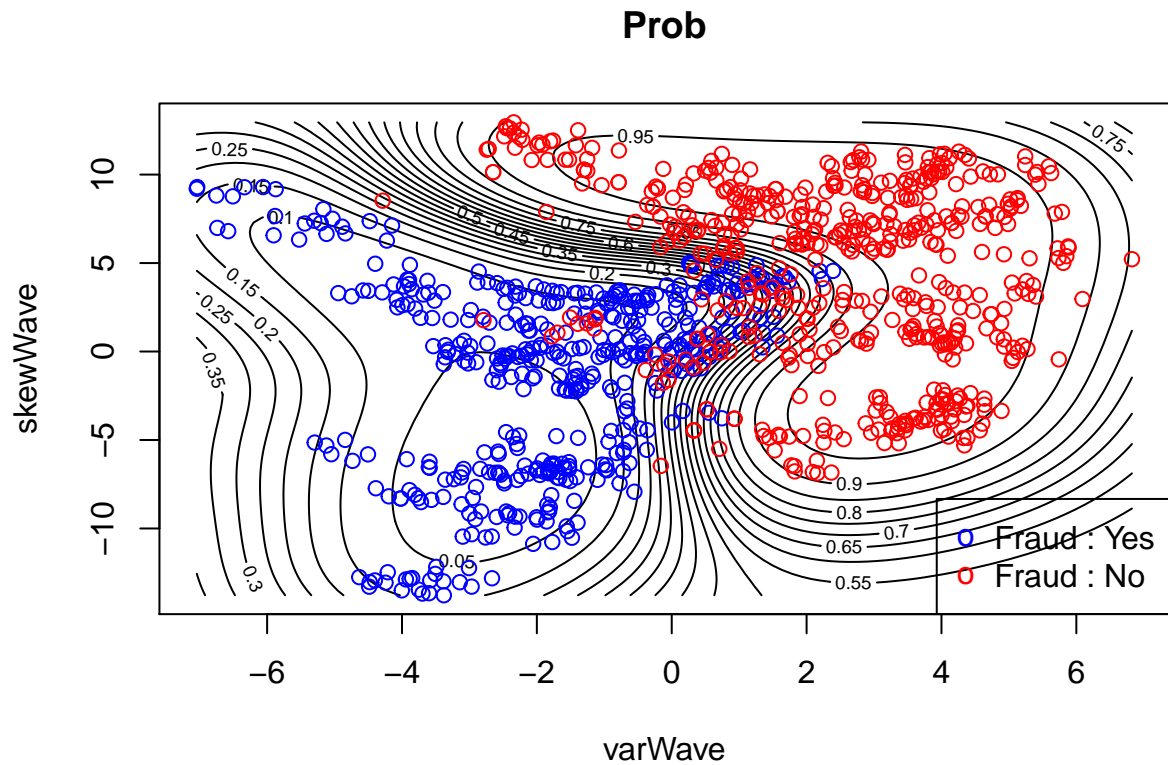
### 3.1

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

```
## Confusion Matrix for Train Data is :
```

```
##
## fraudPred  0   1
##           0 503  18
##           1  41 438
```

```
## Accuracy with Train data is : 0.941
```



### 3.2

## Confusion Matrix for Test Data is :

```
##
## fraudPred.Test    0    1
##                  0 199    9
##                  1   19 145
```

## Accuracy with Test data is : 0.9247312

### 3.3

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

## Confusion Matrix for Test Data using all parameter is :

```
##
## fraudPred.All     0    1
##                  0 216    0
##                  1   2 154
```

## Accuracy for Test data with all parameters is : 0.9946237

We can see test accuracy with test data when only two features were used is 92.42% while when all feature are used it is around 99%. It can be seen that only two features namely varWave and skewWave are important.

```
## rpart variable importance
##
##               Overall
## varWave       100.00
## skewWave       72.53
## kurtWave       11.45
## entropyWave    0.00
```

From above importance values, we can reconfirm our belief that only 2 parameters are majorly important and last one is not at all useful.

## Appendix

```
knitr::opts_chunk$set(echo = TRUE)
# Covariance function
SquaredExpKernel <- function(x1,x2,sigmaF=1,l=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)
}

posteriorGP = function(X , y , XStar, sigmaNoise , sigmaF , l){
  #Inputs
  #X: Vector of training inputs.
  #y: Vector of training targets/outputs.
  #XStar: Vector of inputs where the posterior distribution is evaluated
  #sigmaNoise: Noise standard deviation

  #k: Covariance function or kernel. #SquaredExpKernel
  k = SquaredExpKernel(x1 = X, x2 = X , sigmaF = sigmaF , l = l)

  L_upper = chol(k + (sigmaNoise * diag(length(diag(k))))))

  #since as per documentation of chol function, it returns upper triangle,
  #we have to take transpose of it

  L = t(L_upper)

  #now in order to calculate alpha we have alpha = L.Transpose / (L/y)
  #now using Ax = b => x = b/A so to find L/y solution we can use solve function

  L_by_y = solve(L , y)

  #now trans(x.trans) = x so we can use L_Upper directly
  alpha = solve(L_upper , L_by_y)
```

```

K_Star = SquaredExpKernel(x1 = X, x2 = XStar , sigmaF = sigmaF , l = 1)

#predicted mean
f.Star = t(K_Star) %*% alpha

v = solve(L , K_Star)
#predicted Variance
V_f.Star = SquaredExpKernel(x1 = XStar, x2 = XStar ,
                             sigmaF = sigmaF , l = 1) - (t(v) %*% v)

#taking diagonol elements of covariance matrix for variance in ii
V_f.Star = diag(V_f.Star)
#log marginal likelihood
#logMargLikeli = -(0.5 * t(y) %*% alpha) -

  return(list("mean" = f.Star , "Variance" = V_f.Star))
}#posteriorDist

xGrid = seq(-1,1,length = 100)

#prior
xPrior = 0.4
yPrior = 0.719

#hyperParameter
sigmaF = 1
l = 0.3

SigmaN = 0.1

posteriorF = posteriorGP(X = xPrior , y = yPrior , XStar = xGrid ,
                         sigmaNoise = SigmaN ,
                         sigmaF = sigmaF , l = 1
                         )

#95% Z = 1.96
library(ggplot2)

fnPlot = function(data, xGrid , main.T , xhigh , yhigh , high = TRUE,
                  XStarPlot = FALSE, OrigData = NA ){
  l.band = data$mean - sqrt(1.96 * data$Variance)
  u.band = data$mean + sqrt(1.96 * data$Variance)

  p = ggplot()+
    geom_line(aes(x = xGrid , y = data$mean , color = "posterior mean"))+
    geom_line(aes(x = xGrid , y = l.band , color = "95% Probability (point) Band"))+
    geom_line(aes(x = xGrid , y = u.band , color = "95% Probability (point) Band"))

  if(high == TRUE)
    p = p + geom_point(aes(x = xhigh , y = yhigh ))

```

```

if(XStarPlot == TRUE)
  p = p + geom_point(aes(x = xGrid , y = OrigData , color = "data"))

p + xlab("X Grid") + ylab("Posterior Mean") +
  ggtitle(main.T)

return(p)
}#fnPlot

fnPlot(data = posteriorF , xGrid = xGrid , main.T = "Posterior Mean" ,
  xhigh = 0.4 , yhigh = 0.719 )

xNew = c(0.4 , -0.6 )
yNew = c(0.719 , -0.044)

posteriorF2 = posteriorGP(X = xNew , y = yNew , XStar = xGrid ,
  sigmaNoise = SigmaN ,
  sigmaF = sigmaF , l = 1
)

fnPlot(data = posteriorF2 , xGrid = xGrid , main.T = "Posterior Mean" ,
  xhigh = xNew , yhigh = yNew )

data = c(-1,-0.6,-0.2,0.4,0.8,0.768,-0.044,-0.940,0.719,-0.664)

data = matrix(data,nrow = 2 , byrow = TRUE)
rownames(data) = c("x" , "y")

cat("\n")
cat("      Table of data points")
cat("\n")
cat("\n")
cat("\n")
data
cat("\n")

posteriorF2 = posteriorGP(X = data[1,] , y = data[2,] , XStar = xGrid ,
  sigmaNoise = SigmaN ,
  sigmaF = sigmaF , l = 1
)

fnPlot(data = posteriorF2 , xGrid = xGrid , main.T = "Posterior Mean" ,
  xhigh = data[1,] , yhigh = data[2,] )

#updated l to 1 and sigmaF is already 1

posteriorF2 = posteriorGP(X = data[1,] , y = data[2,] , XStar = xGrid ,

```

```

        sigmaNoise = SigmaN ,
        sigmaF = sigmaF , l = 1
    )

fnPlot(data = posteriorF2 , xGrid = xGrid , main.T = "Posterior Mean" ,
       xhigh = data[1,] , yhigh = data[2,] )

library(kernlab)
library(AtmRay)
#import data

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

#create vector for time and date
#as per task comments
# Estimating a GP on 2190 observations can take some time on slower computers, so let us subsample the
# only every fifth observation. This means that your time and day variables are now time= 1, 6, 11, . . .
# day = 1, 6, 11, . . . , 361, 1, 6, 11, . . . , 361.
n = length(data$date)
time = seq(1 , n , by = 5)
#leap year consideration is not catered for simplicity reasons
data.Day = rep(seq(1 , 365 , by = 5) , times = (n/365))
data.Temp = data$temp[time]

plot(time , data.Temp , xlab = "Days (instead of dates, array of 1:n representing dates)" ,
     ylab = "Temp" , main = "Selected Data"
    )
#given
x = 1
x2 = 2
X = c(1,3,4)
XStar = c(2,3,4)
library(kernlab)
#ell = 1
SqrExpFn <- function(sigmaf = 1, l = 1)
{
    SquaredExpKernel2 <- function(x , y)
    {
        n1 <- length(x)
        n2 <- length(y)
        K <- matrix(NA,n1,n2)
        for (i in 1:n2)
            K[,i] <- sigmaf^2*exp(-0.5*( (x-y[i])/l)^2 )

        return(K)
    }#SquaredExpKernel2

    class(SquaredExpKernel2) <- "kernel"

    return(SquaredExpKernel2)
}

```

```

}#SqrExpFn

#to compute covariance matrix
K = kernelMatrix(kernel = SqrExpFn() , x = X , y = XStar)

cat("Computed CoVariance Matrix is :")
cat("\n")
K
cat("\n")

#calculate sigmaN as residual variance from a simple quadratic regression fit
#since f is distributed with mean 0 , we have to scale our data

scaledData.Temp = scale(data.Temp)
scaleData.Time = scale(time)

quadReg = lm(scaledData.Temp ~ scaleData.Time + I(scaleData.Time)**2)
SigmaN = sd(quadReg$residuals)

#New
#sigmaF = 20
#l = 0.2

#gausspr is an implementation of Gaussian processes for classification and regression

GaussianModel = gausspr(x = time , y = data.Temp ,
                        kernel = SqrExpFn(sigmaF = 20 , l = 0.2) ,
                        var = SigmaN**2,
                        type = "regression"
                        )

meanPredicted = predict(GaussianModel , time)

ggplot()+
  geom_point(aes(x = time , y = data.Temp , color = "Data")) +
  geom_line(aes(x = time , y = meanPredicted[,1] , color = "Predicted Mean"))+
  xlab("Time") + ylab("Temp")

#now posterior mean can be calculated using our function : posteriorGP
#as in this function XStar: Vector of inputs where the posterior distribution is evaluated, we can pass

#we have to use scaled data in order to match output of gausspr function
#scaling is already implemented for LinReg Part

#posteriorGP = function(X , y , XStar, sigmaNoise , sigmaF , l)

posterVariance = posteriorGP(X = scaleData.Time , y = scaledData.Temp ,
                           XStar = scaleData.Time , sigmaNoise = SigmaN,
                           sigmaF = 20 , l = 0.2
                           )$Variance

```



```

#unscaledPostVar = posterVariance * sd(posterVariance) + mean(posterVariance) + posterVariance

lPlot = list("mean" = meanPredicted , "Variance" = posterVariance)

fnPlot(data = lPlot , xGrid = time , main.T = "Posterior Mean and Variance" ,
        xhigh = 0 , yhigh = 0, high = FALSE , XStarPlot = TRUE , OrigData = data.Temp )

scaleData.Day = scale(data.Day)

quadReg2 = lm(scaledData.Temp ~ scaleData.Day + I(scaleData.Day)**2)
SigmaN2 = sd(quadReg2$residuals)

#New
#sigmaF = 20
#l = 0.2

#gausspr is an implementation of Gaussian processes for classification and regression

GaussianModel2 = gausspr(x = data.Day , y = data.Temp ,
                          kernel = SqrExpFn(sigmaF = 20 , l = 0.2) ,
                          var = SigmaN2**2,
                          type = "regression"
                          )

meanPredicted2 = predict(GaussianModel2 , data.Day)

ggplot()+
  geom_point(aes(x = time , y = meanPredicted[,1] , color = "Predicted Mean With Time")) +
  geom_line(aes(x = time , y = meanPredicted2[,1] , color = "Predicted Mean With Day"))+
  xlab("Time") + ylab("Temp") + ggtitle("Predicted Mean")

SqrExpFn2 <- function(sigmaF , l1 , l2, d )
{
  SquaredExpKernel2 <- function(x1,x2)
  {
    e1 = exp(-(2*sin(pi * abs(x1 - x2) / d)**2) / l1**2)
    e2 = exp(-(0.5 * abs(x1 - x2)**2) / l2**2 )
    K = (sigmaF^2) * e1 * e2
    return(K)
  }

  class(SquaredExpKernel2) <- "kernel"

  return(SquaredExpKernel2)
}#SqrExpFn

d = 365 / sd(time)

```

```

GaussianModel2 = gausspr(x = time , y = data.Temp ,
                        kernel = SqrExpFn2(sigmaF = 20 , l1 = 1 , l2 = 10,
                                           d = d) ,
                        var = SigmaN**2,
                        type = "regression"
                        )

predMean3 = predict(GaussianModel2, time)

ggplot() +
  geom_point(aes(x = time , y = data.Temp , color = "data"))+
  geom_line(aes(x = time , y = meanPredicted[,1] , color = "Mean Pred with time" ))+
  geom_line(aes(x = time , y = meanPredicted2[,1] , color = "Predicted Mean With Day"))+
  geom_line(aes(x = time , y = predMean3[,1] , color = "Mean Pred with Periodic" ))+
  xlab("Time") +
  ylab("Temp")+
  ggtitle("Compare Means")

#import data and ranames columns

regData = read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/banknoteFraud.csv")

names(regData) <- c("varWave","skewWave","kurtWave","entropyWave","fraud")

regData[,5] <- as.factor(regData[,5])

#split in test and train
set.seed(111);
SelectTraining <- sample(1:dim(regData)[1], size = 1000, replace = FALSE)
train = regData[SelectTraining,]
test = regData[-SelectTraining,]

gpClassification = gausspr(fraud ~ varWave + skewWave , data = train,
                           type = "classification")

fraudPred = predict(gpClassification , train)

CM = table(fraudPred , train$fraud)

Accuracy = sum(diag(CM)) / sum(CM)

cat("\n")
cat("Confusion Matrix for Train Data is : ")
cat("\n")
CM
cat("\n")

```

```

cat("\n")
cat("Accuracy with Train data is : " , Accuracy)

#inorder to select suitable values we can try with range of values
#between min and max range
#as otherwise it is getting hard to justify min and max values

grid.varWave = seq(min(train$varWave) , max(train$varWave) , length = 100)
grid.skewWave = seq(min(train$skewWave) , max(train$skewWave) , length = 100)

gridPoints <- meshgrid(grid.varWave, grid.skewWave)
gridPoints <- cbind(c(gridPoints$x), c(gridPoints$y))
gridPoints <- data.frame(gridPoints)
names(gridPoints) <- names(train)[1:2]

probPreds <- predict(gpClassification, gridPoints, type="probabilities")

contour( grid.varWave, grid.skewWave , matrix(probPreds[,1],100,byrow = TRUE) ,
         nlevels = 20 ,
         xlab = "varWave", ylab = "skewWave",
         main = 'Prob'
        )
points(x = train$varWave[train$fraud == 1] , y = train$skewWave[train$fraud == 1] ,
       col = "blue" )
points(x = train$varWave[train$fraud == 0] , y = train$skewWave[train$fraud == 0] ,
       col = "red")
legend("bottomright", legend = c("Fraud : Yes" , "Fraud : No") ,
       pch=c("o" , "o"),
       col = c("blue" , "red"))

#Test Data

fraudPred.Test = predict(gpClassification , test)

CM.Test = table(fraudPred.Test , test$fraud)

Accuracy.Test = sum(diag(CM.Test)) / sum(CM.Test)

cat("\n")
cat("Confusion Matrix for Test Data is : ")
cat("\n")
CM.Test
cat("\n")
cat("\n")
cat("Accuracy with Test data is : " , Accuracy.Test)

gpClassification.All = gausspr(fraud ~ . , data = train,
                                type = "classification")

fraudPred.All = predict(gpClassification.All , test)

```

```

CM.All = table(fraudPred.All , test$fraud)

Accuracy.All = sum(diag(CM.All)) / sum(CM.All)

cat("\n")
cat("Confusion Matrix for Test Data using all parameter is : ")
cat("\n")
CM.All
cat("\n")
cat("\n")
cat("Accuracy for Test data with all parameters is : " , Accuracy.All)

library(caret)
set.seed(100)

Mod = train(fraud ~ . , data = train , method = "rpart")

impFeatures = varImp(Mod)

print(impFeatures)

```