Report

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#1. Implementing GP Regression

1.1

We have gaussian regression process model as :

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

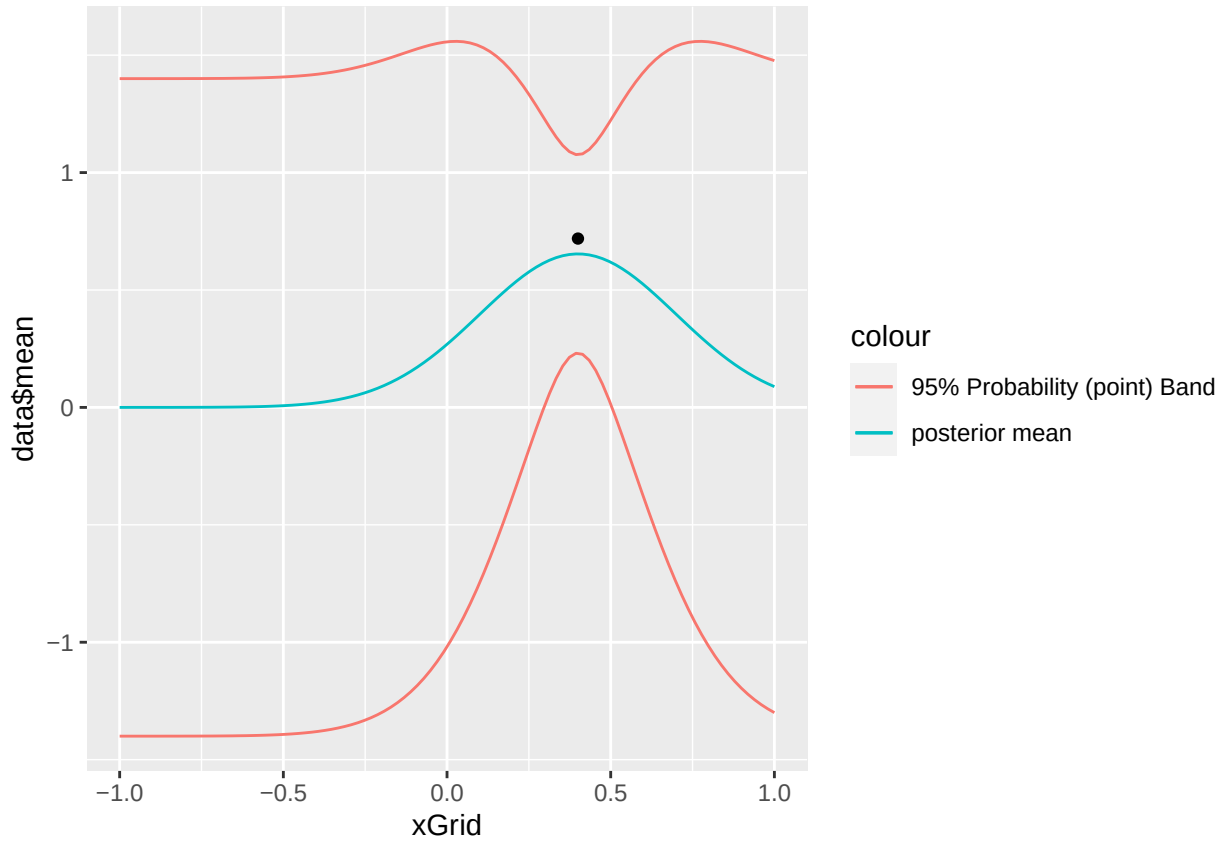
Below is algorithm implemented from Rasmussen and Willams' book which can be found on page 19. Link to book

```
# 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 = l)

  #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 = l) - (t(v) %*% v)

  #taking diagnol 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
```

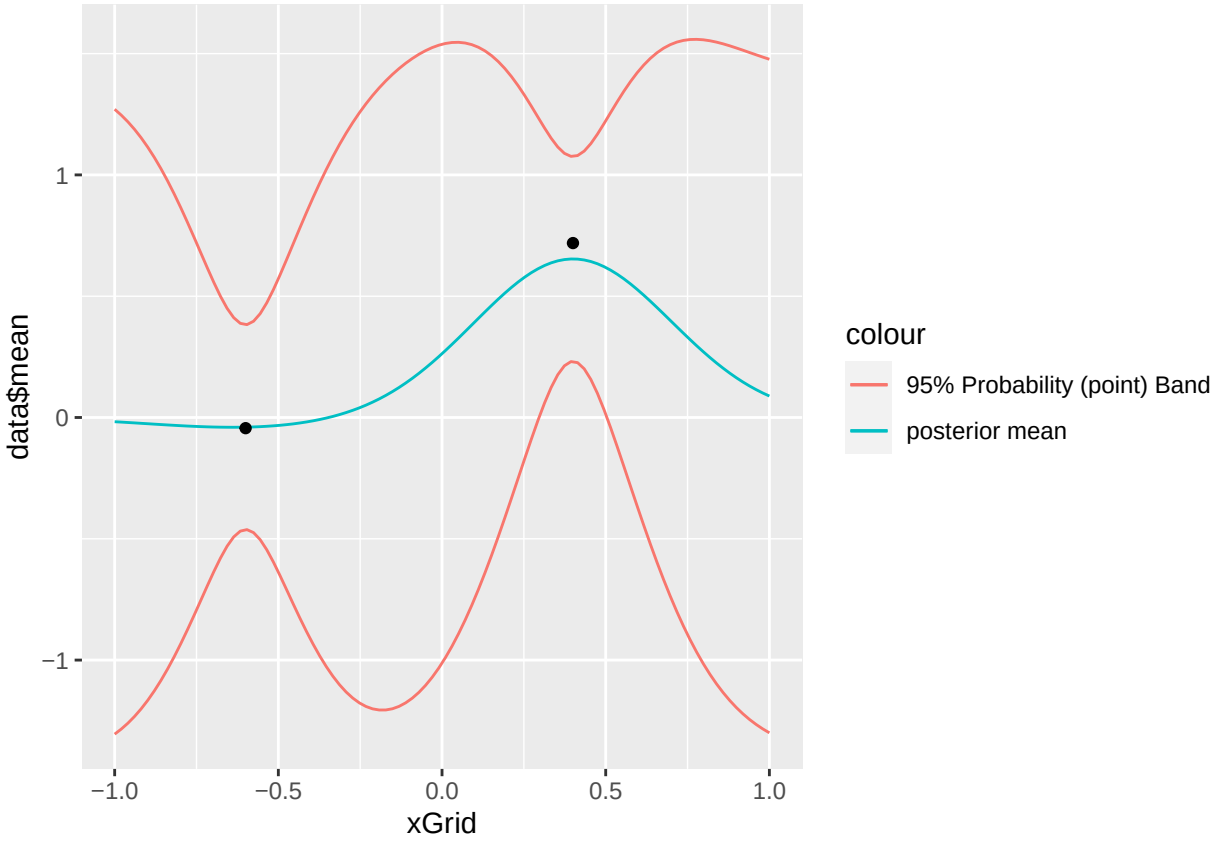
1.2

Now with hyperparameter as $\sigma_f = 1$ and l = 0.3, updating prior with single observation: (x,y) = (0.4,0.719) . Assumed value for σ_n is 0.1 . Below is plot for posterior mean f over the interval of x ϵ [-1,1] with 95% probability (pointwise) band for f.



1.3

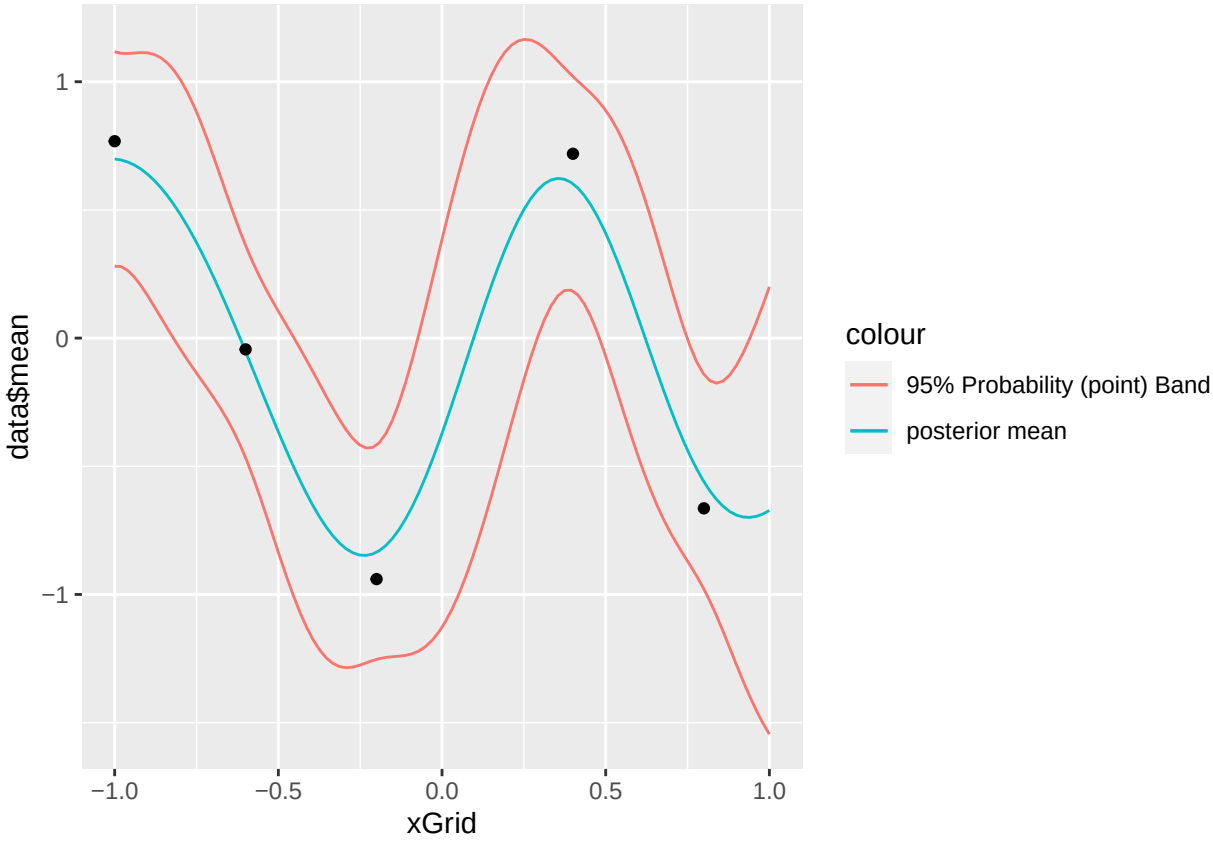
Updating posterior from 1.2 with another observation (x,y) = (-0.6, -0.044) and taking plot:



1.4

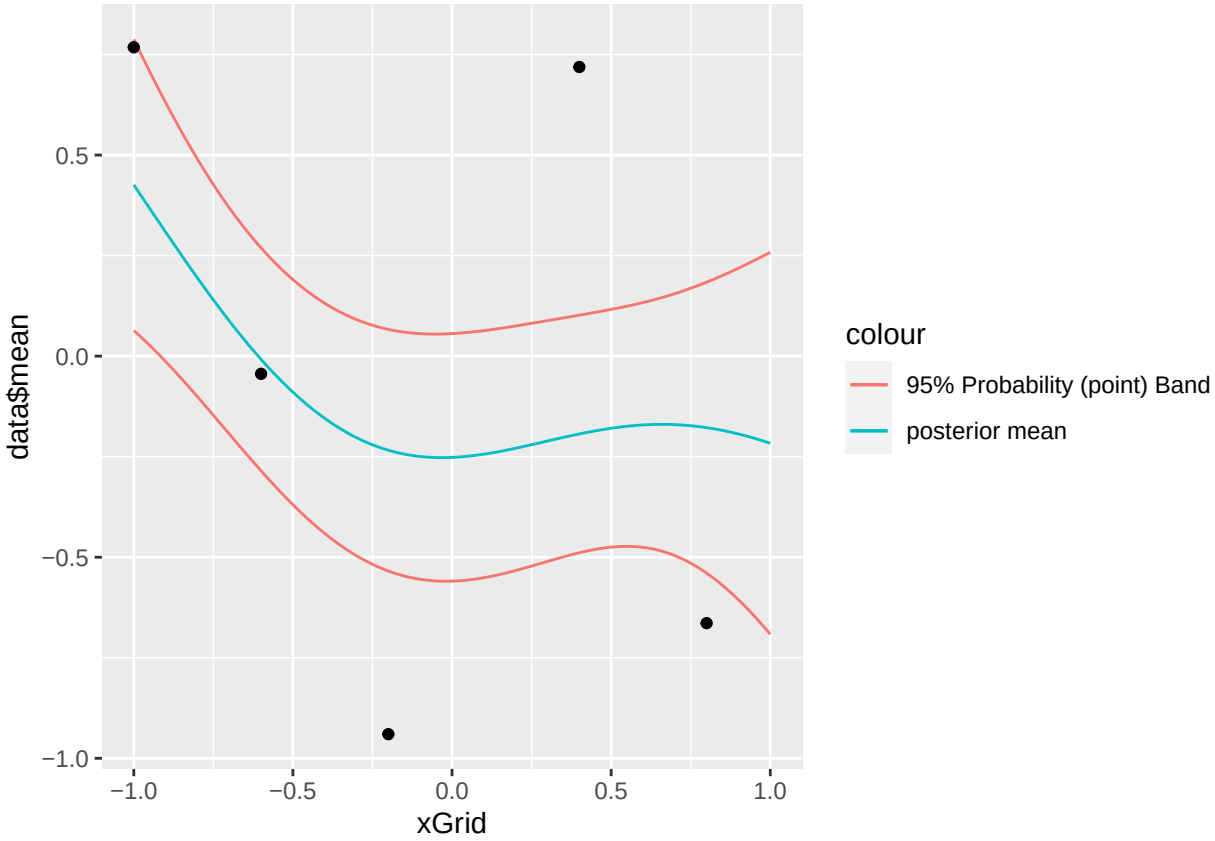
Computing distribution of posterior for below data points and ploting as above:

```
##         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

Repeating step 4 with new hyperparameter value of $\mathrm{l} = 1$ and using same $\sigma_f = 1$.



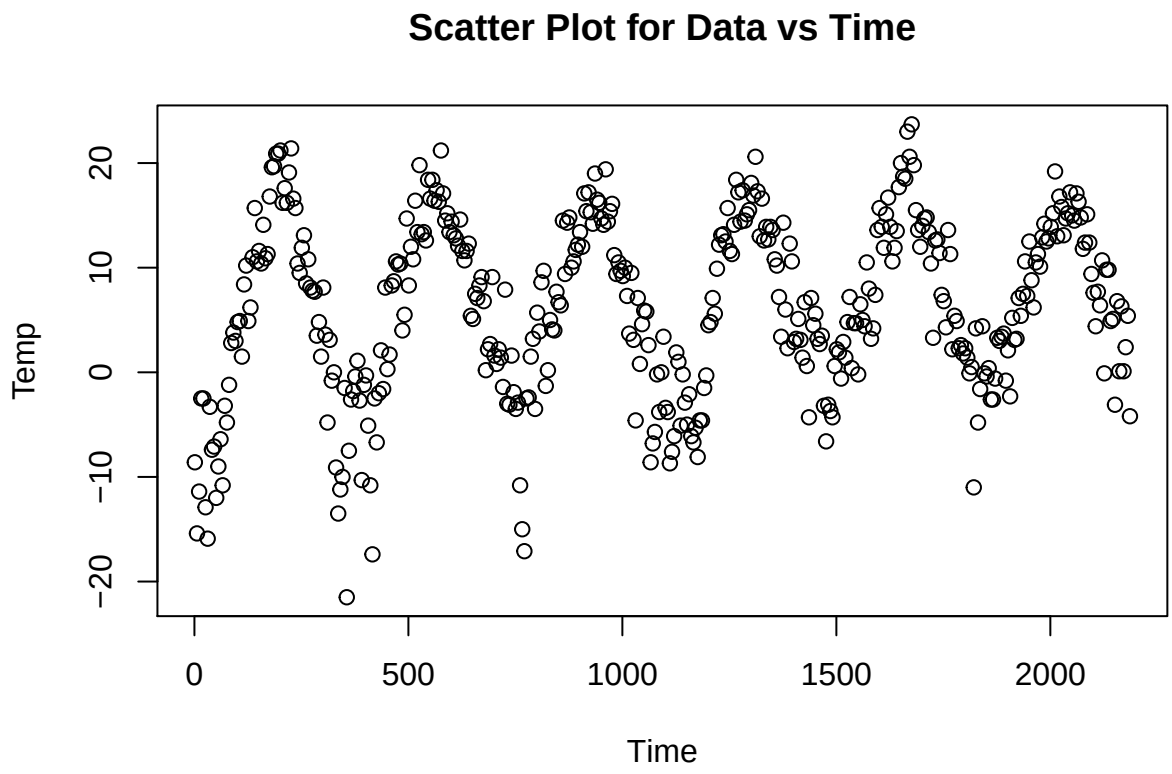
Comparison of Results

In plot for 1.2 to 1.4 observation point's 95% probability band is narrow, as we are assured about the point, thus the obtained 95% band around the observation point is narrow.

In 1.4 and 1.5, when we change the value of "l" from 0.3 to 1, since "l" is acting as a scaling factor, we will obtain a smaller co-variance value and, thus we got a much smoother curve.

#2. GP Regression with kernlab

2.1



Square exponential kernel function:

```
#given
x = 1
x2 = 2
X = c(1,3,4)
XStar = c(2,3,4)
library(kernlab)
#ell = l
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
```

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

cat("Computed CoVariance Matrix is :")
```

```
## Computed CoVariance Matrix is :
```

```r
cat("\n")
```

```r
K
```

```
## 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
```

```r
cat("\n")
```

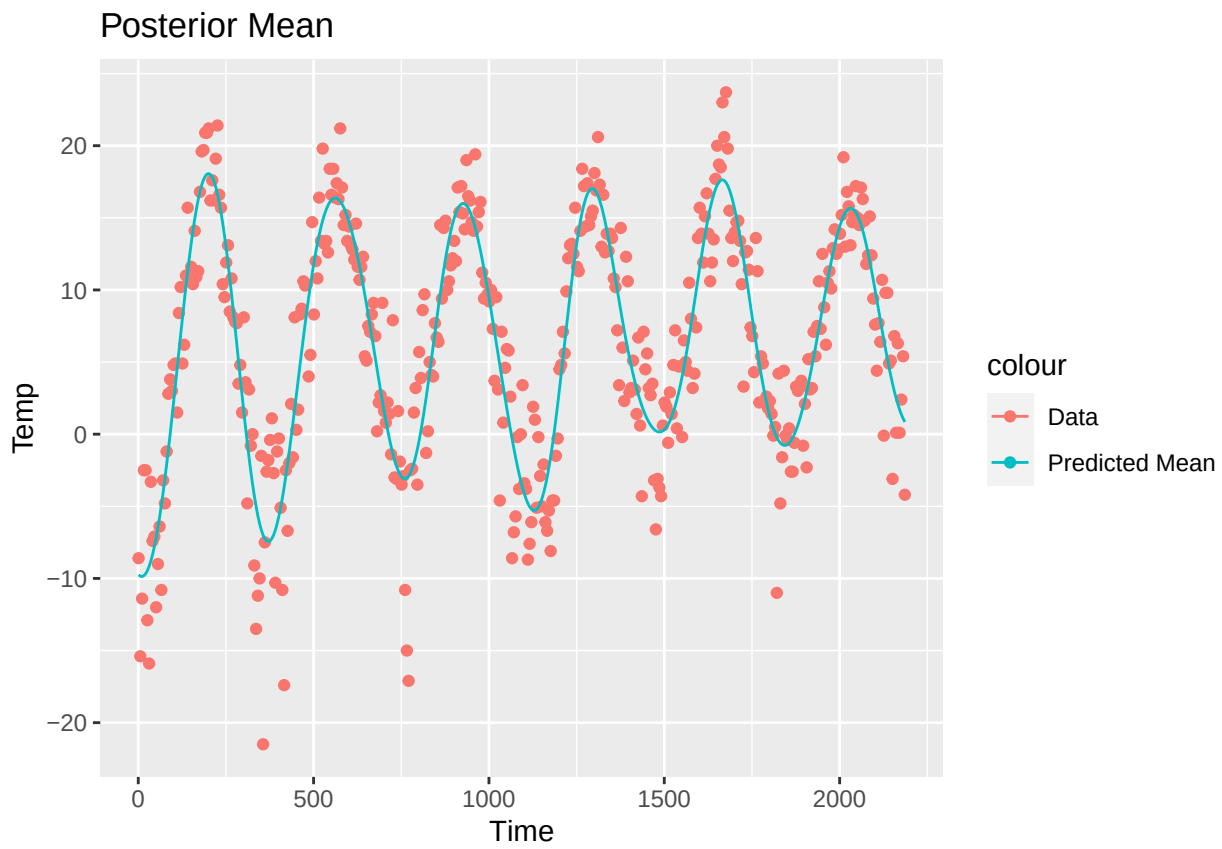
2.2

Given model is :

$temp = f(time) + \epsilon$ with $\epsilon \sim Norm(0, \sigma_n^2)$ and $f \sim GP(0, k(time, time'))$

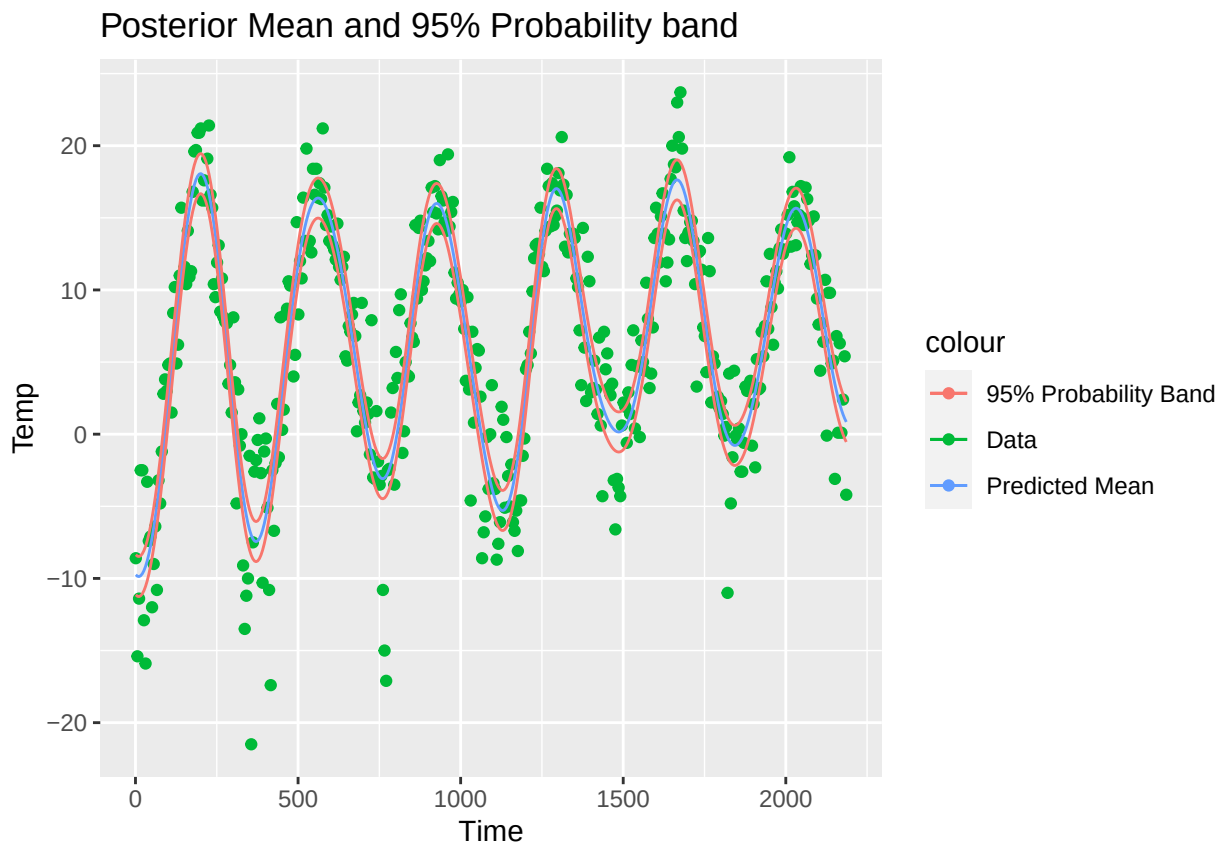
Here σ_n^2 is residual variance from a simple quadratic regression model fit.

Estimating above gaussian process model using the squared exponential function from 2.1 with hyperparameter value as $\sigma_f = 20$ and $l = 0.2$.



2.3

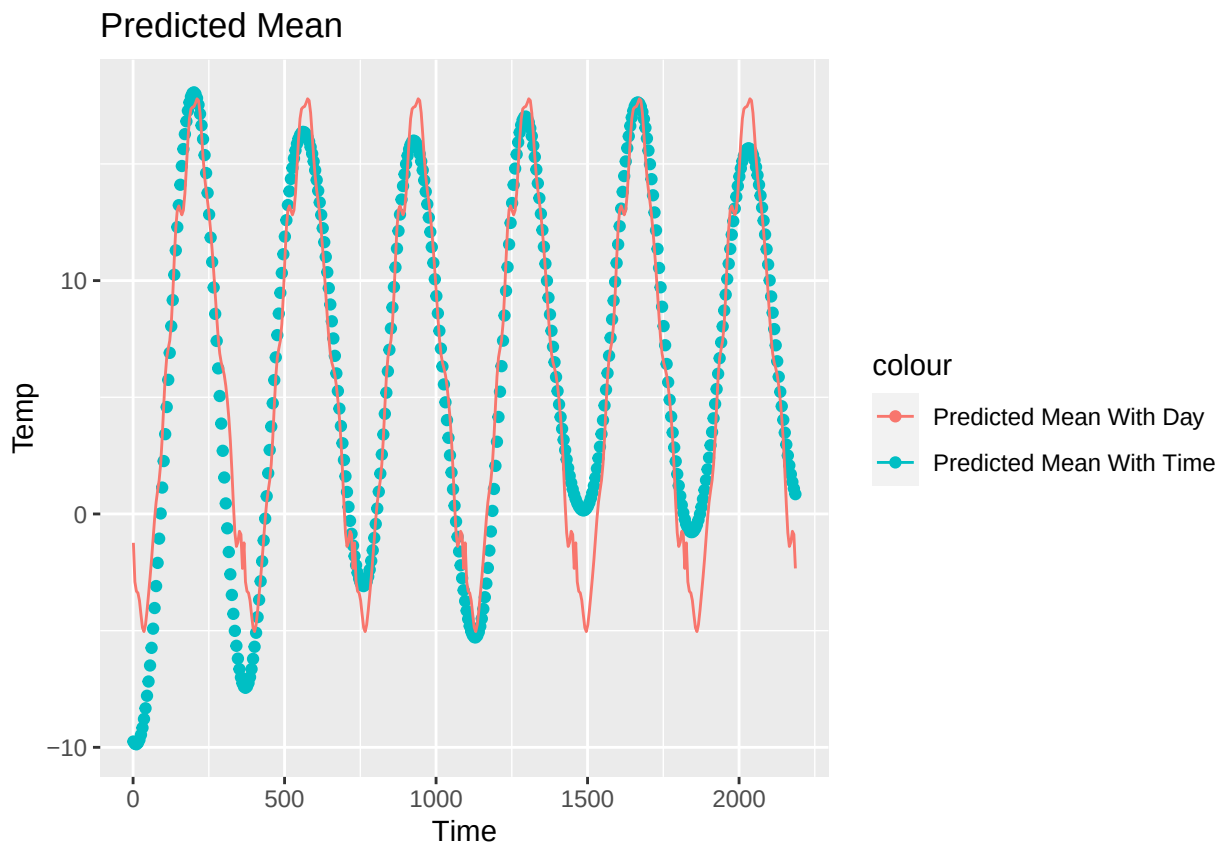
Computing posterior variance for f.



2.4

Considering new model :

$temp = f(day) + \epsilon$ with $\epsilon \sim Norm(0, \sigma_n^2)$ and $f \sim GP(0, k(day, day'))$



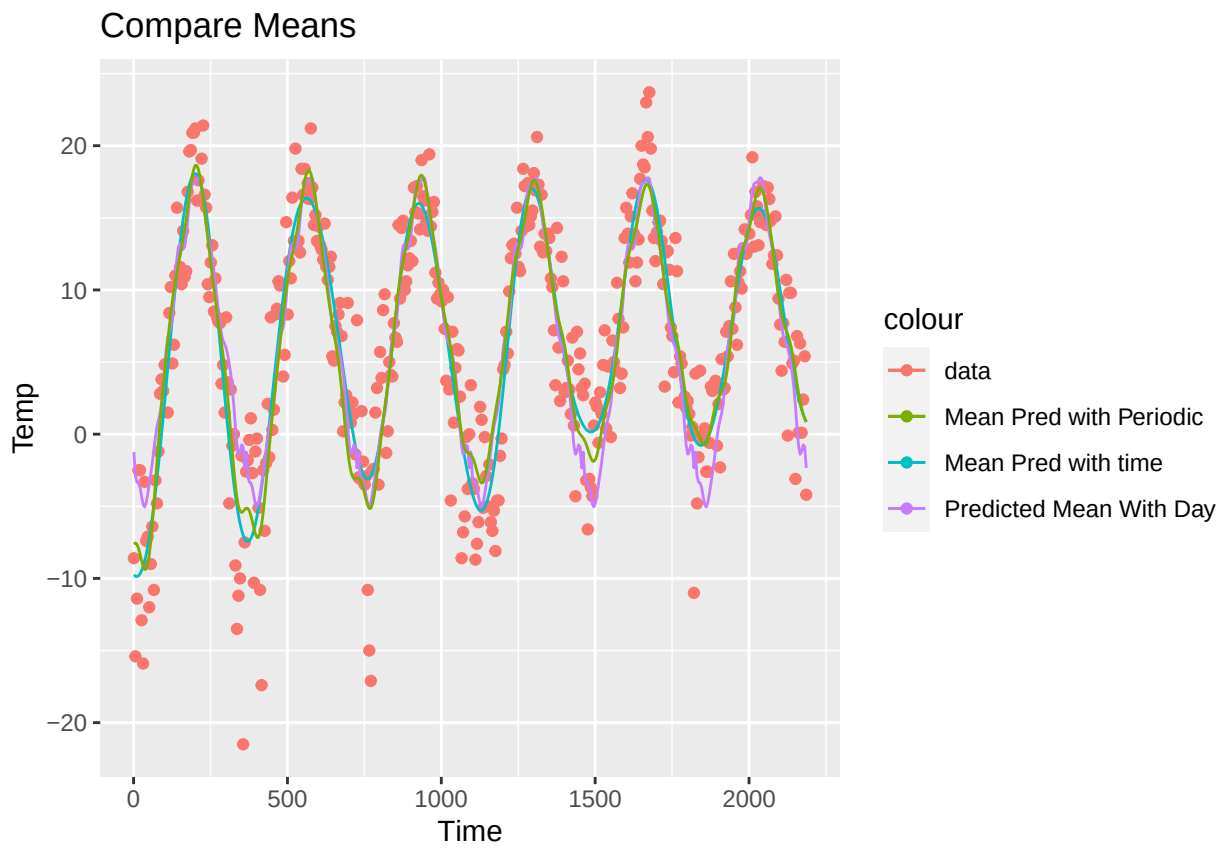
2.5

Generalization of periodic kernel:

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

Setting hyperparameter value as :

$\sigma_f = 20$, $l_1 = 1$ and $l_2 = 10$ and $d = \frac{365}{sd(time)}$

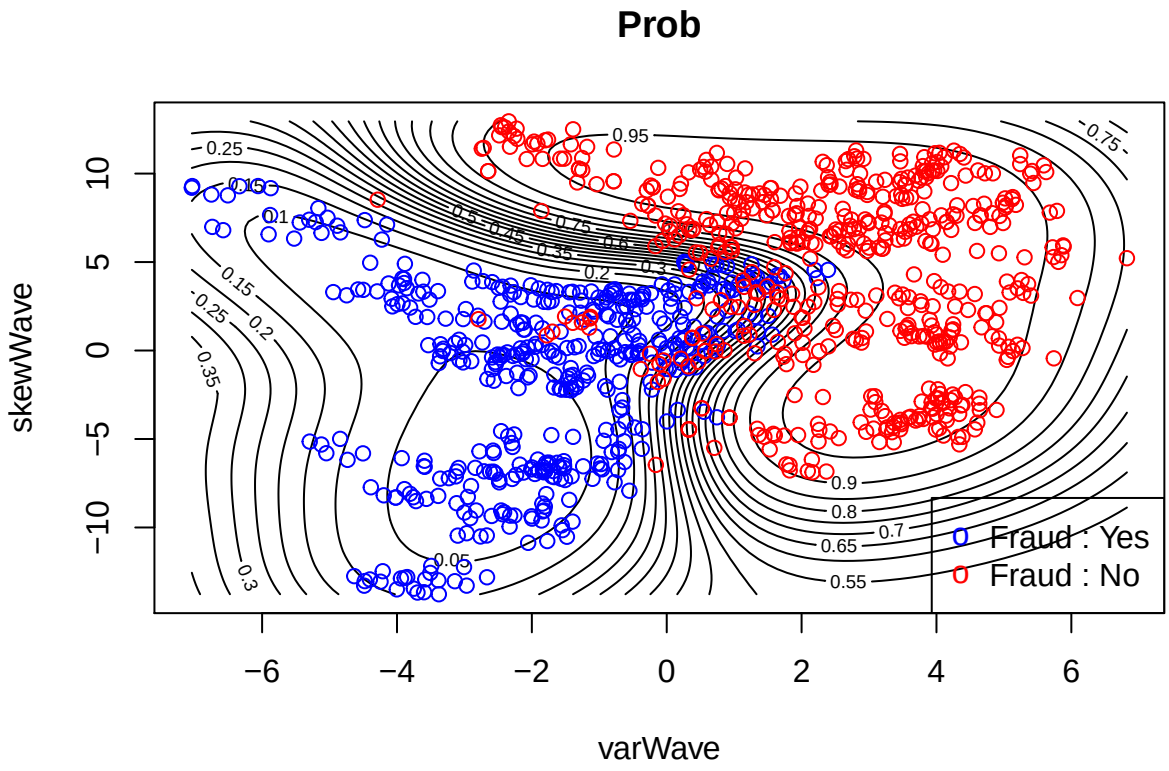


With mean value predicted with day values we can that it is repeating in cycle which could be understood in terms of repeating value of days in band of 1 to 365 while mean predicted by Time is very smooth but it does not follow shift in data mass which is accurately captured in mean calculated by periodic kernel as it take consideration for periodic year nature given by day (1:365) with trend change over time.

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

One more thing of interest here is that, while including all 4 Parameters, our False Positive and False Negative reduces sharply which could be an important parameter of interest. For such cases, it is expected to use all parameters.

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 = l)

   #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 = l) - (t(v) %*% v)

   #taking diagnol 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 = l
                        )


#95% Z = 1.96
library(ggplot2)

fnPlot = function(data, xGrid , main.T , xhigh , yhigh , high = TRUE,
                  XStarPlot = FALSE, OrigData = NA , Xlab = NA , Ylab = 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"))

   if(is.null(Xlab) & is.null(Ylab))
      {
         p + xlab("X Grid") + ylab("Posterior Mean")
      }else{
         p + xlab(Xlab) + ylab(Ylab)
      }

   p + ggtitle(main.T)

   return(p)

}#fnPlot


fnPlot(data = posteriorF , xGrid = xGrid , main.T = "Posterior Mean for f" ,
       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 = l
                         )

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")
data
cat("\n")

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

```
                          sigmaNoise = SigmaN ,
                          sigmaF = sigmaF , l = l
                         )

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.cs

#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 = "Time" ,
     ylab = "Temp" , main = "Scatter Plot for Data vs Time" )

#given
x = 1
x2 = 2
X = c(1,3,4)
XStar = c(2,3,4)
library(kernlab)
#ell = l
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") + ggtitle("Posterior Mean")

#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
```

```r
#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 = time , y = scaledData.Temp ,
                             XStar = 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 95% Probability Band" ,
#        xhigh = 0  , yhigh =0, high = FALSE , XStarPlot = TRUE , OrigData = data.Temp ,
#        Xlab = "Time" , Ylab = "Temp")

l.band = meanPredicted - sqrt(1.96 * posterVariance)
u.band = meanPredicted + sqrt(1.96 * posterVariance)


ggplot()+
   geom_point(aes(x = time , y = data.Temp , color = "Data"))  +
   geom_line(aes(x = time , y = meanPredicted[,1] , color = "Predicted Mean"))+
   geom_line(aes(x = time , y = l.band , color = "95% Probability Band"))+
   geom_line(aes(x = time , y = u.band , color = "95% Probability Band"))+
   xlab("Time") + ylab("Temp") + ggtitle("Posterior Mean and 95% Probability band")




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 = SigmaN**2,
                         type = "regression"
                         )
```

```r
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/banknoteFrau

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)
```