## Lab4

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#### Contributions

We solved all questions individually and discussed together, we wrote our comment together.

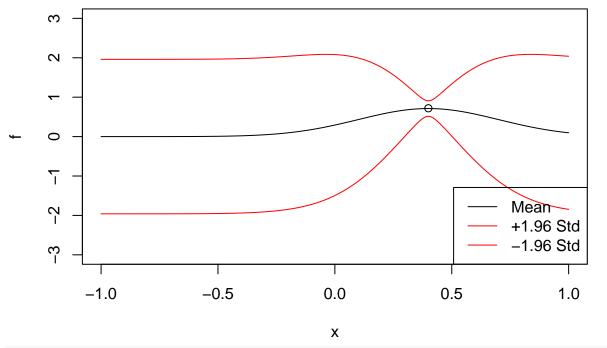
## Q2.1

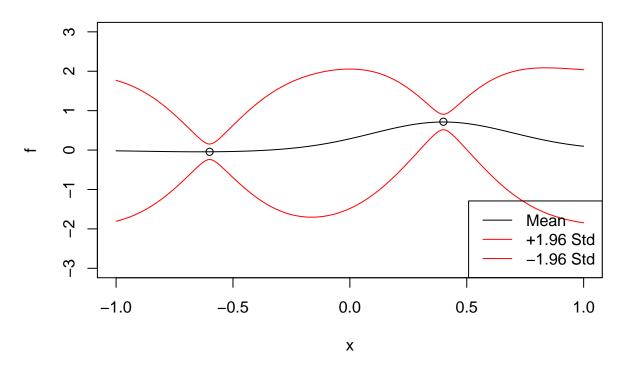
```
SquaredExpKernel <- function(x1,x2,sigmaF=1,l=3){</pre>
  n1 \leftarrow length(x1)
  n2 <- length(x2)
  K <- matrix(NA,n1,n2)</pre>
  for (i in 1:n2){
    K[,i] \leftarrow sigmaF^2*exp(-0.5*((x1-x2[i])/1)^2)
  return(K)
}
posteriorGP <- function(X, y, Xstar, sigmaNoise, K, ...){</pre>
  n <- length(X)
  C \leftarrow K(X, X, ...) + sigmaNoise^2 * diag(n)
  L <- t(chol(C))
  L_inv <- solve(L)
  C_inv <- t(L_inv) %*% L_inv</pre>
  mean <- K(Xstar, X, ...) %*% C_inv %*% y
  var <- K(Xstar, Xstar, ...) - K(Xstar, X, ...) %*% C_inv %*% t(K(Xstar, X, ...))</pre>
  return(list(mean=mean, var=var))
}
```

## Q2.2

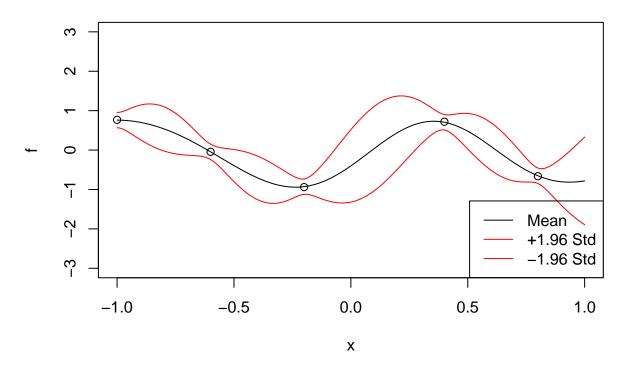
```
X = 0.4
y = 0.719
Xstar = seq(-1, 1, 0.01)
sigmaNoise = 0.1
K = SquaredExpKernel
f = posteriorGP(X, y, Xstar, sigmaNoise, K, sigmaF=1, l=0.3)

up_bound <- f$mean+1.96*sqrt(diag(f$var))
low_bound <- f$mean-1.96*sqrt(diag(f$var))
plot(Xstar, f$mean, type='l', ylim =c(-3,3), xlab = "x", ylab = "f")
lines(Xstar, up_bound, col='red')
lines(Xstar, low_bound, col='red')</pre>
```

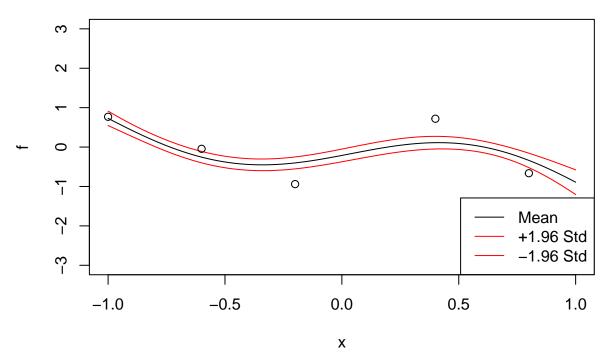




## **Q2.4**



## Q2.5



When change I from 0.3 to 1, we got a smoother curve, this is because when we have a lager I, the gaussian kernel will have a lager variance, therefore x\_star will depend more on far distance points.

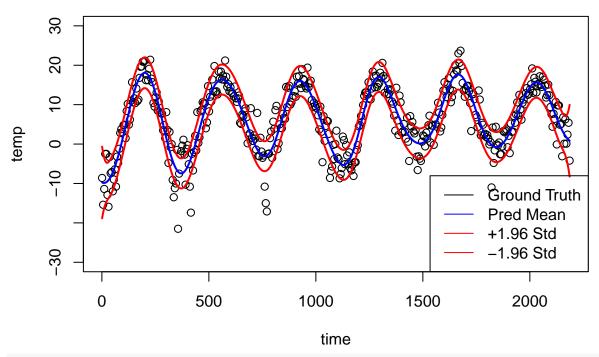
## Q3.1

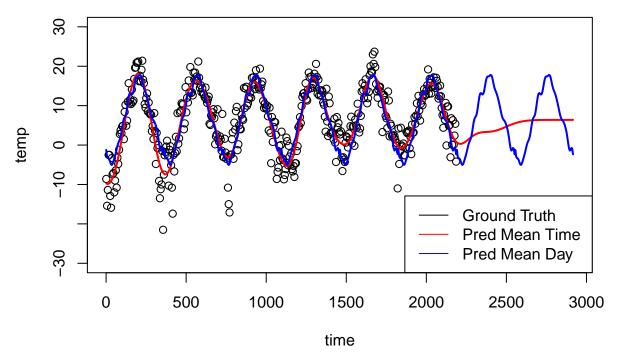
```
df <- read.csv("TempTullinge.csv", sep=";", header=TRUE)</pre>
time \leftarrow seq(1, 2190, 5)
df = df[time,]
df$time <- time
day \leftarrow rep(seq(1, 365, 5), 6)
df$day <- day
RBFkernel <- function(sigmaf = 1, ell = 1) {</pre>
  rval <- function(x, y = NULL) {</pre>
      res - sigmaf^2*exp(-0.5*((x-y)/ell)^2)
      return(res)
    }
  class(rval) <- "kernel"</pre>
  return(rval)
SEkernel <- RBFkernel(sigmaf = 1, ell = 1)</pre>
SEkernel(1,2)
## [1] 0.6065307
X \leftarrow matrix(c(1,3,4), 3, 1)
Xstar \leftarrow matrix(c(2,3,4), 3, 1)
kernelMatrix(kernel = SEkernel, x = X, y = Xstar)
## 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
```

#### Q3.2

```
temp <- df$temp
temp <- (temp - mean(temp)) / sd(temp)</pre>
time <- (time - mean(time)) / sd(time)</pre>
day <- (day - mean(day)) / sd(day)</pre>
plot(df$time, df$temp, ylim=c(-30, 30), xlab='time', ylab='temp')
polyFit <- lm(temp ~ time + I(time^2))</pre>
sigmaNoise <- sd(polyFit$residuals)</pre>
sigmaf <- 20
ell <- 0.2
RBF <- RBFkernel(sigmaf = sigmaf, ell=ell)</pre>
GPfit <- gausspr(time, temp, kernel = RBF, var = sigmaNoise^2)</pre>
extr_time \leftarrow seq(2191, 8*365, 5)
extr_time_norm <- (extr_time - mean(df$time)) / sd(df$time)</pre>
meanPred <- predict(GPfit, time)</pre>
EXTmeanPred <- predict(GPfit, extr time norm)</pre>
lines(df$time, meanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
x<-time
xs<-time
n <- length(x)
Kss <- kernelMatrix(kernel = RBF, x = xs, y = xs)</pre>
Kxx <- kernelMatrix(kernel = RBF, x = x, y = x)</pre>
Kxs <- kernelMatrix(kernel = RBF, x = x, y = xs)</pre>
Covf = Kss-t(Kxs)%*%solve(Kxx + sigmaNoise^2*diag(n), Kxs) # Covariance matrix of fStar.
ub <- meanPred + 1.96*sqrt(diag(Covf))</pre>
lb <- meanPred - 1.96*sqrt(diag(Covf))</pre>
lines(df$time, lb * sd(df$temp) + mean(df$temp), col = "red", lwd = 2)
lines(df$time, ub * sd(df$temp) + mean(df$temp), col = "red", lwd = 2)
legend("bottomright", legend=c("Ground Truth", "Pred Mean ","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1,1), col=c("black","blue","red","red"))
```





They actually get very similar results, but this input data only has seasonal component without trend component.

#### • Time:

GP on the whole time period, this allow us to prediction temperature only based on recent time but ignored information on the same day in another year. There might have some trend information ignored ( i.e. climate change )

#### • Day:

GP on the whole single year, this is actually a GP on the mean temperature of each day over 6 years, so we can see above plot, the blue line just repeat the same pattern in every year. This is because our GP only learned the average temperature for each day over 6 years.

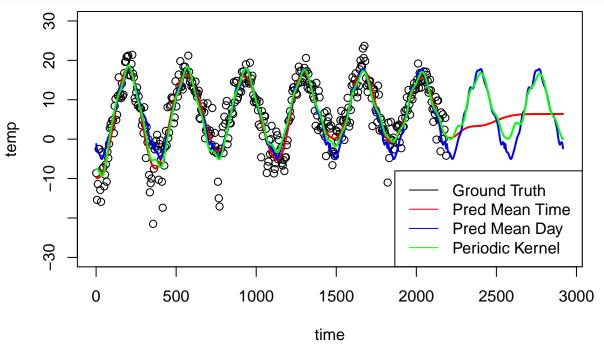
#### Q3.5

```
RBFPeriodickernel <- function(sigmaf = 1, ell1 = 1, ell2 = 1, d = 1) {
    rval <- function(x, y = NULL) {
        res <- sigmaf^2*exp(-0.5*( (x-y)/ell2)^2 )*exp(-2*(sin(pi*abs(x-y)/d)/ell1)^2 )
        return(res)
    }
    class(rval) <- "kernel"
    return(rval)
}

sigmaf <- 20
ell1 <- 1
ell2 <- 10
d <- 365 / sd(c(1:2190))

RBF_P <- RBFPeriodickernel(sigmaf = sigmaf, ell1 = ell1, ell2 = ell2, d = d)
GPfit_PK <- gausspr(time, temp, kernel = RBF_P, var = sigmaNoise^2)</pre>
```

```
meanPred_PK <- predict(GPfit_PK, time)
EXTmeanPred_PK <- predict(GPfit_PK, extr_time_norm)
plot(df$time, df$temp, ylim=c(-30, 30), xlab='time', ylab='temp', xlim=c(0, 8*365))
lines(df$time, meanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='red')
lines(extr_time, EXTmeanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='red')
lines(df$time, meanPred_day * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
lines(extr_time, EXTmeanPred_day * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
lines(df$time, meanPred_PK * sd(df$temp) + mean(df$temp), lwd = 2, col='green')
lines(extr_time, EXTmeanPred_PK * sd(df$temp) + mean(df$temp), lwd = 2, col='green')
legend("bottomright", legend=c("Ground Truth", "Pred Mean Time ", "Pred Mean Day", "Periodic Kernel"),
lwd=c(1,1,1,1), col=c("black", "red", "blue", "green"))</pre>
```



This approach fit original data very well, locally periodic kernel might be better than previous two approaches, since it could be seen as the product of periodic kernel and a ordinary RBF Kernel, which will use both periodic information and local information.

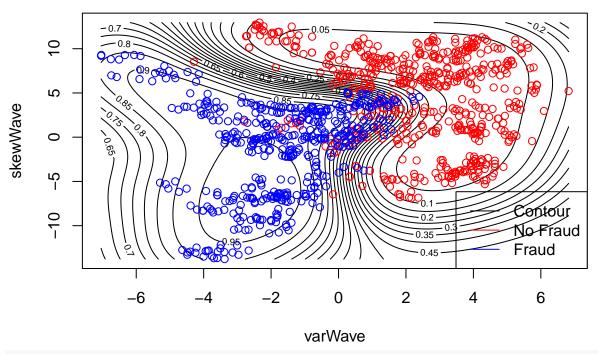
## Q4.1

```
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])

set.seed(111)
SelectTraining <- sample(1:dim(data)[1], size = 1000, replace = FALSE)
train=data[SelectTraining,]
test=data[-SelectTraining,]</pre>
GPClassifier <- gausspr(fraud ~ varWave + skewWave, data=train)
```

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

# Prob(Fraud)



```
print('Confusion matrix and accuracy of training set')

## [1] "Confusion matrix and accuracy of training set"

confmatrix <- table(predict(GPClassifier,train[,1:2]), train[,5])

confmatrix

##

##

0 1

## 0 503 18</pre>
```

1 41 438

##

```
sum(diag(confmatrix)) / sum(confmatrix)
## [1] 0.941
print('Confusion matrix and accuracy of test set')
## [1] "Confusion matrix and accuracy of test set"
confmatrix <- table(predict(GPClassifier,test[,1:2]), test[,5])</pre>
confmatrix
##
##
         0
     0 199
##
             9
     1 19 145
sum(diag(confmatrix)) / sum(confmatrix)
## [1] 0.9247312
Q4.3
GPClassifier <- gausspr(fraud ~ ., data=train)</pre>
## Using automatic sigma estimation (sigest) for RBF or laplace kernel
print('Confusion matrix and accuracy of test set with all 4 features')
## [1] "Confusion matrix and accuracy of test set with all 4 features"
confmatrix <- table(predict(GPClassifier,test[,1:4]), test[,5])</pre>
confmatrix
##
##
         0
             1
    0 216
##
##
    1
         2 154
sum(diag(confmatrix)) / sum(confmatrix)
## [1] 0.9946237
```

# Appendix

```
knitr::opts_chunk$set(echo = TRUE)
library(kernlab)
library(AtmRay)

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])/1)^2 )
    }
    return(K)
}</pre>
```

```
posteriorGP <- function(X, y, Xstar, sigmaNoise, K, ...){</pre>
  n <- length(X)
  C \leftarrow K(X, X, ...) + sigmaNoise^2 * diag(n)
  L \leftarrow t(chol(C))
  L_inv <- solve(L)</pre>
  C_inv <- t(L_inv) %*% L_inv</pre>
  mean <- K(Xstar, X, ...) %*% C_inv %*% y
  var <- K(Xstar, Xstar, ...) - K(Xstar, X, ...) %*% C_inv %*% t(K(Xstar, X, ...))</pre>
  return(list(mean=mean, var=var))
}
X = 0.4
y = 0.719
Xstar = seq(-1, 1, 0.01)
sigmaNoise = 0.1
K = SquaredExpKernel
f = posteriorGP(X, y, Xstar, sigmaNoise, K, sigmaF=1, 1=0.3)
up_bound <- f$mean+1.96*sqrt(diag(f$var))</pre>
low bound <- f$mean-1.96*sqrt(diag(f$var))</pre>
plot(Xstar, f\$mean, type='l', ylim = c(-3,3), xlab = "x", ylab = "f")
lines(Xstar, up bound, col='red')
lines(Xstar, low_bound, col='red')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
X = c(0.4, -0.6)
y = c(0.719, -0.044)
Xstar = seq(-1, 1, 0.01)
sigmaNoise = 0.1
K = SquaredExpKernel
f = posteriorGP(X, y, Xstar, sigmaNoise, K, sigmaF=1, l=0.3)
up_bound <- f$mean+1.96*sqrt(diag(f$var))</pre>
low_bound <- f$mean-1.96*sqrt(diag(f$var))</pre>
plot(Xstar, f$mean, type='1', ylim =c(-3,3), xlab = "x", ylab = "f")
lines(Xstar, up_bound, col='red')
lines(Xstar, low_bound, col='red')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
X = c(0.4, -0.6, -1, -0.2, 0.8)
y = c(0.719, -0.044, 0.768, -0.940, -0.664)
Xstar = seq(-1, 1, 0.01)
sigmaNoise = 0.1
K = SquaredExpKernel
f = posteriorGP(X, y, Xstar, sigmaNoise, K, sigmaF=1, l=0.3)
up_bound <- f$mean+1.96*sqrt(diag(f$var))</pre>
low_bound <- f$mean-1.96*sqrt(diag(f$var))</pre>
plot(Xstar, f\$mean, type='l', ylim = c(-3,3), xlab = "x", ylab = "f")
```

```
lines(Xstar, up_bound, col='red')
lines(Xstar, low_bound, col='red')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
X = c(0.4, -0.6, -1, -0.2, 0.8)
y = c(0.719, -0.044, 0.768, -0.940, -0.664)
Xstar = seq(-1, 1, 0.01)
sigmaNoise = 0.1
K = SquaredExpKernel
f = posteriorGP(X, y, Xstar, sigmaNoise, K, sigmaF=1, l=1)
up_bound <- f$mean+1.96*sqrt(diag(f$var))</pre>
low_bound <- f$mean-1.96*sqrt(diag(f$var))</pre>
plot(Xstar, f\$mean, type='l', ylim = c(-3,3), xlab = "x", ylab = "f")
lines(Xstar, up_bound, col='red')
lines(Xstar, low_bound, col='red')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
df <- read.csv("TempTullinge.csv", sep=";", header=TRUE)</pre>
time \leftarrow seq(1, 2190, 5)
df = df[time,]
df$time <- time
day \leftarrow rep(seq(1, 365, 5), 6)
df$day <- day
RBFkernel <- function(sigmaf = 1, ell = 1) {
  rval <- function(x, y = NULL) {</pre>
      res < sigmaf<sup>2</sup>*exp(-0.5*( (x-y)/ell)<sup>2</sup> )
      return(res)
    }
  class(rval) <- "kernel"</pre>
  return(rval)
}
SEkernel <- RBFkernel(sigmaf = 1, ell = 1)</pre>
SEkernel(1,2)
X \leftarrow matrix(c(1,3,4), 3, 1)
Xstar \leftarrow matrix(c(2,3,4), 3, 1)
kernelMatrix(kernel = SEkernel, x = X, y = Xstar)
temp <- df$temp
temp <- (temp - mean(temp)) / sd(temp)</pre>
time <- (time - mean(time)) / sd(time)</pre>
day <- (day - mean(day)) / sd(day)</pre>
plot(df$time, df$temp, ylim=c(-30, 30), xlab='time', ylab='temp')
polyFit <- lm(temp ~ time + I(time^2))</pre>
sigmaNoise <- sd(polyFit$residuals)</pre>
sigmaf <- 20
ell <- 0.2
```

```
RBF <- RBFkernel(sigmaf = sigmaf, ell=ell)</pre>
GPfit <- gausspr(time, temp, kernel = RBF, var = sigmaNoise^2)</pre>
extr_time \leftarrow seq(2191, 8*365, 5)
extr_time_norm <- (extr_time - mean(df$time)) / sd(df$time)</pre>
meanPred <- predict(GPfit, time)</pre>
EXTmeanPred <- predict(GPfit, extr_time_norm)</pre>
lines(df$time, meanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
x<-time
xs<-time
n <- length(x)
Kss <- kernelMatrix(kernel = RBF, x = xs, y = xs)</pre>
Kxx \leftarrow kernelMatrix(kernel = RBF, x = x, y = x)
Kxs \leftarrow kernelMatrix(kernel = RBF, x = x, y = xs)
Covf = Kss-t(Kxs)%*%solve(Kxx + sigmaNoise^2*diag(n), Kxs) # Covariance matrix of fStar.
ub <- meanPred + 1.96*sqrt(diag(Covf))</pre>
lb <- meanPred - 1.96*sqrt(diag(Covf))</pre>
lines(df$time, lb * sd(df$temp) + mean(df$temp), col = "red", lwd = 2)
lines(df$time, ub * sd(df$temp) + mean(df$temp), col = "red", lwd = 2)
legend("bottomright", legend=c("Ground Truth", "Pred Mean ","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1,1), col=c("black","blue","red","red"))
extr day \leftarrow rep(seq(1, 365, 5), 2)
extr_day_norm <- (extr_day - mean(df$day)) / sd(df$day)</pre>
sigmaf <- 20
ell <- 0.2
RBF <- RBFkernel(sigmaf = sigmaf, ell=ell)</pre>
GPfit_day <- gausspr(day, temp, kernel = RBF, var = sigmaNoise^2)</pre>
meanPred_day <- predict(GPfit_day, day)</pre>
EXTmeanPred_day <- predict(GPfit_day, extr_day_norm)</pre>
plot(df$time, df$temp, ylim=c(-30, 30), xlab='time', ylab='temp', xlim=c(0, 8*365))
lines(df$time, meanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='red')
lines(extr_time, EXTmeanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='red')
lines(df$time, meanPred_day * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
lines(extr_time, EXTmeanPred_day * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
legend("bottomright", legend=c("Ground Truth", "Pred Mean Time ", "Pred Mean Day"),
        lwd=c(1,1,1), col=c("black","red","blue"))
RBFPeriodickernel <- function(sigmaf = 1, ell1 = 1, ell2 = 1, d = 1) {
  rval <- function(x, y = NULL) {</pre>
      res <- sigmaf^2*exp(-0.5*((x-y)/ell2)^2)*exp(-2*(sin(pi*abs(x-y)/d)/ell1)^2)
      return(res)
  class(rval) <- "kernel"</pre>
  return(rval)
}
```

```
sigmaf <- 20
ell1 <- 1
ell2 <- 10
d \leftarrow 365 / sd(c(1:2190))
RBF_P <- RBFPeriodickernel(sigmaf = sigmaf, ell1 = ell1, ell2 = ell2, d = d)
GPfit_PK <- gausspr(time, temp, kernel = RBF_P, var = sigmaNoise^2)</pre>
meanPred_PK <- predict(GPfit_PK, time)</pre>
EXTmeanPred_PK <- predict(GPfit_PK, extr_time_norm)</pre>
plot(df$time, df$temp, ylim=c(-30, 30), xlab='time', ylab='temp', xlim=c(0, 8*365))
lines(df$time, meanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='red')
lines(extr_time, EXTmeanPred * sd(df$temp) + mean(df$temp), lwd = 2, col='red')
lines(df$time, meanPred_day * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
lines(extr_time, EXTmeanPred_day * sd(df$temp) + mean(df$temp), lwd = 2, col='blue')
lines(df$time, meanPred_PK * sd(df$temp) + mean(df$temp), lwd = 2, col='green')
lines(extr_time, EXTmeanPred_PK * sd(df$temp) + mean(df$temp), lwd = 2, col='green')
legend("bottomright", legend=c("Ground Truth", "Pred Mean Time ", "Pred Mean Day", "Periodic Kernel"),
        lwd=c(1,1,1,1), col=c("black","red","blue","green"))
data <- read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/banknoteFraud
names(data) <- c("varWave", "skewWave", "kurtWave", "entropyWave", "fraud")</pre>
data[,5] <- as.factor(data[,5])</pre>
set.seed(111)
SelectTraining <- sample(1:dim(data)[1], size = 1000, replace = FALSE)
train=data[SelectTraining,]
test=data[-SelectTraining,]
GPClassifier <- gausspr(fraud ~ varWave + skewWave, data=train)</pre>
# class probabilities
probPreds <- predict(GPClassifier, train[,1:2], type="probabilities")</pre>
x1 <- seq(min(train[,1]),max(train[,1]),length=100)</pre>
x2 <- seq(min(train[,2]),max(train[,2]),length=100)</pre>
gridPoints <- meshgrid(x1, x2)</pre>
gridPoints <- cbind(c(gridPoints$x), c(gridPoints$y))</pre>
gridPoints <- data.frame(gridPoints)</pre>
names(gridPoints) <- names(train)[1:2]</pre>
probPreds <- predict(GPClassifier, gridPoints, type="probabilities")</pre>
# Plotting for Prob(setosa)
contour(x1,x2,matrix(probPreds[,2],100,byrow = TRUE), 20, xlab = "varWave", ylab = "skewWave", main = "
points(train[train[,5]=='0',1],train[train[,5]=='0',2],col="red")
points(train[train[,5]=='1',1],train[train[,5]=='1',2],col="blue")
legend("bottomright", legend=c("Contour", "No Fraud", "Fraud"),
        lwd=c(1,1,1), col=c("black","red","blue"))
print('Confusion matrix and accuracy of training set')
confmatrix <- table(predict(GPClassifier,train[,1:2]), train[,5])</pre>
sum(diag(confmatrix)) / sum(confmatrix)
```

```
print('Confusion matrix and accuracy of test set')
confmatrix <- table(predict(GPClassifier,test[,1:2]), test[,5])
confmatrix
sum(diag(confmatrix)) / sum(confmatrix)
GPClassifier <- gausspr(fraud ~ ., data=train)
print('Confusion matrix and accuracy of test set with all 4 features')
confmatrix <- table(predict(GPClassifier,test[,1:4]), test[,5])
confmatrix
sum(diag(confmatrix)) / sum(confmatrix)</pre>
```