Lab4

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Contributions

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

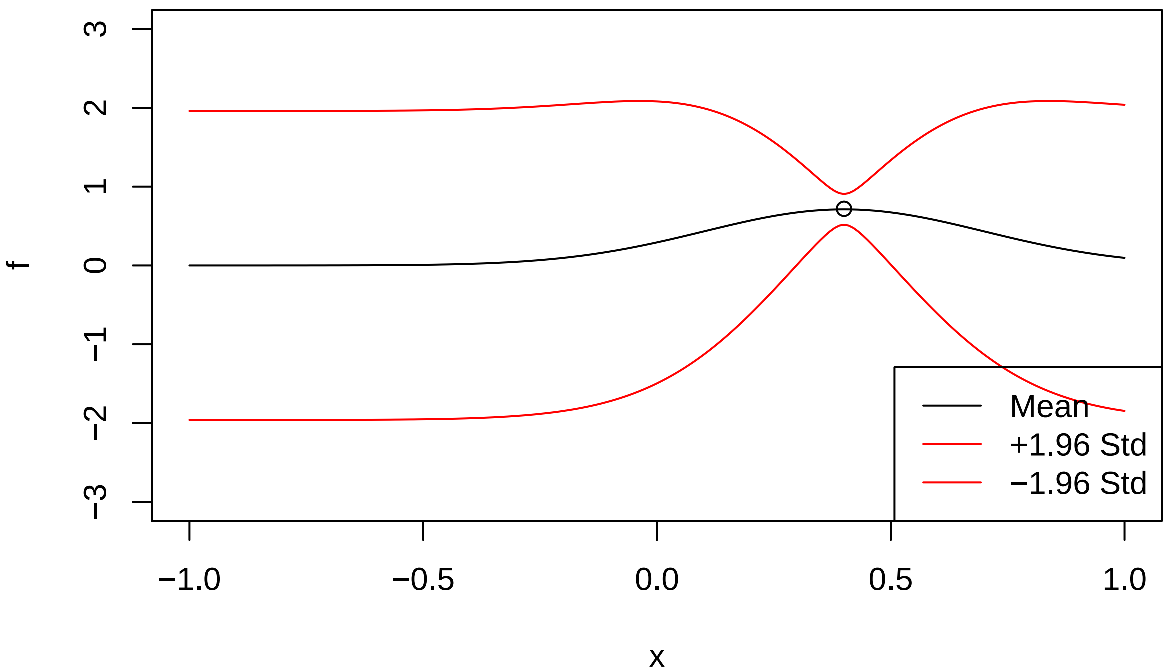
Q2.1

```
SquaredExpKernel <- function(x1,x2,sigmaF=1,l=3){
  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, K, ...){
  n <- length(X)
  C <- K(X, X, ...) + sigmaNoise ^ 2 * diag(n)
  L <- t(chol(C))
  L_inv <- solve(L)
  C_inv <- t(L_inv) %*% L_inv
  mean <- K(Xstar, X, ...) %*% C_inv %*% y
  var <- K(Xstar, Xstar, ...) - K(Xstar, X, ...) %*% C_inv %*% t(K(Xstar, X, ...))
  return(list(mean=mean, var=var))

}
```

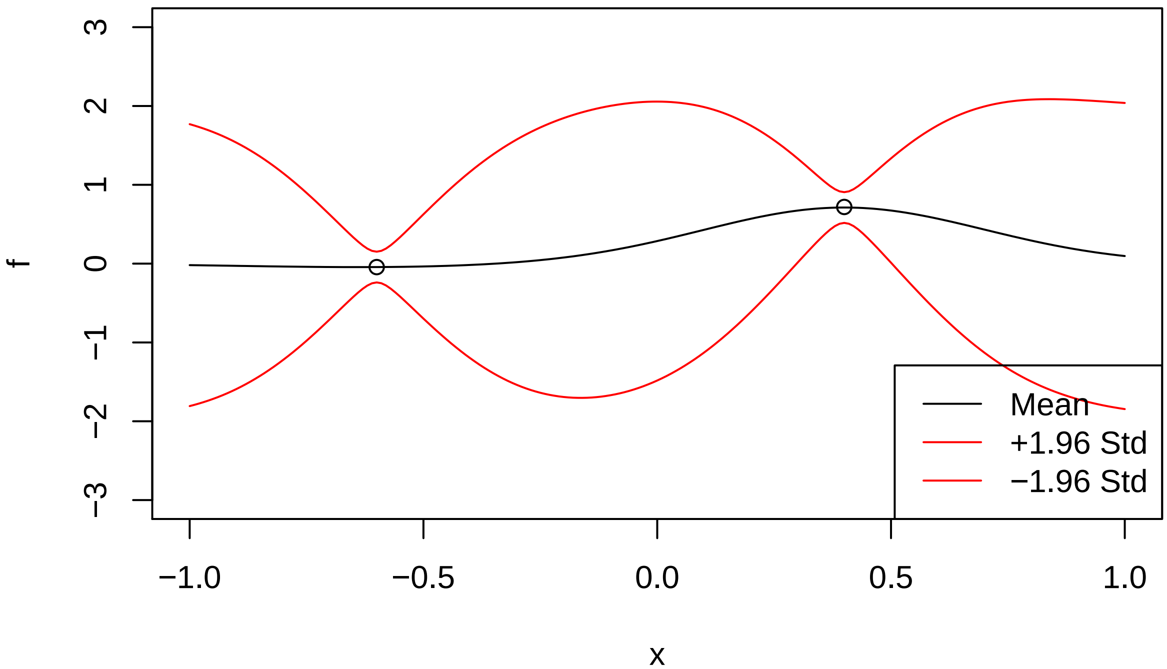
Q2.2

```
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')
```

```r
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
```

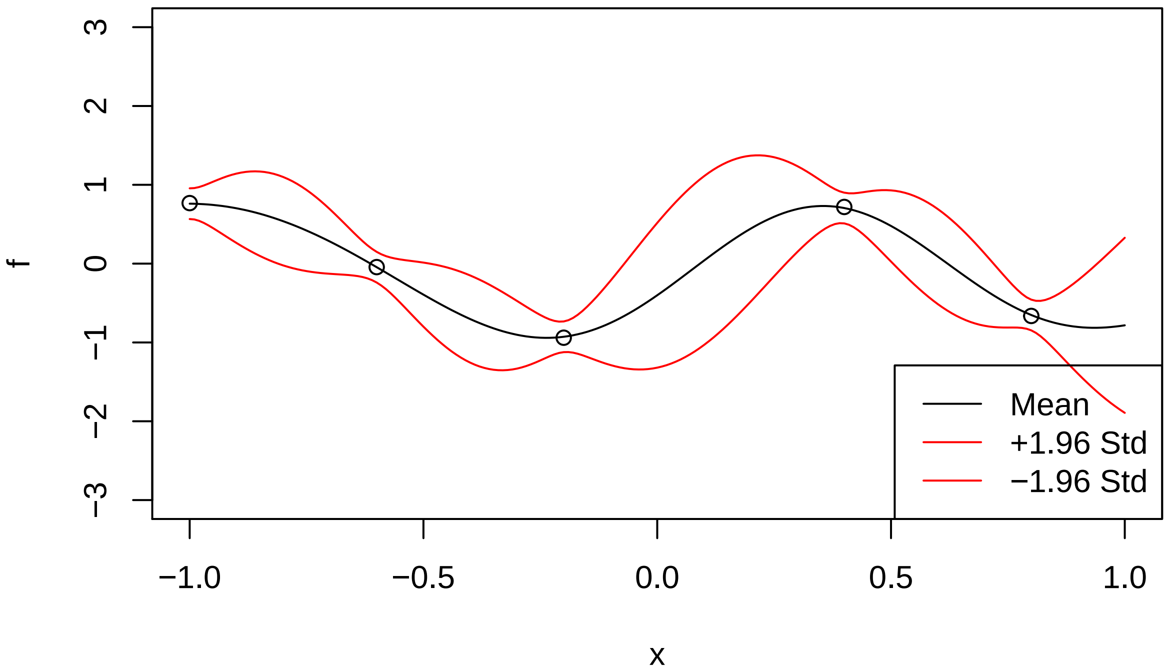



```r
X = c(0.4, -0.6)
y = c(0.719, -0.044)
Xstar = seq(-1, 1, 0.01)
sigmaNoise = 0.1
K = SquaredExpKernel
f = posteriorGP(X, y, Xstar, sigmaNoise, K, sigmaF=1, l=0.3)

up_bound <- f$mean+1.96*sqrt(diag(f$var))
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')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
```



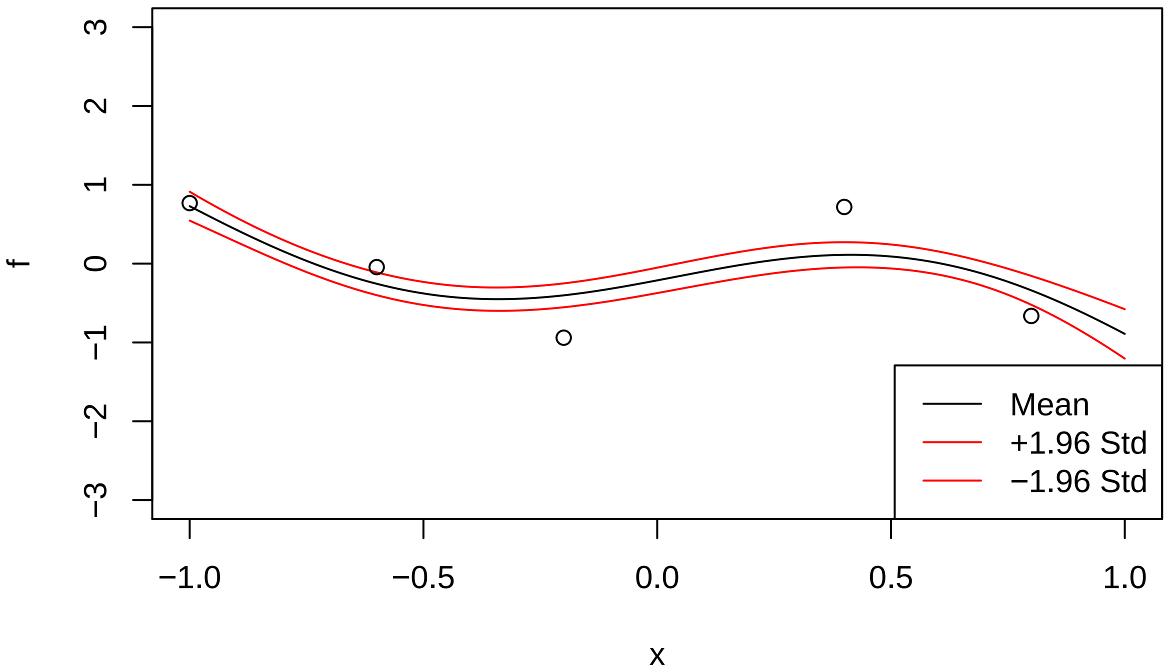
Q2.4

```
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))
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')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
```



Q2.5

```
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))
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')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
```



When change l from 0.3 to 1, we got a smoother curve, this is because when we have a lager l, 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)
time <- seq(1, 2190)
time <- (time -mean(time)) / sd(time)
day <- rep(1:365,6)
day <- (day -mean(day)) / sd(day)
df$time <- time

RBFkernel <- function(sigmaf = 1, ell = 1) {
  rval <- function(x, y = NULL) {
      res <- sigmaf^2*exp(-0.5*( (x-y)/ell)^2 )
      return(res)
    }
  class(rval) <- "kernel"
  return(rval)
}

SEkernel <- RBFkernel(sigmaf = 1, ell = 1)
SEkernel(1,2)
```

```
## [1] 0.6065307
```

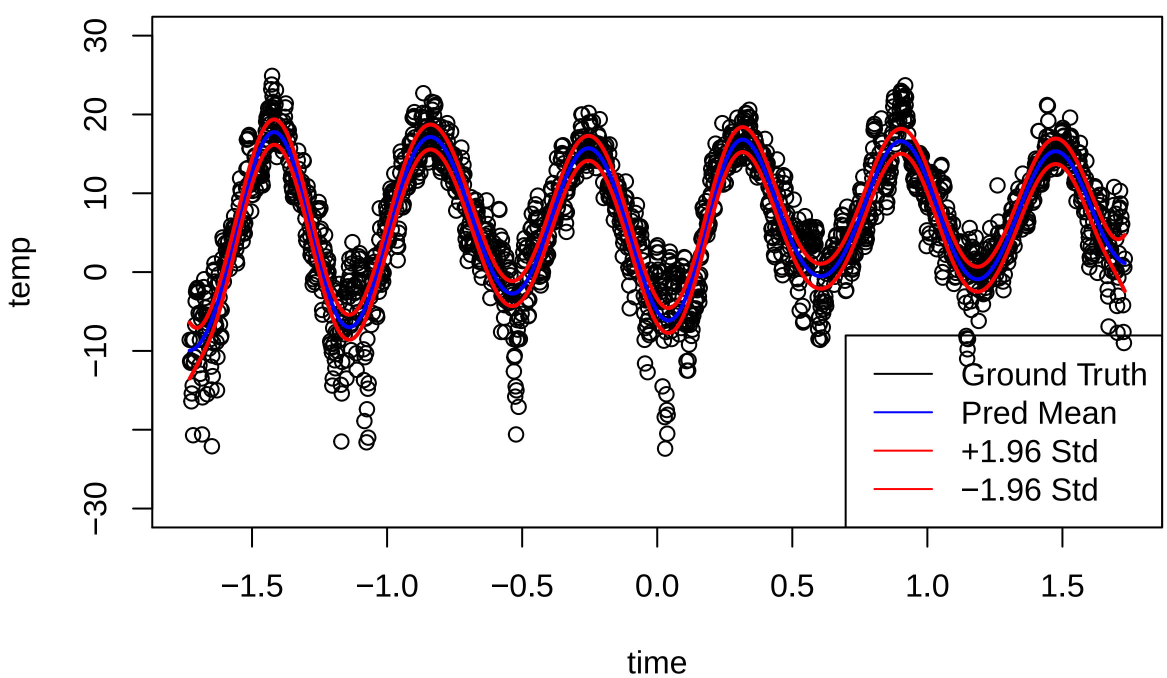
```
X <- matrix(c(1,3,4), 3, 1)
Xstar <- matrix(c(2,3,4), 3, 1)
kernelMatrix(kernel = SEkernel, x = X, y = Xstar)
```

```
## 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
```

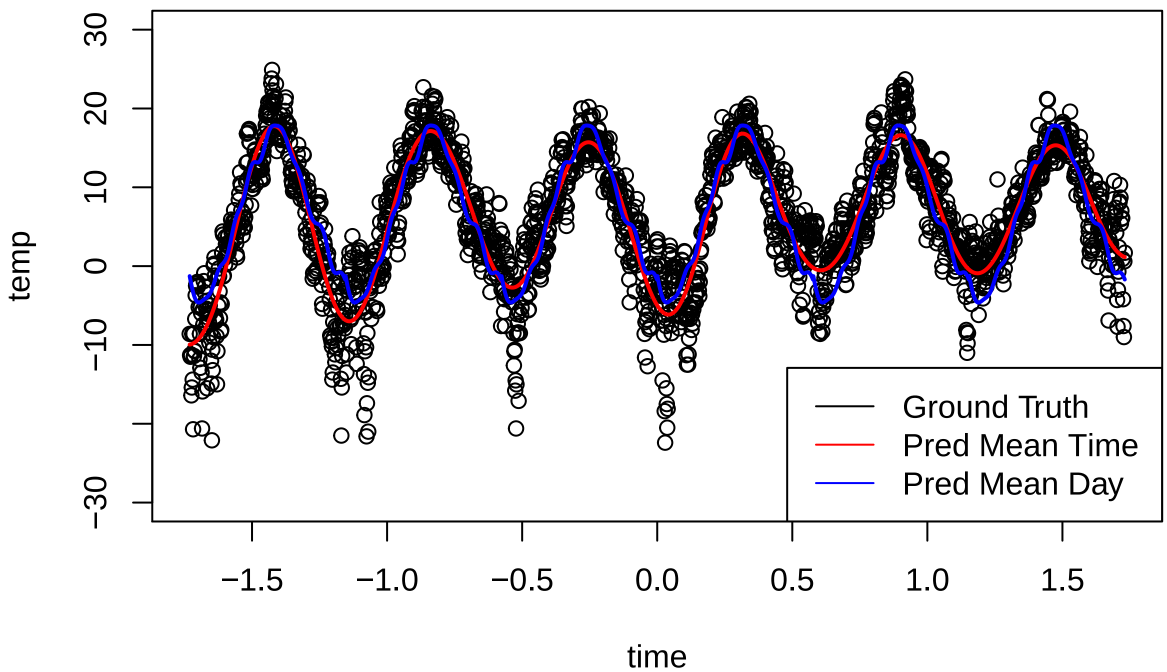
Q3.2

```
temp <- df$temp
plot(time, temp, ylim=c(-30, 30))

polyFit <- lm(temp ~  time + I(time^2))
sigmaNoise <- sd(polyFit$residuals)
sigmaf <- 20
ell <- 0.2
RBF <- RBFkernel(sigmaf = sigmaf, ell=ell)
GPfit <- gausspr(time, temp, kernel = RBF, var = sigmaNoise^2)
meanPred <- predict(GPfit, time)
lines(time, meanPred, lwd = 2, col='blue')

x<-time
xs<-time # XStar.
n <- length(x)
Kss <- kernelMatrix(kernel = RBF, x = xs, y = xs)
Kxx <- kernelMatrix(kernel = RBF, x = x, y = x)
Kxs <- kernelMatrix(kernel = RBF, x = x, y = xs)
Covf = Kss-t(Kxs)%*%solve(Kxx + sigmaNoise^2*diag(n), Kxs) # Covariance matrix of fStar.
lines(xs, meanPred - 1.96*sqrt(diag(Covf)), col = "red", lwd = 2)
lines(xs, meanPred + 1.96*sqrt(diag(Covf)), 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"))
```




```
temp <- df$temp
plot(time, temp, ylim=c(-30, 30))
```

```r
polyFit <- lm(temp ~  time + I(time^2))
sigmaNoise <- sd(polyFit$residuals)
sigmaf <- 20
ell <- 0.2
RBF <- RBFkernel(sigmaf = sigmaf, ell=ell)
GPfit_day <- gausspr(day, temp, kernel = RBF, var = sigmaNoise^2)
meanPred_day <- predict(GPfit_day, day)
plot(time, temp, ylim=c(-30, 30))
lines(time, meanPred, lwd = 2, col='red')
lines(time, meanPred_day, 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"))
```



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)

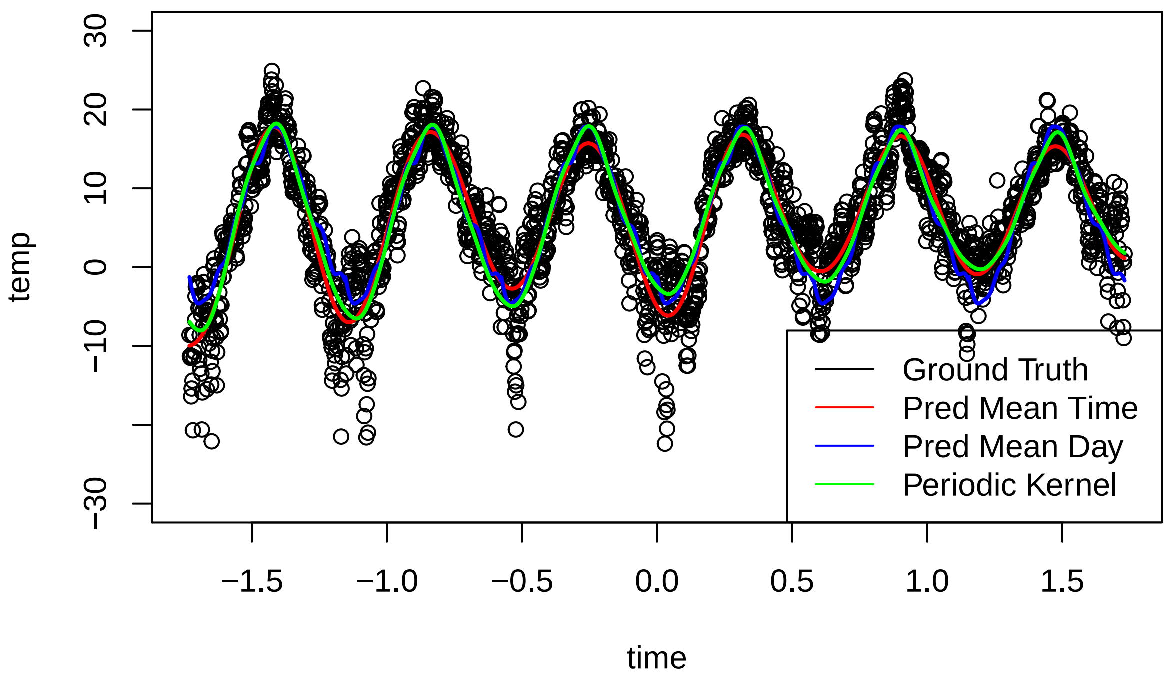
- Day:

GP on the whole single year, this approach might introduce some ambiguities, it has the same day as input but multiple outputs. This approach seems assuming temperature will always be the same on the same day in different years.

Q3.5

```r
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)
meanPred_PK <- predict(GPfit_PK, time)
plot(time, temp, ylim=c(-30, 30))
lines(time, meanPred, lwd = 2, col='red')
lines(time, meanPred_day, lwd = 2, col='blue')
lines(time, meanPred_PK, 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"))
```



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.

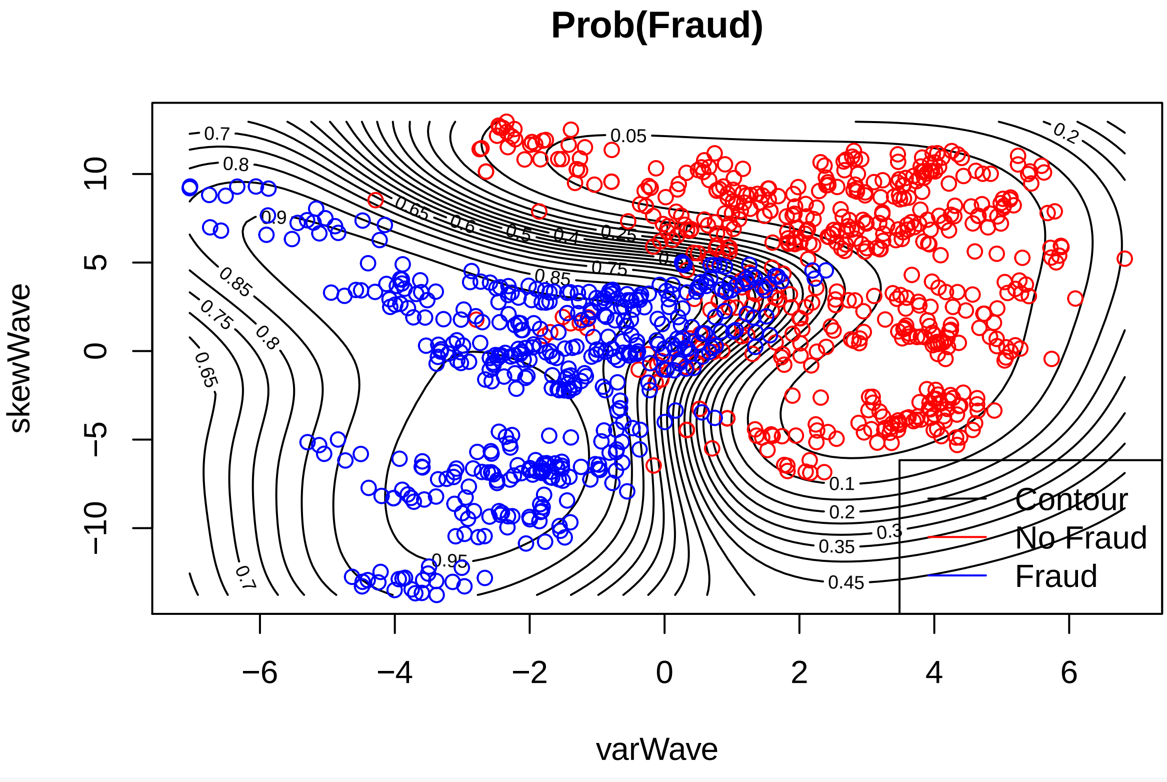
Q4.1

```
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)
```

```r
SelectTraining <- sample(1:dim(data)[1], size = 1000, replace = FALSE)
train=data[SelectTraining,]
test=data[-SelectTraining,]


GPClassifier <- gausspr(fraud ~  varWave + skewWave, data=train)
```

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

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

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

# Plotting for Prob(setosa)
contour(x1,x2,matrix(probPreds[,2],100,byrow = TRUE), 20, xlab = "varWave", ylab = "skewWave", main = 'P
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"))
```




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

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

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

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

```r
sum(diag(confmatrix)) / sum(confmatrix)
```

```
## [1] 0.941
```

```r
print('Confusion matrix and accuracy of test set')
```

```
## [1] "Confusion matrix and accuracy of test set"
```

```r
confmatrix <- table(predict(GPClassifier,test[,1:2]), test[,5])
confmatrix
```

```
##
##       0   1
##   0 199   9
##   1  19 145
```

```r
sum(diag(confmatrix)) / sum(confmatrix)
```

```
## [1] 0.9247312
```

Q4.3

```r
GPClassifier <- gausspr(fraud ~ ., data=train)
```

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

```r
print('Confusion matrix and accuracy of test set with all 4 features')
```

```
## [1] "Confusion matrix and accuracy of test set with all 4 features"
```

```r
confmatrix <- table(predict(GPClassifier,test[,1:4]), test[,5])
confmatrix
```

```
##
##       0   1
##   0 216   0
##   1   2 154
```

```r
sum(diag(confmatrix)) / sum(confmatrix)
```

```
## [1] 0.9946237
```

Appendix

```r
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])/l)^2 )
  }
  return(K)
}

posteriorGP <- function(X, y, Xstar, sigmaNoise, K, ...){
  n <- length(X)
  C <- K(X, X, ...) + sigmaNoise ^ 2 * diag(n)
  L <- t(chol(C))
  L_inv <- solve(L)
  C_inv <- t(L_inv) %*% L_inv
  mean <- K(Xstar, X, ...) %*% C_inv %*% y
  var <- K(Xstar, Xstar, ...) - K(Xstar, X, ...) %*% C_inv %*% t(K(Xstar, X, ...))
  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, 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')
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))
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')
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)
```

```r
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')
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))
low_bound <- f$mean-1.96*sqrt(diag(f$var))
plot(Xstar, f$mean, type='l', ylim =c(-3,3), xlab = "x", ylab = "f")
lines(Xstar, up_bound, col='red')
lines(Xstar, low_bound, col='red')
points(X, y)
legend("bottomright", legend=c("Mean","+1.96 Std", "-1.96 Std"),
        lwd=c(1,1,1), col=c("black","red","red"))
df <- read.csv("TempTullinge.csv", sep=";", header=TRUE)
time <- seq(1, 2190)
time <- (time -mean(time)) / sd(time)
day <- rep(1:365,6)
day <- (day -mean(day)) / sd(day)
df$time <- time

RBFkernel <- function(sigmaf = 1, ell = 1) {
  rval <- function(x, y = NULL) {
      res <- sigmaf^2*exp(-0.5*( (x-y)/ell)^2 )
      return(res)
    }
  class(rval) <- "kernel"
  return(rval)
}

SEkernel <- RBFkernel(sigmaf = 1, ell = 1)
SEkernel(1,2)

X <- matrix(c(1,3,4), 3, 1)
Xstar <- matrix(c(2,3,4), 3, 1)
kernelMatrix(kernel = SEkernel, x = X, y = Xstar)

temp <- df$temp
plot(time, temp, ylim=c(-30, 30))
```

```r
polyFit <- lm(temp ~  time + I(time^2))
sigmaNoise <- sd(polyFit$residuals)
sigmaf <- 20
ell <- 0.2
RBF <- RBFkernel(sigmaf = sigmaf, ell=ell)
GPfit <- gausspr(time, temp, kernel = RBF, var = sigmaNoise^2)
meanPred <- predict(GPfit, time)
lines(time, meanPred, lwd = 2, col='blue')

x<-time
xs<-time # XStar.
n <- length(x)
Kss <- kernelMatrix(kernel = RBF, x = xs, y = xs)
Kxx <- kernelMatrix(kernel = RBF, x = x, y = x)
Kxs <- kernelMatrix(kernel = RBF, x = x, y = xs)
Covf = Kss-t(Kxs)%*%solve(Kxx + sigmaNoise^2*diag(n), Kxs) # Covariance matrix of fStar.
lines(xs, meanPred - 1.96*sqrt(diag(Covf)), col = "red", lwd = 2)
lines(xs, meanPred + 1.96*sqrt(diag(Covf)), 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"))
temp <- df$temp
plot(time, temp, ylim=c(-30, 30))

polyFit <- lm(temp ~  time + I(time^2))
sigmaNoise <- sd(polyFit$residuals)
sigmaf <- 20
ell <- 0.2
RBF <- RBFkernel(sigmaf = sigmaf, ell=ell)
GPfit_day <- gausspr(day, temp, kernel = RBF, var = sigmaNoise^2)
meanPred_day <- predict(GPfit_day, day)
plot(time, temp, ylim=c(-30, 30))
lines(time, meanPred, lwd = 2, col='red')
lines(time, meanPred_day, 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) {
      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)
meanPred_PK <- predict(GPfit_PK, time)
```

```r
plot(time, temp, ylim=c(-30, 30))
lines(time, meanPred, lwd = 2, col='red')
lines(time, meanPred_day, lwd = 2, col='blue')
lines(time, meanPred_PK, 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")
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,]


GPClassifier <- gausspr(fraud ~  varWave + skewWave, data=train)


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

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

# 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])
confmatrix
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)
```