Lab 4 - Gaussian Processes

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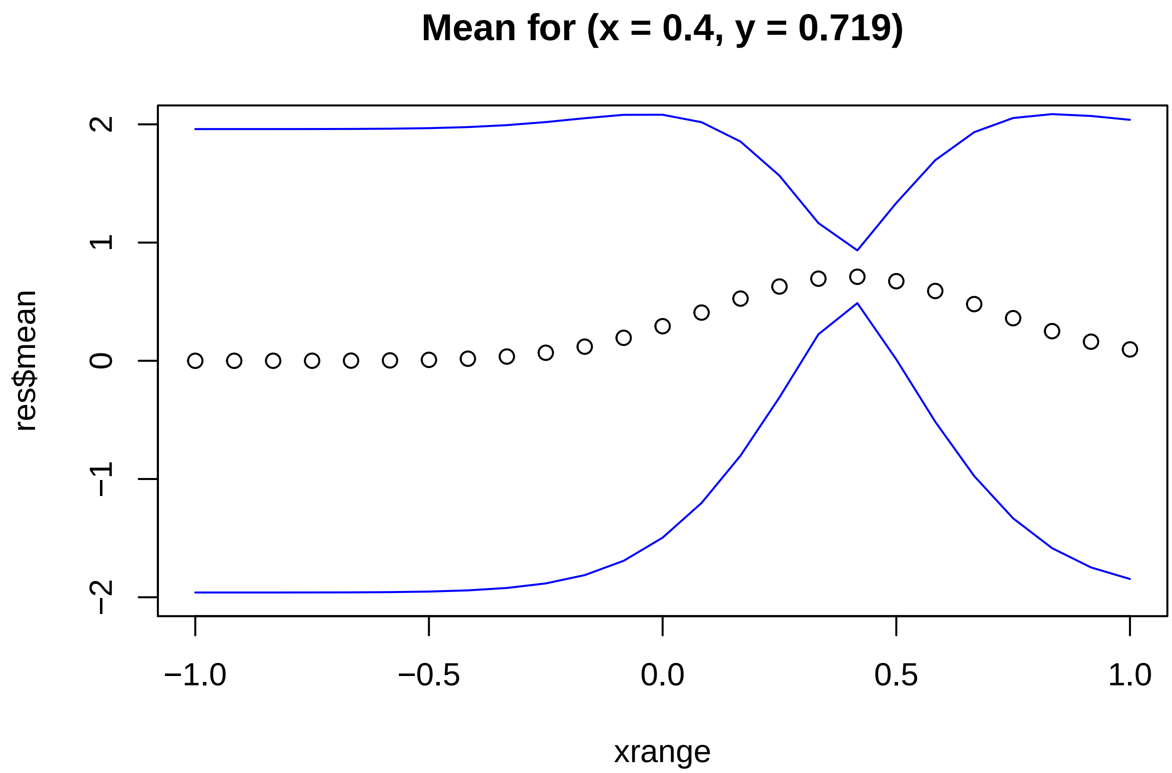
Assignment 1

2.1) (1) Implementing GP Regression

```
# Simulating from posterior distribution of f
posteriorGP = function(X, y, XStar, sigmaNoise, k, sigmaF, l){

  K = k(X,X, sigmaF, l)
  n = length(XStar)
  L = t(chol(K + sigmaNoise*diag(dim(K)[1])))
  kStar = k(X,XStar, sigmaF, l)
  alpha = solve(t(L), solve(L,y))

  FStar = t(kStar) %*% alpha
  v = solve(L, kStar)
  vf = k(XStar, XStar, sigmaF, l) - t(v)%*%v #+ sigmaNoise*diag(n) #Adding sigma for noise
  logmarglike = -t(y)%*%alpha/2 - sum(diag(L)) - n/2*log(2*pi)
  # Returns a vector with the posterior mean and variance
  return(list("mean" = FStar,"variance" = vf,"logmarglike" = logmarglike))
}
```

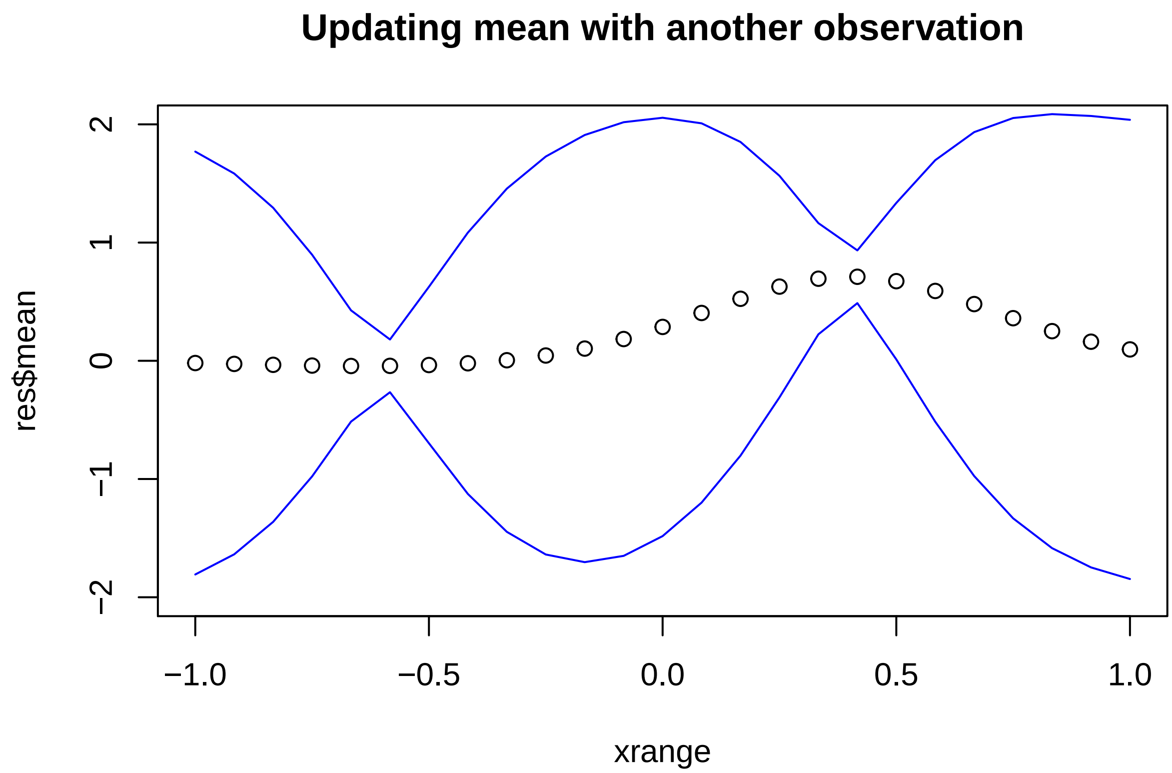
2.1) (2) GP Regression with kernlab

```
sigmaf = 1^2
sigman = 0.1^2
l = 0.3
x = 0.4
y = 0.719
xrange = seq(-1,1, length=25)

res = posteriorGP(x, y, xrange, sigman, SquaredExpKernel, sigmaF = sigmaf, l=l)

# (2) Plotting posterior mean and 95% interval bands
plot(x = xrange, y = res$mean, ylim = c(-2,2), main = "Mean for (x = 0.4, y = 0.719)")
lines(x = xrange, y = res$mean + sqrt(diag(res$variance))*1.96, col="blue", type="l")
lines(x = xrange, y = res$mean - sqrt(diag(res$variance))*1.96, col="blue",  type="l")
```



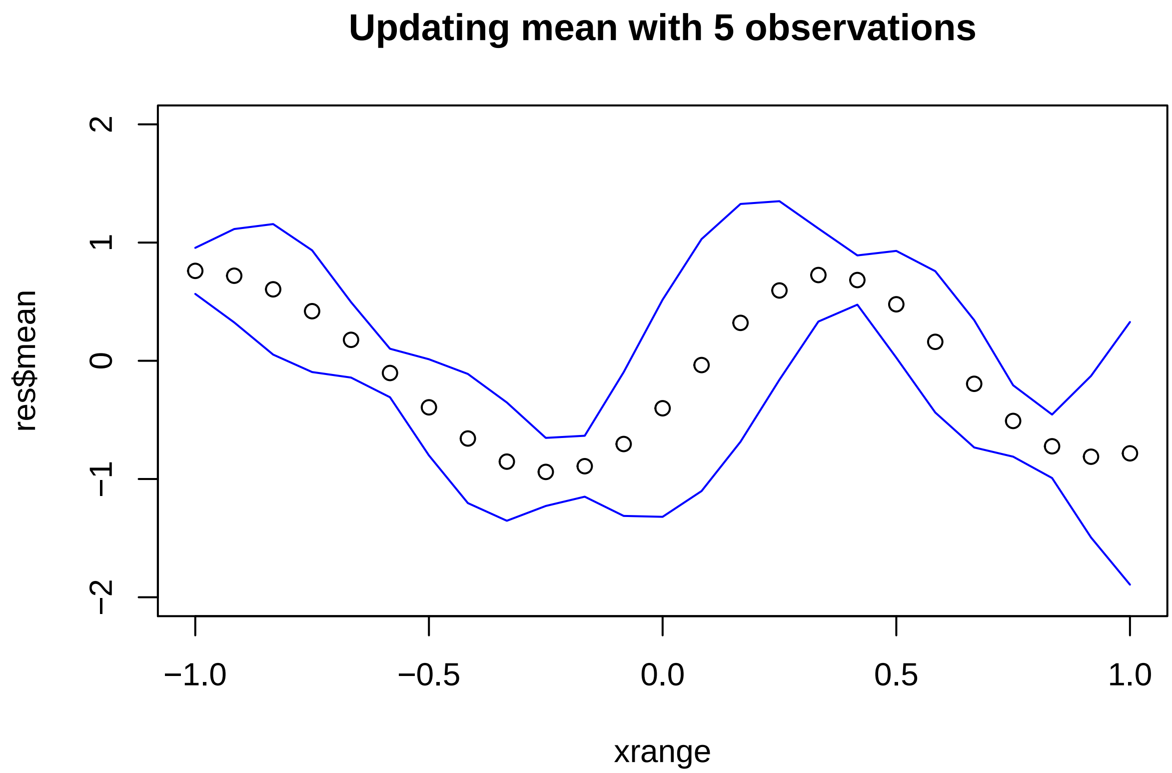
2.1) (3)

```
# (3)
x = c(0.4,-0.6)
y = c(0.719,-0.044)

res = posteriorGP(x, y, xrange, sigman, SquaredExpKernel, sigmaF = sigmaf, l=l)
plot(x = xrange, y = res$mean, ylim = c(-2,2), main = "Updating mean with another observation")
lines(x = xrange, y = res$mean + sqrt(diag(res$variance))*1.96, col="blue", type="l")
lines(x = xrange, y = res$mean - sqrt(diag(res$variance))*1.96, col="blue",  type="l")
```



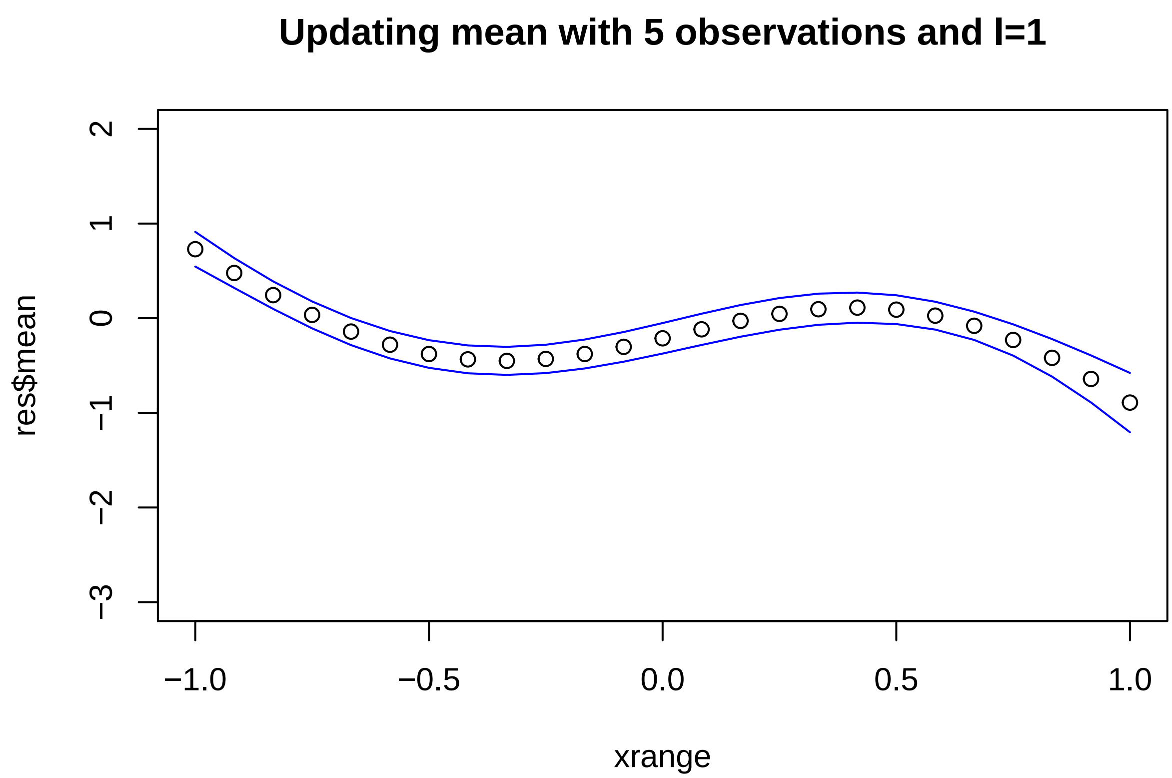
2.1) (4)

```
# (4)
x = c(-1.0, -0.6, -0.2, 0.4, 0.8)
y = c(0.768, -0.044, -0.940, 0.719, -0.664)
sigmaf = 1^2
l = 0.3
res = posteriorGP(x, y, xrange, sigman, SquaredExpKernel, sigmaF = sigmaf, l=l)
plot(x = xrange, y = res$mean, ylim = c(-2,2), main = "Updating mean with 5 observations")
lines(x = xrange, y = res$mean + sqrt(diag(res$variance))*1.96, col="blue", type="l")
lines(x = xrange, y = res$mean - sqrt(diag(res$variance))*1.96, col="blue",  type="l")
```



2.1) (5)

```
# (5)
x = c(-1.0, -0.6, -0.2, 0.4, 0.8)
y = c(0.768, -0.044, -0.940, 0.719, -0.664)
sigmaf = 1
l = 1
res = posteriorGP(x, y, xrange, sigman, SquaredExpKernel, sigmaF = sigmaf, l=l)

plot(x = xrange, y = res$mean, ylim = c(-3,2), main = "Updating mean with 5 observations and l=1")
lines(x = xrange, y = res$mean + sqrt(diag(res$variance))*1.96, col="blue", type="l")
lines(x = xrange, y = res$mean - sqrt(diag(res$variance))*1.96, col="blue",  type="l")
```



Since **l=1**, the produced function will be more smooth compared to (4). We also see that the bands created are much more narrow compared to plot produced in (4).

Assignment 2

2.2 (1) GP Regression with kernlab

```
time = seq(from=1, to=2190, by=5)
temps = temps[time]
day = rep(seq(from=1, to=361, by=5), times=6)
# Data scaling
daymean = mean(day)
daysd = sd(day)
timemean = mean(time)
timesd = sd(time)
tempsmean = mean(temps)
tempssd = sd(temps)

day_s = scale(day)
time_s = scale(time)
temps_s = scale(temps)
```

2.2 (1)

```r
SEKernel = function(x1, x2, ell = 1, sigmaf = 1){
  r = sqrt(sum((x1 - x2)^2))
  return(sigmaf^2*exp(-r^2/(2*ell^2)))
}

SEKernel(x1=1, x2=2, ell = l, sigmaf = sigmaf)
```

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

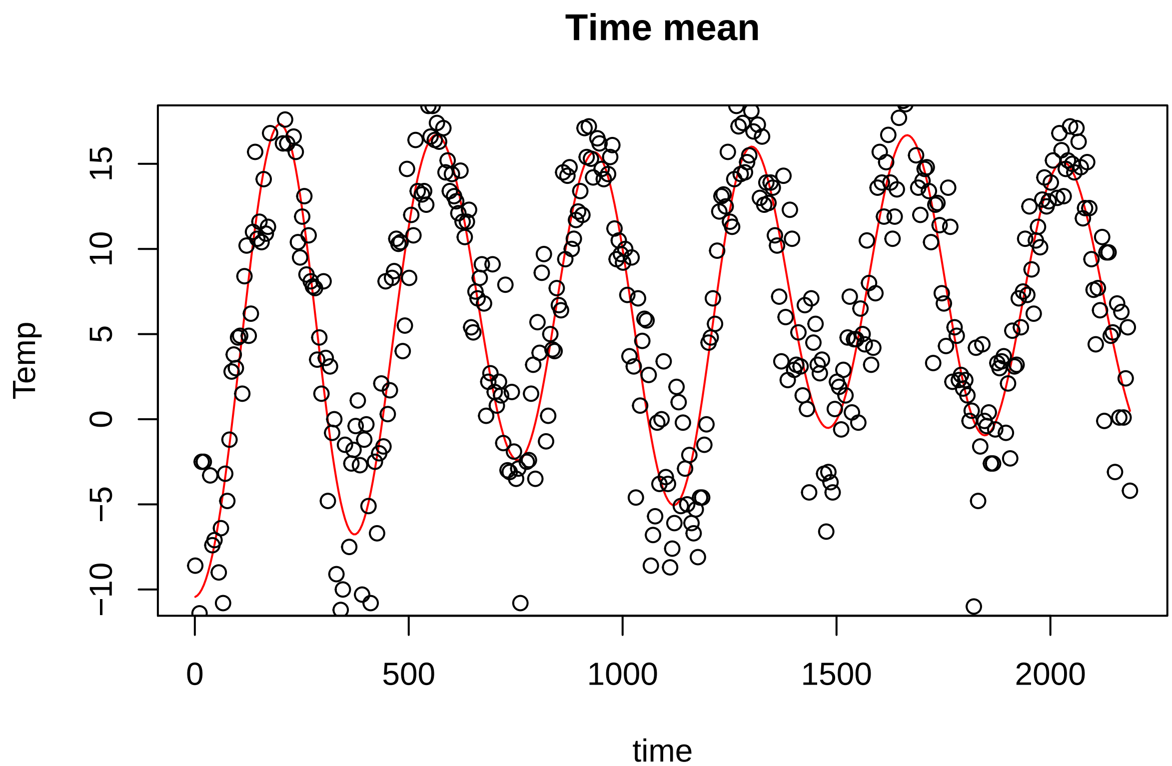
```r
X = c(1,3,4)
XStar = c(2,3,4)
kernelMatrix(kernel = SEKernel, x=X, y=XStar)
```

```
## 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
```

```r
SEKernelfunc = function(ell, sigmaf){
  kernel = function(x1, x2){
  r = sqrt(sum((x1 - x2)^2))
  return(sigmaf^2*exp(-r^2/(2*ell^2)))
  }
  class(kernel) <- "kernel"
  return(kernel)
}
```

2.2 (2)

```r
ell = 0.2
sigmaf = 20

# Getting the error term for the GP
polyFit <- lm(temps ~  time_s + I(time_s^2))
sigma = sd(polyFit$residuals)
GPfit = gausspr(x=time_s, y=temps_s, kernel = SEKernelfunc(ell, sigmaf), var = sigma^2, type="regressio
meanpred = predict(GPfit, time_s)

# Plotting the means from time data
plot(time, meanpred*tempssd+tempsmean, col="red", type='l', ylab="Temp", main="Time mean")
lines(x = time, y = temps,  type="p")
```

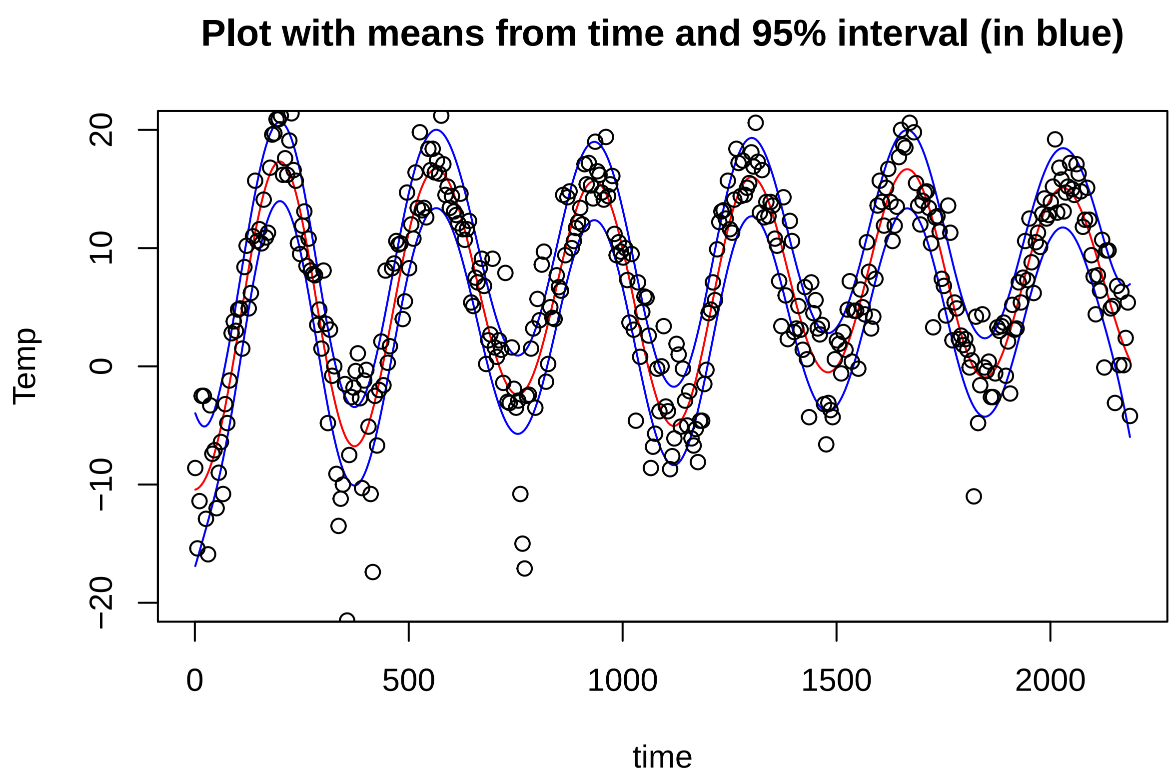


A higher value for ell increases smoothness. A higher value for sigmaf increases the possible ranges of the predicted means. A lower value gives lower covariance between prediction. This explains the difference in the highest and lowest values for different sigmaf's.

2.2 (3)

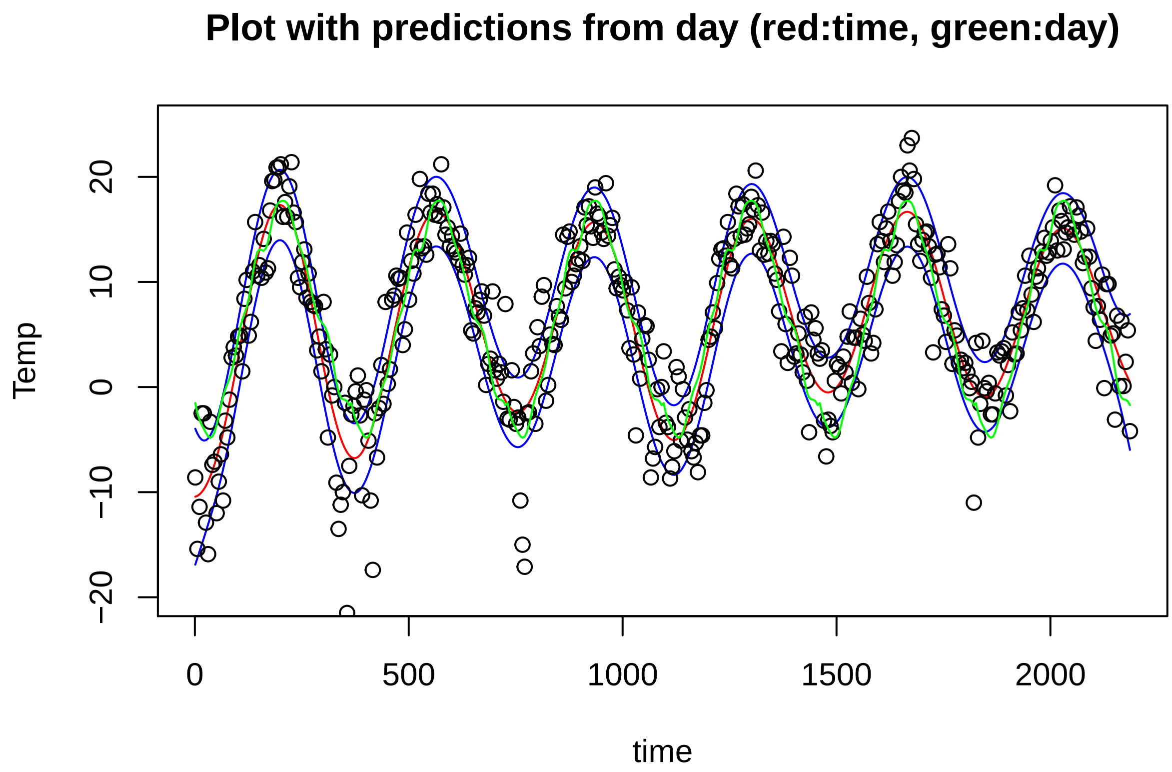
```
# Modified posteriorGP function
posteriorGP = function(X, y, XStar, sigmaNoise, k){
  K = kernelMatrix(k,X,X)
  n = length(XStar)
  L = t(chol(K + sigmaNoise*diag(dim(K)[1])))
  kStar = kernelMatrix(k,X,XStar)
  alpha = solve(t(L), solve(L,y))
  FStar = (t(kStar)) %*% alpha
  v = solve(L, kStar)
  vf = kernelMatrix(k,XStar, XStar) - t(v)%*%v #+ sigmaNoise*diag(n) #Adding sigma for noise
  logmarglike = -t(y)%*%alpha/2 - sum(diag(L)) - n/2*log(2*pi)

  # Returns a vector with the posterior mean and variance
  return(list("mean" = FStar,"variance" = vf,"logmarglike" = logmarglike))
}
sigmaf = 20
var = posteriorGP(X=time_s, y=temps_s, XStar=time_s, sigmaNoise=sigma^2, k=SEKernelfunc(ell, sigmaf))

plot(time, meanpred*tempssd+tempsmean, col="red", type='l', ylim=c(-20,20), main="Plot with means from
```

```
lines(x = time, y = meanpred*tempssd+tempsmean + sqrt(diag(var$variance))*1.96, col="blue", type="l")
lines(x = time, y = meanpred*tempssd+tempsmean - sqrt(diag(var$variance))*1.96, col="blue",  type="l")
lines(x = time, y = temps,  type="p")
```



2.2 (4)

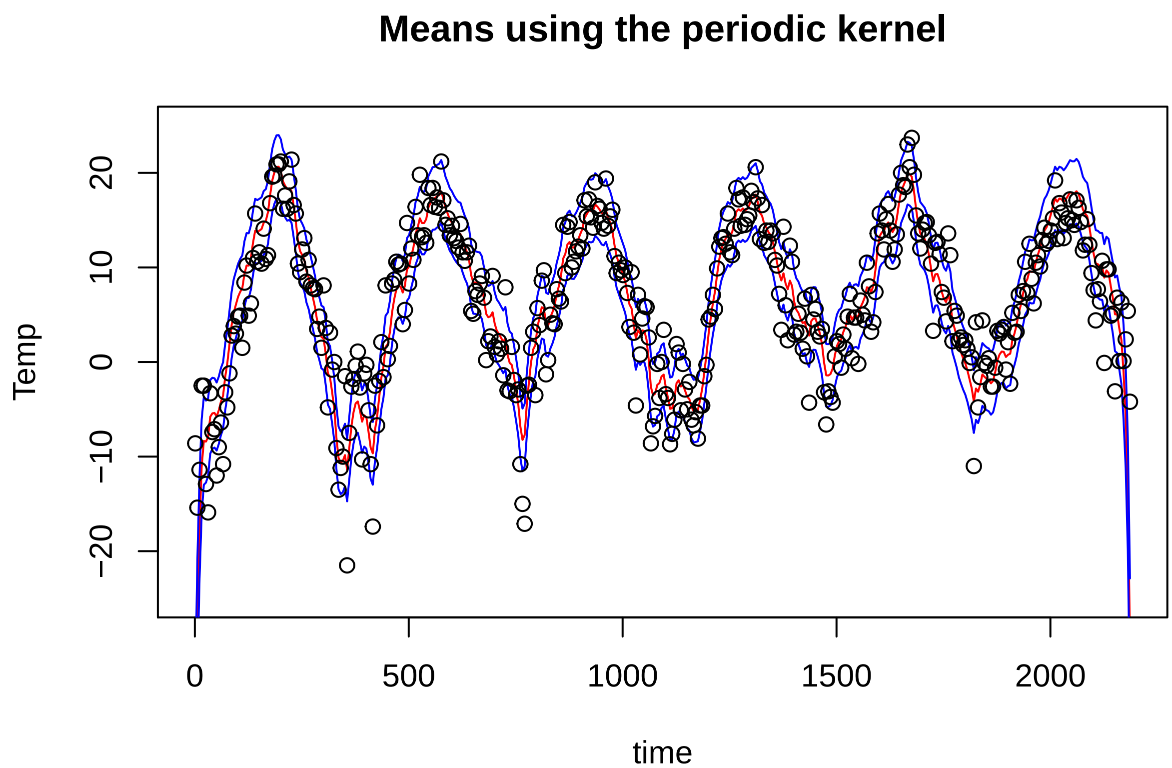
```
ell = 0.2
sigmaf = 20

# Getting the error term for the GP, using day instead of time
polyFit <- lm(temps ~  day_s + I(day_s^2))
sigma = sd(polyFit$residuals)
GPfit = gausspr(x=day_s, y=temps_s, kernel = SEKernelfunc(ell, sigmaf), var = sigma^2, type="regression
meanpred_day = predict(GPfit, day_s)

plot(time, meanpred*tempssd+tempsmean, col="red", type='l', ylim=c(-20,25), main="Plot with predictions
lines(x = time, y = meanpred*tempssd+tempsmean + sqrt(diag(var$variance))*1.96, col="blue", type="l")
lines(x = time, y = meanpred*tempssd+tempsmean - sqrt(diag(var$variance))*1.96, col="blue",  type="l")
lines(x = time, y = temps,  type="p")
lines(x = time, y = meanpred_day*tempssd+tempsmean, col="green",  type="l")
```



2.2 (5)

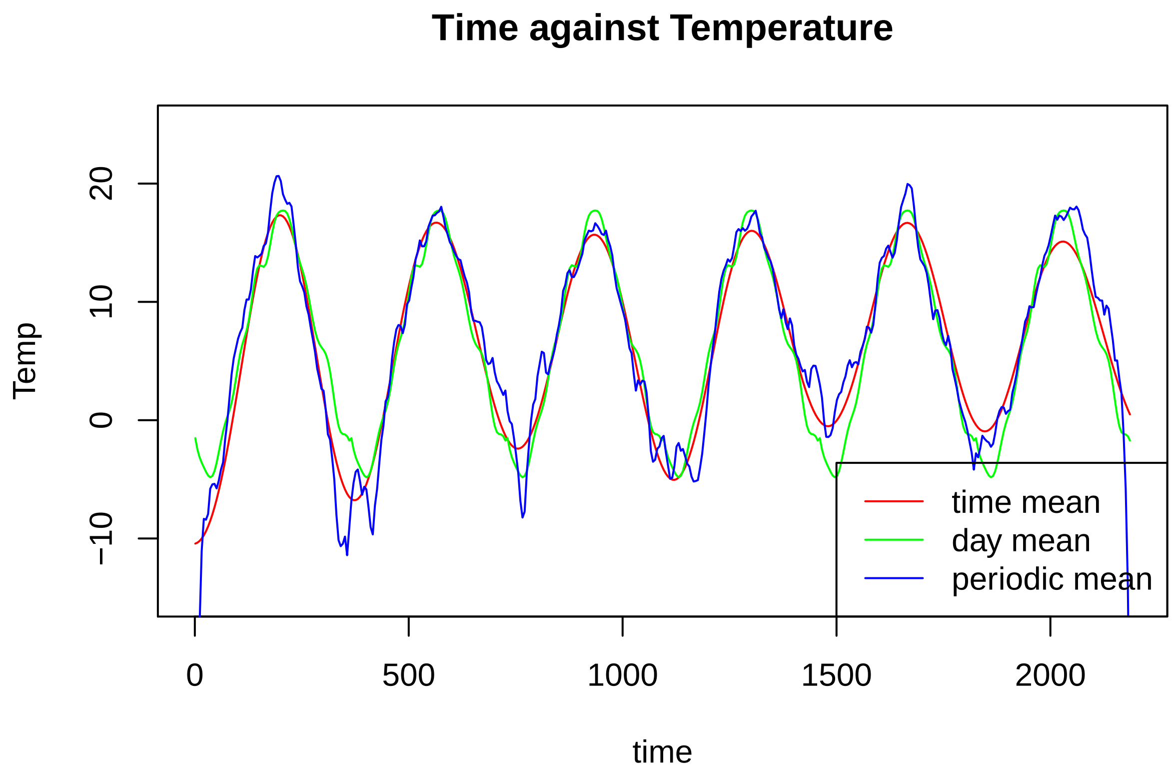
```
periodickernelfunc = function(sigmaf, l1, l2, d){
  periodicKernel = function(x1, x2){
  r = sqrt(sum((x1 - x2)^2))
  one = exp(-2*sin(r/d)/l1^2)
  two = exp(-r^2/(2*l2^2))
  return(sigmaf^2*one*two)
  }
  class(periodicKernel) <- "kernel"
  return(periodicKernel)
}

# Hyperparameters
sigmaf = 20
l1 = 1
l2 = 10
d = 365/sd(time)

# Getting the error term for the GP
polyFit <- lm(temps ~  time_s + I(time_s^2))
sigma = sd(polyFit$residuals)
GPfit = gausspr(x=time_s, y=temps_s, kernel = periodickernelfunc(sigmaf, l1, l2, d), var = sigma^2, typ
meanpred_5 = predict(GPfit, time_s)
```

```
# Plotting the means!
plot(x = time, y = meanpred_5*tempssd+tempsmean, col="red", type='l', ylim=c(-25,25), main = "Means usi
lines(x = time, y = meanpred_5*tempssd+tempsmean + sqrt(diag(var$variance))*1.96, col="blue", type="l")
lines(x = time, y = meanpred_5*tempssd+tempsmean - sqrt(diag(var$variance))*1.96, col="blue",  type="l"
lines(x = time, y = temps,  type="p")
```



Plot of all the means

```
plot(x = time, y = meanpred*tempssd+tempsmean, col="red", type='l', ylim=c(-15,25),main = "Time against
lines(x = time, y = meanpred_day*tempssd+tempsmean, col="green", type='l')
lines(x = time, y = meanpred_5*tempssd+tempsmean, col="blue", type='l')
legend("bottomright", legend=c("time mean", "day mean", "periodic mean"), lty=c(1, 1, 1),col=c("red", "
```



We can see that the periodic kernel produces produces more sharp "valleys" and more even "tops" compared to the more smooth Squared Exponential kernel. This can be explained by the use of the periodic kernel. The model now takes into consideration

Assignment 3

2.3 (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 = data[SelectTraining,]
test_data = data[-SelectTraining,]


GPfitfraud <- gausspr(fraud ~  varWave + skewWave, data=train_data)
```

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

```
GPfitfraud
```

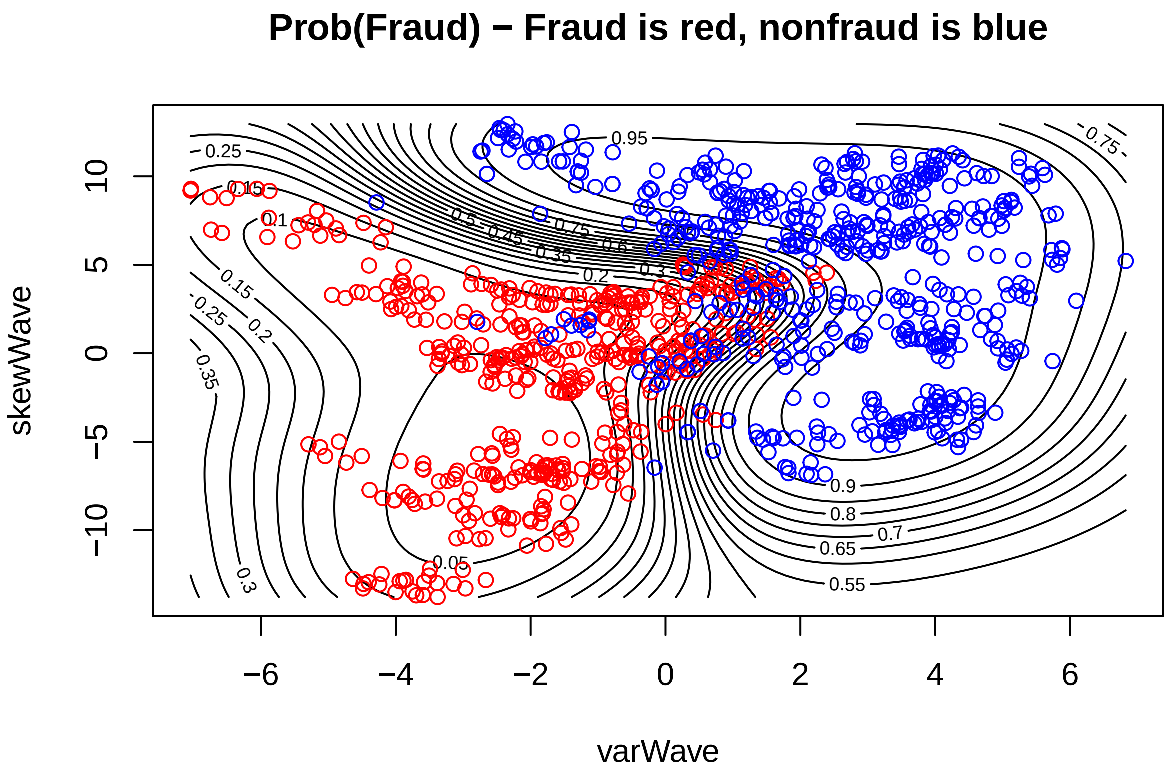
```
## Gaussian Processes object of class "gausspr"
## Problem type: classification
##
## Gaussian Radial Basis kernel function.
##  Hyperparameter : sigma =  1.42415004757028
##
## Number of training instances learned : 1000
## Train error : 0.059
```

```
# Predict on the training set
pred = predict(GPfitfraud,train_data)
# Confusion matrix
table(pred, data[SelectTraining,5])
```

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

Plotting the data

```
probPreds <- predict(GPfitfraud, test_data, type="probabilities")
varWave <- seq(min(data[,1]),max(data[,1]),length=100)
skewWave <- seq(min(data[,2]),max(data[,2]),length=100)
gridPoints <- meshgrid(varWave, skewWave)
gridPoints <- cbind(c(gridPoints$x), c(gridPoints$y))

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

# Plotting for Prob(fraud)
contour(varWave, skewWave, matrix(probPreds[,1], 100, byrow = TRUE), 20, xlab = "varWave", ylab = "skew
points(train_data[train_data$fraud==1,1], train_data[train_data$fraud==1,2],col="red")
points(train_data[train_data$fraud==0,1], train_data[train_data$fraud==0,2],col="blue")
```



2.3 (2)

```r
# Predict on the test set
pred = predict(GPfitfraud,test_data)
# Confusion matrix (test)
conf = table(pred, data[-SelectTraining,5])
print(conf)
```

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

```r
# Computing accuracy
sum(diag(conf))/sum(conf)
```

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

2.3 (3)

```r
GPfitfraud <- gausspr(fraud ~  varWave + skewWave + kurtWave + entropyWave, data=train_data)
```

```
## 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 =  0.438275644976386
##
## Number of training instances learned : 1000
## Train error : 0.003
```

```r
# Predict on the test set
pred_new = predict(GPfitfraud,test_data)
# Confusion matrix (test)
conf_new = table(pred_new, data[-SelectTraining,5])
print(conf_new)
```

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

```r
# Computing accuracy
sum(diag(conf_new))/sum(conf_new)
```

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

We can see that accuracy is much higher when using all four covariates. Only two cases were incorrectly classified!