Lab 3 - Advanced Machine Learning

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Assignment 1

a)

The implementation of a function that simulates from the posterior distribution *f(x)* by using the squared exponential kernel is done in two steps. In the first step a function that computes the squared exponential kernel is created. The formula for the squared exponential kernel can be seen below:

$$K(x, x') = \sigma_f^2 \times exp(-0.5 \times (\frac{x - x'}{\iota})^2)$$

The second step is to build the function *PosteriorGP*. The aim with this function is to calculate the posterior mean and variance of f over a grid of x-values. This is done by implementing algorithm 2.1 from the book *Gaussian Processes for Machine Learning* (Rasmussen and Williams).

The code that has been used to implement the functions can be seen in the appendix *R-code*.

The prior mean of f is assumed to be zero for all x, which gives the following prior distribution for *f(x)*:

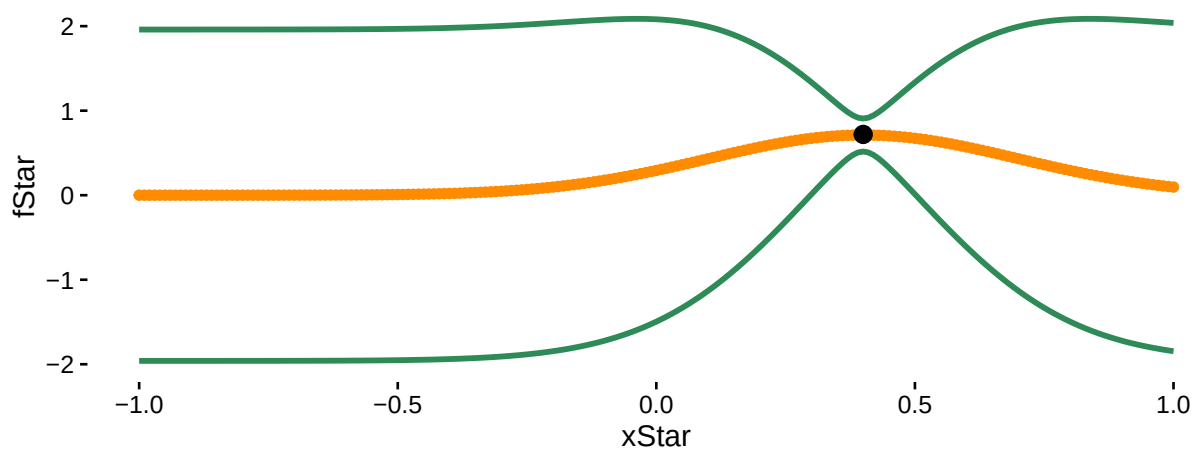
$$f(x) \sim GP(0, K(x, x'))$$

Then, the posterior guassian distribution looks as following:

$$f_* \mid x, y, x_* \sim N(\bar{f}_*, cov(\bar{f}_*)$$

b)

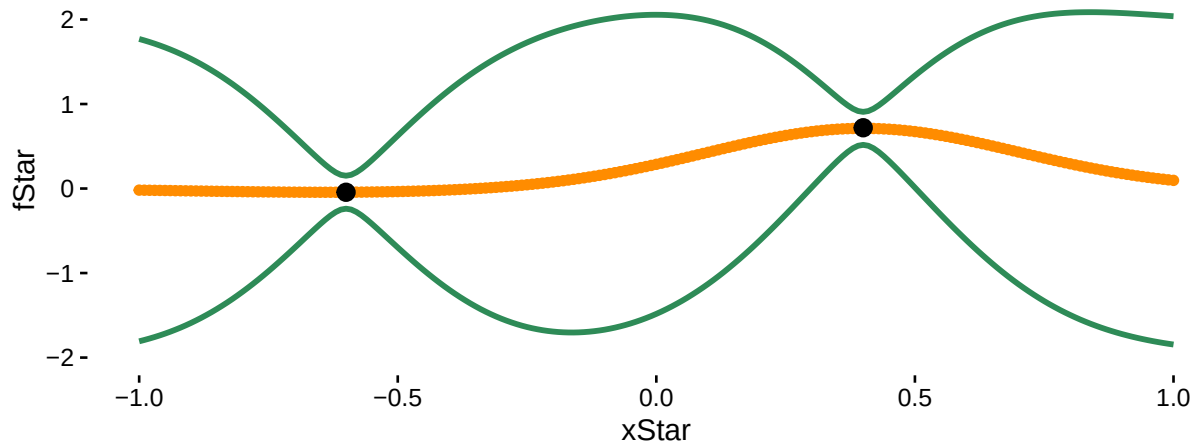
Since the noise standard deviation is assumed to be known the parameter σ_n is set to 0.1. The prior hyperparameter σ_f is set to 1 and the second prior hyperparameter ι is set to 0.3. Furthermore the prior is updated with one observation, *(x,y)*=(0.4, 0.719). A plot over the posterior mean of f over the interval $x \in$ [-1,1] with 95 % probability bands for f can be seen below.



The black dot is the observed value and it can be seen that the probability bands are more narrow around this value.

c)

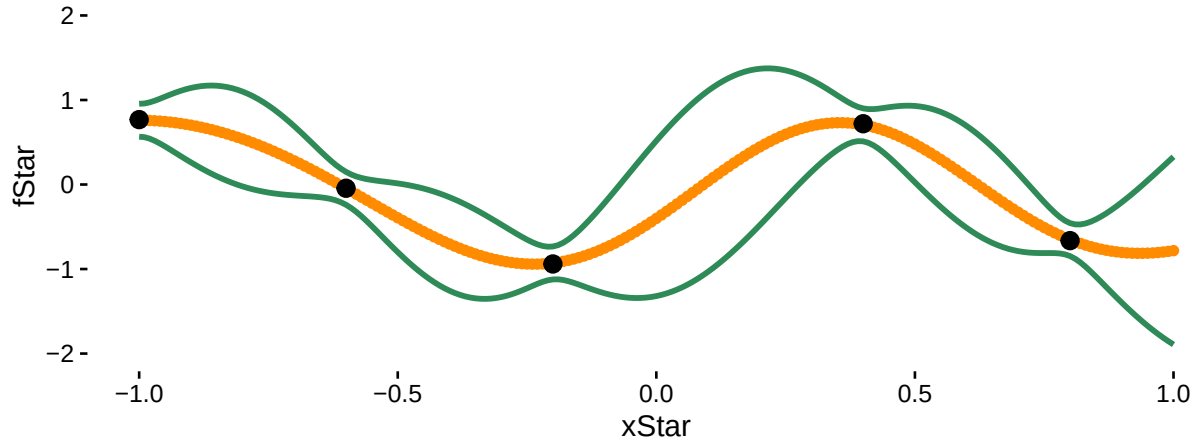
The posterior from *b)* is updated with another observation, *(x,y)*=(-0.6, -0.044).



Again it can be seen that the probability bands are more narrow around the observed values, and that they are quite wide for the other values.

d)

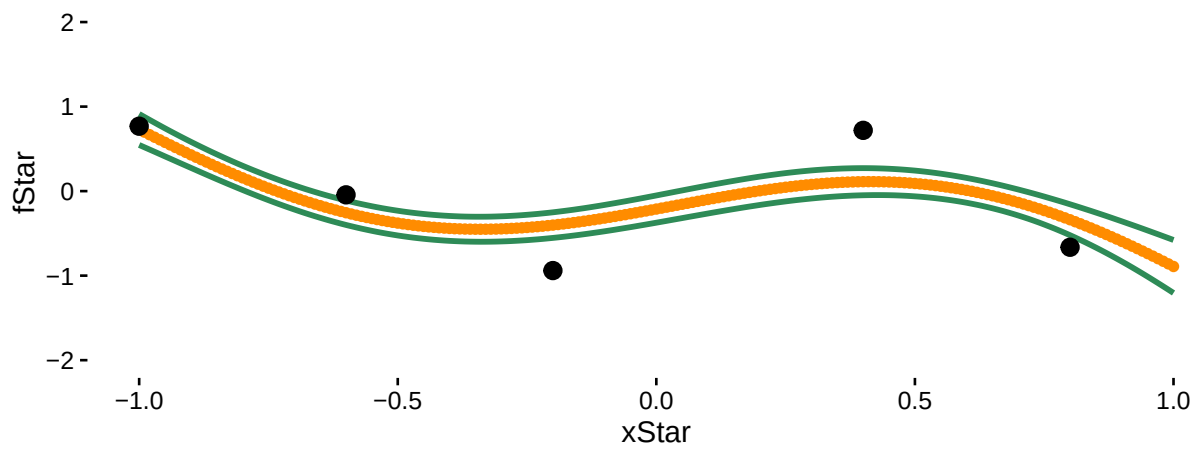
In *d)* the number of observations rises to five, resulting in the following plot over the posterior mean of f and its 95 % probability intervals.



Compared to the plots in *b)* and *c)*, the curve for the posterior mean of f is less straight/ more curvaceous than before. The probability bands has also changed and are thanks to the rise from two to five observed values more narrow, but also quite wiggly.

e)

The hyperparameter ι is now set to 1. The other parameters are unchanged and the same observations as in *d)* are used.



Compared to the plot in *d)*, the probability bands obtained with ι set to 1 looks much smoother and lies much closer to the curve for the posterior mean of *f*. Another change is that curve for the posterior mean of f no longer goes through all of the observed values. Instead the fitted curve appears to be an average between the observed values that lies closest to each other.

Assignment 2

a)

The code where I define my own square exponential kernel function can be seen below.

```
sqExpK <- function(sigmaf = 1, ell = 1) {
  rval <- function(x, xStar = NULL) {
    return(sigmaf * exp (-1/2 * ((x-xStar)/ell)^2 ))
  }
  class(rval) <- "kernel"
  return(rval)
}
```

When evaluated in the point $x = 1$ and $x' = 2$ the following value is given.

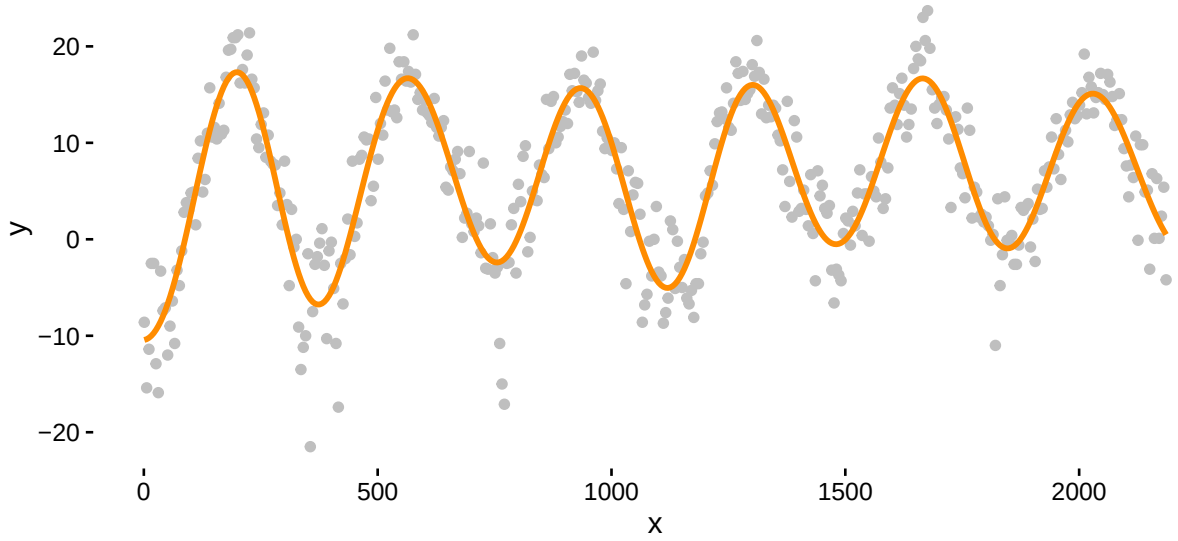
```
## [1] 0.8824969
```

The *kernelMatrix* is tested for the vectors $\mathbf{x} = (1, 3, 4)^T$ and $x_* = (2, 3, 4)^T$. Returned by this function is the covariance matrix $\mathbf{K}(x, x_*)$.

```
## An object of class "kernelMatrix"
##           [,1]      [,2]      [,3]
## [1,] 0.8824969 0.6065307 0.3246525
## [2,] 0.8824969 1.0000000 0.8824969
## [3,] 0.6065307 0.8824969 1.0000000
```

b)

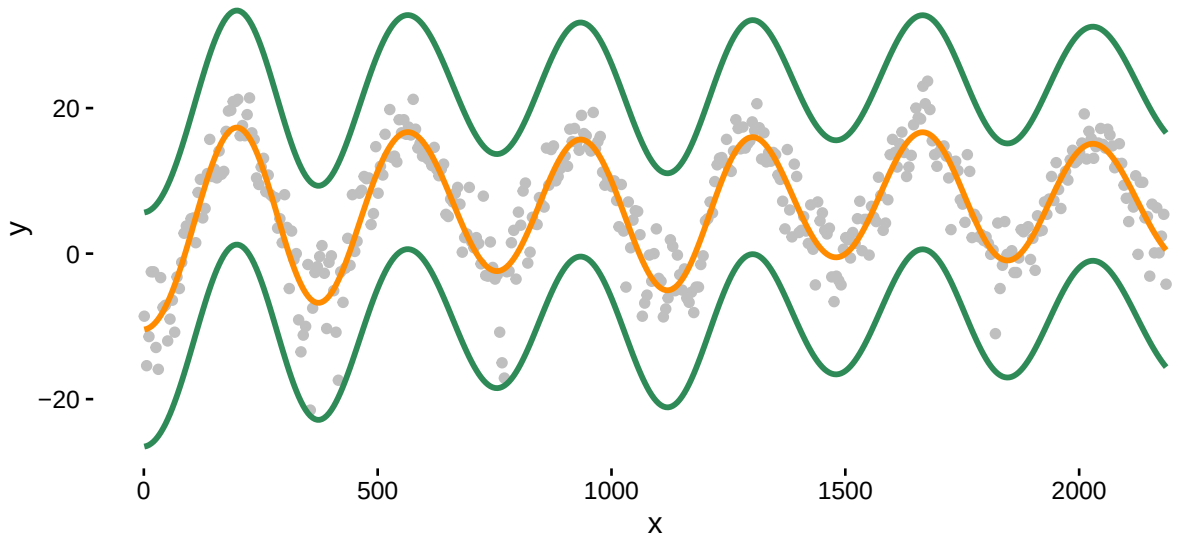
The gaussian process regression model where the temperature is a function of time is estimated. At every data point in the training set is the posterior mean computed. In the graph below are the points in the data plotted together with the posterior mean.



The orange curve are the predicted values and the grey dots the observed temperature. For the temperatures a general pattern can be seen and this pattern appears to be relatively well modelled. In general does the orange line lie quite close to the observed values.

c)

The algorithm implemented in *1.a)* that was used for computing the posterior distribution of f is now used for computing the posterior variance of the results presented in *2.b)*. The result is presented by adding 95 % posterior probability bands to the plot of the posterior means presented in the previous exercise.

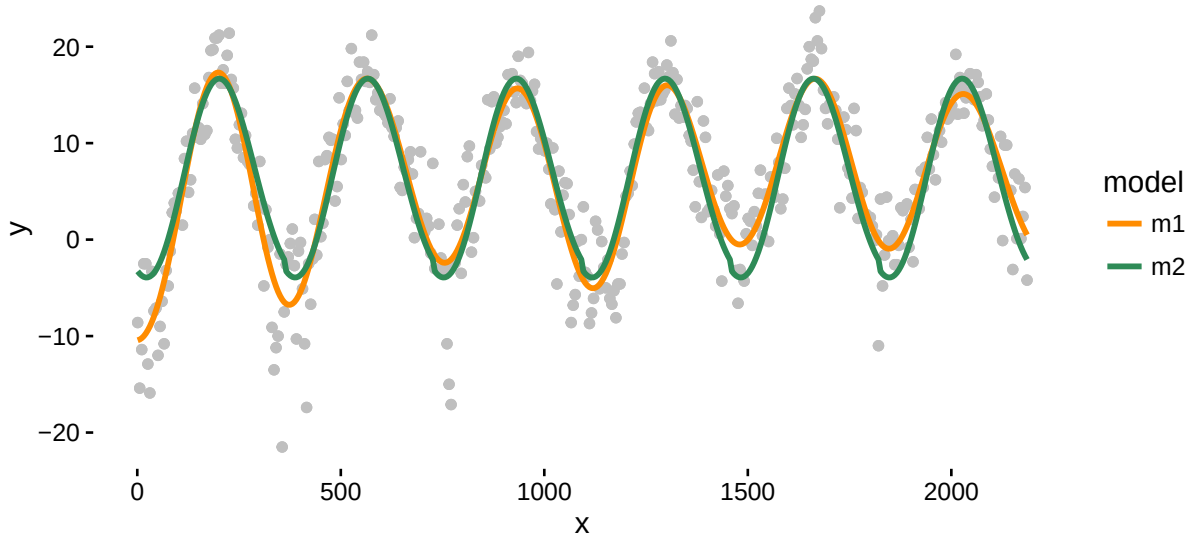


The 95 % posterior probability bands are quite wide, meaning that at a specific time point the 95 % posterior

interval also is relatively wide. It does appear to be a large uncertainty around the models estimated posterior mean values.

d)

A model with temperature as a function of day is estimated. The posterior mean of this model is compared to the posterior mean of the model which had temperature as a function of time.



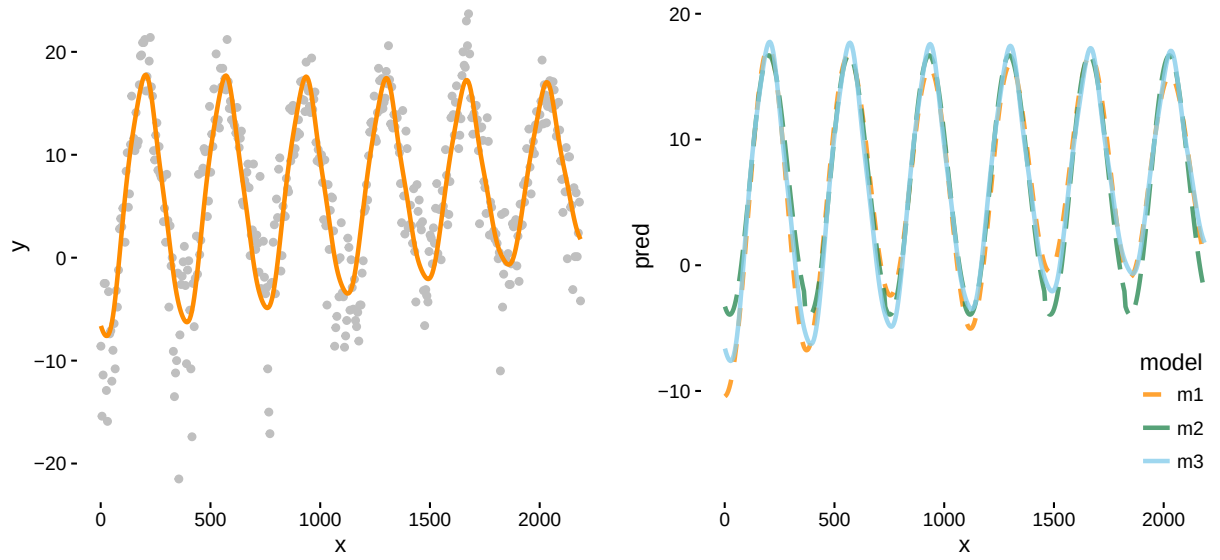
The posterior mean of the two models are very similar. Although, model 2 which has day as variable is less flexible and does not adjust its posterior mean from year to year. The second model therefore has the same posterior mean value for each day in all different years.
Pros with first model is the flexibility which let the model use nearby data points for only the current year to estimate the temperature. Negative is that it does not take so much of earlier years data into account when making the estimations. The reversed conclusion can be conducted for the second model. It is a positive aspect that it uses data for all years available but negative that it is unflexible in the sense that it gives the same posterior mean for a day in all years.

e)

A periodic kernel is implemented and the formula for the kernel is given below.

$$K(x, x') = \sigma_f^2 \times exp(\frac{2sin^2(\pi|x - x'|/d)}{\iota_1^2}) \times exp(-0.5 \times (\frac{x - x'}{\iota_2^2})^2)$$

Two new parameters are then introduced. The correlation between the same day in different years is controlled by the parameter ι_2^2 and the period is specified with the parameter d. A Gaussian process model is estimated with time as explanatory variable.

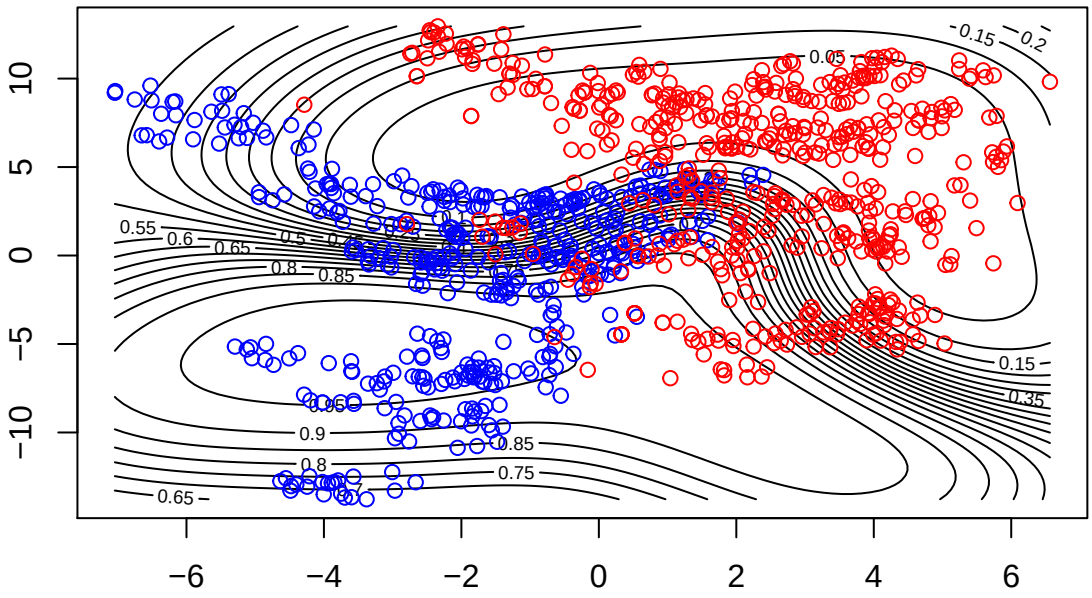


The periodic kernel produces a combination of the models estimated in *b)* and *d)*. It uses both data from the year before and data from points in time close to the one that is estimated. The posterior means obtained when using this kernel in the GP model is shown together with the observed temperature in the plot to the left. A comparsion of the posterior means for all models is illustrated with the plot to the right.
Unlike the two first models does the GP with the periodic kernel show a clear trend over the six years of observed data. The posterior mean for the temperature during the winter has increased from year to year. Regarding the temperatures during the summer is the posterior mean instead constant as it takes the same values during all years.
The general appearance of the posterior means is relatively similar for the respective models. The differences lies, as mentioned earlier, in which values the kernel gives high or low correlation for.

Assignment 3

a)

A model with the variables *varWave* and *skewWave* as input variables and fraud as target variable is estimated. The contours of the prediction probability for an observation to get classified as fraud or not is plotted below. In the contour plot is also training data added where fraud=1 are coloured blue and observations with fraud=0 coloured red.



It can be seen that the model relatively well separates the training data correct with the prediction probabilities obtained with the model. This conclusion is also confirmed by the confusion matrix for the classifier on the training data and the accuracy.

```
##
##       0   1
##   0 512  24
##   1  44 420
```

```
## Accuracy: 0.932
```

b)

The estimated model is then used for making predictions on the test set and the results are presented in a confusion matrix. The accuracy for the test data is almost the same as for the training data. In order words does the model seem to be a rather good fit.

```
##
##       0   1
##   0 191   9
##   1  15 157
```

```
## Accuracy: 0.9354839
```

c)

A new model with two more input variables, *kurtWave* and *entropyWave*, is fitted. The confusion matrix and the accuracy of this model when the observations in the test data are predicted is presented below. A higher accuracy is recieved as all but one of the observations are classified correctly with this model.

```
## Accuracy: 0.9973118
```

Appendix - R-code

```
library(ggplot2)
# Lab 3 Assignment 1
SqExpKernel <- function(x1, x2, hyperParam) {
    K <- matrix(nrow = length(x1), ncol = length(x2))
    for (i in 1:length(x2)) {
        K[, i] <- hyperParam[1]^2 * exp(-0.5 * ((x1 - x2[i])/hyperParam[2])^2)
    }
    return(K)
}
PosteriorGP <- function(x, y, xStar, hyperParam, sigmaNoise) {
    # Calculates f star bar
    K <- SqExpKernel(x, x, hyperParam)
    L <- t(chol(K + sigmaNoise * diag(dim(K)[1])))
    alpha <- solve(t(L), solve(L, y))
    # Posterior mean
    fStar <- (SqExpKernel(xStar, x, hyperParam)) %*% alpha
    # Posterior variance
    v_f <- solve(L, t(SqExpKernel(xStar, x, hyperParam)))
    cov_fStar <- SqExpKernel(xStar, xStar, hyperParam) - (t(v_f) %*% v_f)
    # Store all values in a list
    val_list <- list(fStar = fStar, xStar = xStar, cov_fStar = cov_fStar, xStar = xStar)
    return(val_list)
}
assign1B <- PosteriorGP(x = 0.4, y = 0.719, xStar = seq(-1, 1, 0.01), hyperParam = c(1,
    0.3), sigmaNoise = 0.1^2)
Upper1B <- assign1B$fStar + 1.96 * sqrt(diag(assign1B$cov_fStar))
Lower1B <- assign1B$fStar - 1.96 * sqrt(diag(assign1B$cov_fStar))
plotD <- data.frame(fStar = assign1B$fStar, xStar = assign1B$xStar, Lower = Lower1B,
    Upper = Upper1B)
xy <- data.frame(x = 0.4, y = 0.719)
ggplot(plotD, aes(y = fStar, x = xStar)) + geom_point(col = "darkorange") +
    ylim(-2, 2.2) + geom_line(data = plotD, aes(xStar, Lower), col = "seagreen",
    size = 1.1) + geom_line(data = plotD, aes(xStar, Upper), col = "seagreen",
    size = 1.1) + geom_point(data = xy, aes(x, y), size = 3) + theme_classic()
assign1C <- PosteriorGP(x = c(0.4, -0.6), y = c(0.719, -0.044), xStar = seq(-1,
    1, 0.01), hyperParam = c(1, 0.3), sigmaNoise = 0.1^2)
Upper1C <- assign1C$fStar + 1.96 * sqrt(diag(assign1C$cov_fStar))
Lower1C <- assign1C$fStar - 1.96 * sqrt(diag(assign1C$cov_fStar))

plotD <- data.frame(fStar = assign1C$fStar, xStar = assign1C$xStar, Lower = Lower1C,
    Upper = Upper1C)
```

```r
xy <- data.frame(x = c(0.4, -0.6), y = c(0.719, -0.044))
ggplot(plotD, aes(y = fStar, x = xStar)) + geom_point(col = "darkorange") +
    ylim(-2, 2.2) + geom_line(data = plotD, aes(xStar, Lower), col = "seagreen",
    size = 1.1) + geom_line(data = plotD, aes(xStar, Upper), col = "seagreen",
    size = 1.1) + geom_point(data = xy, aes(x, y), size = 3) + theme_classic()
assign1D <- PosteriorGP(x = c(0.8, 0.4, -0.2, -0.6, -1), y = c(-0.664, 0.719,
    -0.94, -0.044, 0.768), xStar = seq(-1, 1, 0.01), hyperParam = c(1, 0.3),
    sigmaNoise = 0.1^2)
Upper1D <- assign1D$fStar + 1.96 * sqrt(diag(assign1D$cov_fStar))
Lower1D <- assign1D$fStar - 1.96 * sqrt(diag(assign1D$cov_fStar))

plotD <- data.frame(fStar = assign1D$fStar, xStar = assign1D$xStar, Lower = Lower1D,
    Upper = Upper1D)
xy <- data.frame(x = c(0.8, 0.4, -0.2, -0.6, -1), y = c(-0.664, 0.719, -0.94,
    -0.044, 0.768))
ggplot(plotD, aes(y = fStar, x = xStar)) + geom_point(col = "darkorange") +
    ylim(-2, 2.2) + geom_line(data = plotD, aes(xStar, Lower), col = "seagreen",
    size = 1.1) + geom_line(data = plotD, aes(xStar, Upper), col = "seagreen",
    size = 1.1) + geom_point(data = xy, aes(x, y), size = 3) + theme_classic()
assign1E <- PosteriorGP(x = c(0.8, 0.4, -0.2, -0.6, -1), y = c(-0.664, 0.719,
    -0.94, -0.044, 0.768), xStar = seq(-1, 1, 0.01), hyperParam = c(1, 1), sigmaNoise = 0.1^2)
Upper1E <- assign1E$fStar + 1.96 * sqrt(diag(assign1E$cov_fStar))
Lower1E <- assign1E$fStar - 1.96 * sqrt(diag(assign1E$cov_fStar))

plotD <- data.frame(fStar = assign1E$fStar, xStar = assign1E$xStar, Lower = Lower1E,
    Upper = Upper1E)
xy <- data.frame(x = c(0.8, 0.4, -0.2, -0.6, -1), y = c(-0.664, 0.719, -0.94,
    -0.044, 0.768))
ggplot(plotD, aes(y = fStar, x = xStar)) + geom_point(col = "darkorange") +
    ylim(-2, 2.2) + geom_line(data = plotD, aes(xStar, Lower), col = "seagreen",
    size = 1.1) + geom_line(data = plotD, aes(xStar, Upper), col = "seagreen",
    size = 1.1) + geom_point(data = xy, aes(x, y), size = 3) + theme_classic()
# Assignment 2
library(kernlab)
temps <- read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/TempTullinge
    header = TRUE, sep = ";")
temps$time <- 1:2190
temps$day <- rep(1:365, 6)
temps$index <- rep(1:5, 438)
thinTemps <- subset(temps, temps$index == 1)[, 1:4]
sqExpK <- function(sigmaf = 1, ell = 1) {
    rval <- function(x, xStar = NULL) {
        return(sigmaf * exp(-1/2 * ((x - xStar)/ell)^2))
    }
    class(rval) <- "kernel"
    return(rval)
}
sqExpKFunc = sqExpK(sigmaf = 1, ell = 2)  # sqExpKFunc is a kernel FUNCTION
sqExpKFunc(1, 2)  # Evaluating the kernel in x=1, x'=2
# Computing the whole covariance matrix K from the kernel.
x <- as.matrix(c(1, 3, 4))
xStar <- as.matrix(c(2, 3, 4))
K <- kernelMatrix(kernel = sqExpKFunc, x = x, y = xStar)  # So this is K(X,Xstar)
```

```
K
quadLM <- lm(temp ~ time + time^2, data = temps)
sigma_n <- var(quadLM$residuals)

# Correct parametrizesed?
sqExpKFunc = sqExpK(sigmaf = 20^2, ell = 0.2)
reg <- gausspr(thinTemps$time, thinTemps$temp, kernel = sqExpKFunc, var = sigma_n)
postMean <- data.frame(pred = predict(reg), y = thinTemps$temp, x = thinTemps$time)
plotB <- ggplot(postMean, aes(x = x, y = y)) + geom_point(col = "grey75") +
    geom_line(data = postMean, aes(x = x, y = pred), col = "darkorange", size = 1.1) +
    theme_classic()
plotB
covar_f <- PosteriorGP(x = thinTemps$time, y = thinTemps$temp, xStar = thinTemps$time,
    hyperParam = c(20^2, 0.2), sigmaNoise = sigma_n)
probBands <- data.frame(Upper = postMean[, 1] + 1.96 * sqrt(diag(covar_f$cov_fStar)),
    Lower = postMean[, 1] - 1.96 * sqrt(diag(covar_f$cov_fStar)), x = thinTemps$time)
plotB + geom_line(data = probBands, aes(x = x, y = Upper), size = 1.1, col = "seagreen") +
    geom_line(data = probBands, aes(x = x, y = Lower), size = 1.1, col = "seagreen")
quadLM2 <- lm(temp ~ day + day^2, data = temps)
sigma_n2 <- var(quadLM2$residuals)
# Small difference, 67.3641 vs 64.10528
sqExpKFuncD = sqExpK(sigmaf = 20^2, ell = 1.2)
regD <- gausspr(thinTemps$day, thinTemps$temp, kernel = sqExpKFuncD, var = sigma_n2)
postMeanD <- data.frame(pred = predict(regD), y = thinTemps$temp, x = thinTemps$time)
postMT <- data.frame(rbind(postMean, postMeanD), model = c(rep("m1", 438), rep("m2",
    438)))
ggplot(postMT, aes(y = y, x = x)) + geom_point(col = "grey75") + geom_line(aes(x = x,
    y = pred, col = model), size = 1.1) + theme_classic() + scale_color_manual(values = c("darkorange",
    "seagreen"))
PeriodicK <- function(sigmaf = 1, ell_one = 1, ell_two = 1, d = 1) {
    rval <- function(x, xStar = NULL) {
        return(sigmaf * exp(-(2 * sin(pi * abs(x - xStar)/d)^2)/ell_one^2) *
            exp(-0.5 * (abs(x - xStar)^2/ell_two^2)))
    }
    class(rval) <- "kernel"
    return(rval)
}
PeriodicKFunc = PeriodicK(sigmaf = 20^2, ell_one = 1, ell_two = 10, d = 365/sd(thinTemps$time))
# PeriodicKFunc is a kernel FUNCTION
regE <- gausspr(thinTemps$time, thinTemps$temp, kernel = PeriodicKFunc, var = sigma_n)
postMeanE <- data.frame(pred = predict(regE), y = thinTemps$temp, x = thinTemps$time)
plotE <- ggplot(postMeanE, aes(x = x, y = y)) + geom_point(col = "grey75") +
    geom_line(data = postMeanE, aes(x = x, y = pred), col = "darkorange", size = 1.1) +
    theme_classic()
postMT <- rbind(postMT, data.frame(postMeanE, model = "m3"))
plotAll <- ggplot(postMT, aes(x = x, y = pred)) + geom_line(aes(col = model,
    linetype = model), size = 1.1, alpha = 0.8) + theme_classic() + scale_color_manual(values = c("dark
    "seagreen", "skyblue")) + scale_linetype_manual(values = c("dashed", "longdash",
    "solid")) + theme(legend.justification = c(1, 0), legend.position = c(1,
    0)) + scale_y_continuous(limits = c(-17, 20))
library(gridExtra)
grid.arrange(plotE, plotAll, ncol = 2)
# Assignment 3
```

```r
library(AtmRay)
data <- read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/banknoteFraud
    header = FALSE, sep = ",")
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, ]
# a)
cfA <- gausspr(fraud ~ varWave + skewWave, data = Train)
gridX <- seq(min(Train$varWave), max(Train$varWave), length = 100)
gridY <- seq(min(Train$skewWave), max(Train$skewWave), length = 100)
gridP <- meshgrid(gridX, gridY)
gridP <- cbind(c(gridP$x), c(gridP$y))
gridP <- data.frame(gridP)
names(gridP) <- names(Train)[1:2]
probPredsA <- predict(cfA, gridP, type = "probabilities")
contour(x = gridX, y = gridY, z = matrix(probPredsA[, 2], 100), 20)
points(Train[Train[, 5] == 1, 1], Train[Train[, 5] == 1, 2], col = "blue")
points(Train[Train[, 5] == 0, 1], Train[Train[, 5] == 0, 2], col = "red")
# predict on the training set
confMatA <- table(predict(cfA, Train[, 1:2]), Train[, 5])  # confusion matrix
confMatA
cat("Accuracy:", sum(diag(confMatA))/sum(confMatA))
confMatB <- table(predict(cfA, Test[, 1:2]), Test[, 5])  # confusion matrix
confMatB
cat("Accuracy:", sum(diag(confMatB))/sum(confMatB))
cfC <- gausspr(fraud ~ varWave + skewWave + kurtWave + entropyWave, data = Train)
confMatC <- table(predict(cfC, Test[, 1:4]), Test[, 5])  # confusion matrix
cat("Accuracy:", sum(diag(confMatC))/sum(confMatC))
## NA
```