Advanced Machine Learning

Lab 3

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```
library(kernlab)
library(AtmRay)
library(knitr)
```

1)

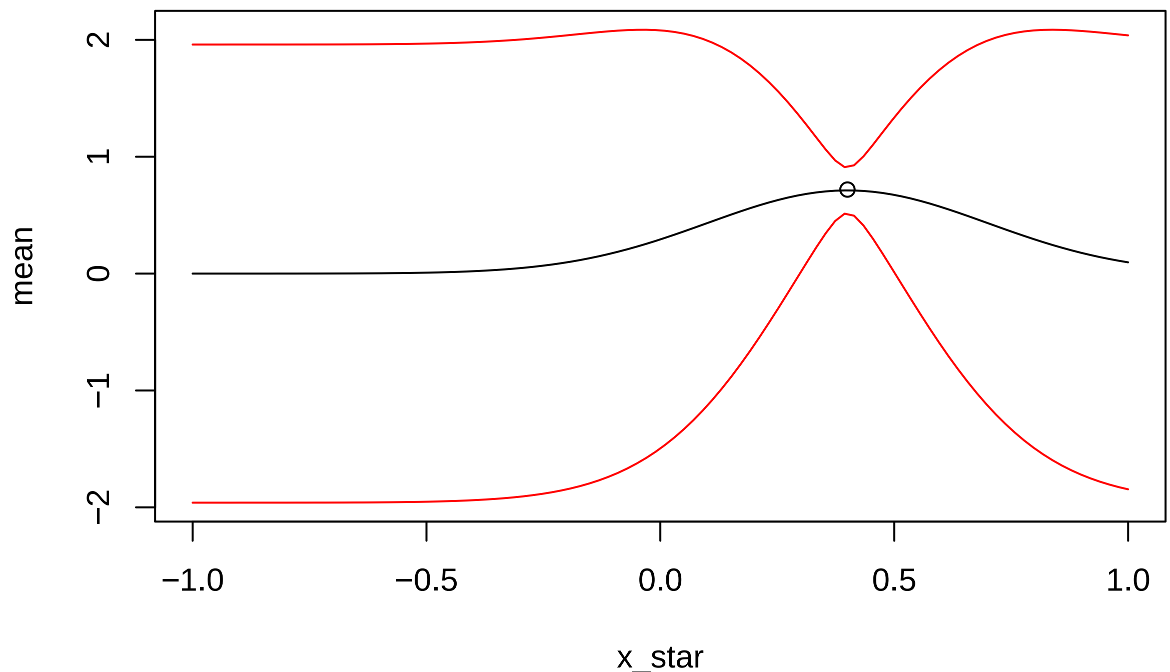
a)

```
squared_exp_kernel <- function(sigma, l){
    function(x1, x2) {
        n1 <- length(x1)
        n2 <- length(x2)
        K <- matrix(NA, n1, n2)

        for (i in 1:n2){
            K[, i] <- sigma^2 * exp(-0.5 * ((x1 - x2[i]) / l)^2)
        }

        K
    }
}

posterior_gp <- function(x_new, x, y, noise, kernel) {
    Kxx <- kernel(x, x)
    Kxs <- kernel(x, x_new)
    Kss <- kernel(x_new, x_new)

    L <- t(chol(Kxx + diag(noise^2, nrow(Kxx), ncol(Kxx))))
    alpha <- solve(t(L), solve(L, y))
    mean <- t(Kxs) %*% alpha
    v <- solve(L, Kxs)
    covariance <- Kss - t(v) %*% v
    list(mean=mean, variance=covariance)
}

plot_gp <- function(posterior, x_star) {
    mean <- posterior$mean
    lower_band <- mean - 1.96 * sqrt(diag(posterior$variance))
    upper_band <- mean + 1.96 * sqrt(diag(posterior$variance))

    plot(x_star, mean, type="l", ylim=c(min(lower_band), max(upper_band)))
    lines(x_star, lower_band, col="red")
```

```
    lines(x_star, upper_band, col="red")
}
```

b)

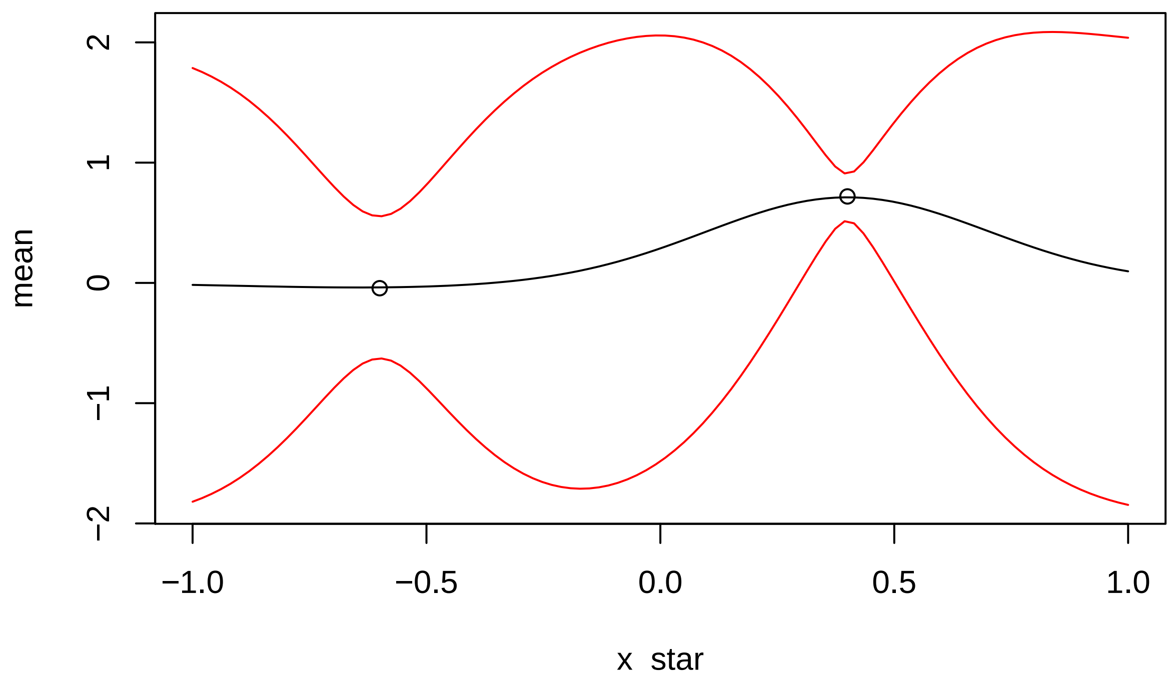
```
kernel <- squared_exp_kernel(1, 0.3)
x_star <- seq(-1, 1, length=100)
x <- c(0.4)
y <- c(0.719)
noise <- 0.1

pgp <- posterior_gp(x_star, x, y, noise, kernel)

plot_gp(pgp, x_star)
points(x, y)
```



c)

```
kernel <- squared_exp_kernel(1, 0.3)
x_star <- seq(-1, 1, length=100)
x <- c(0.4)
y <- c(0.719)
noise <- 0.1

x_new <- c(-0.6)
y_new <- c(-0.044)

prior_mean <- pgp$mean
prior_covariance <- pgp$variance
```

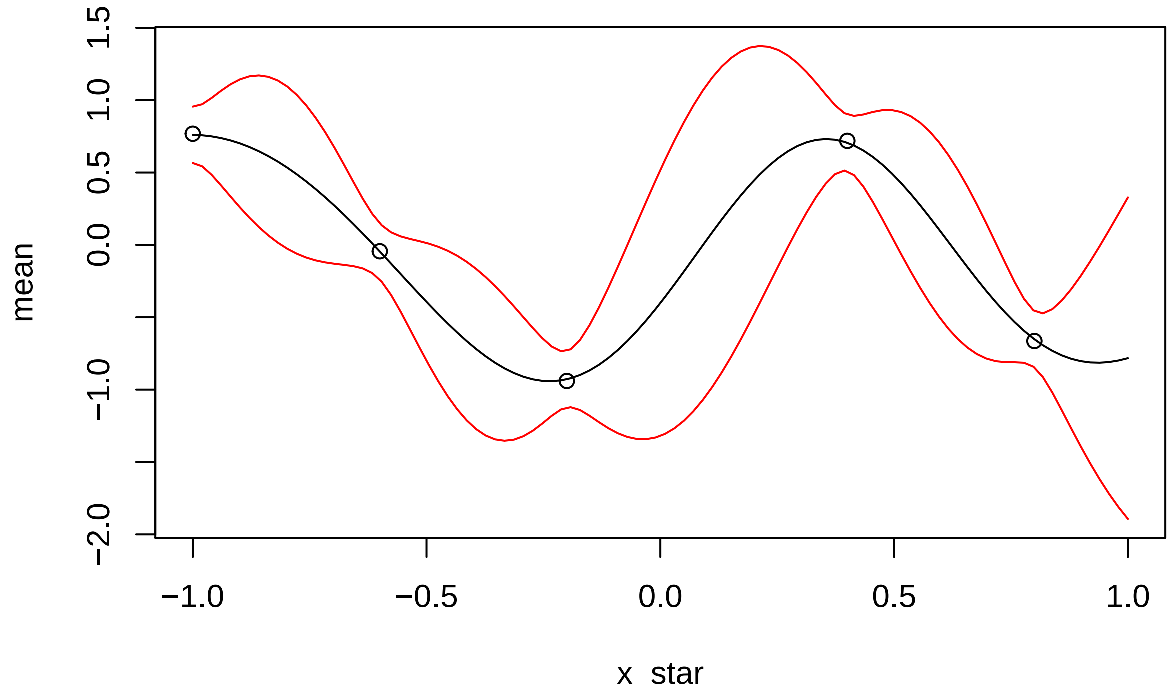
```r
## Should it be noise here?
posterior_mean <- prior_mean +
    kernel(x_star, x_new) %*%
    solve(kernel(x_new, x_new) + diag(noise, length(x_new), length(x_new))) %*%
    t(y_new)

posterior_covariance <- prior_covariance -
    kernel(x_star, x_new) %*%
    solve(kernel(x_new, x_new) + diag(noise, length(x_new), length(x_new))) %*%
    kernel(x_new, x_star)

mean <- posterior_mean
lower_band <- mean - 1.96 * sqrt(diag(posterior_covariance))
upper_band <- mean + 1.96 * sqrt(diag(posterior_covariance))

plot(x_star, mean, type="l", ylim=c(min(lower_band), max(upper_band)))
points(c(x, x_new), c(y, y_new))
lines(x_star, lower_band, col="red")
lines(x_star, upper_band, col="red")
```



d)

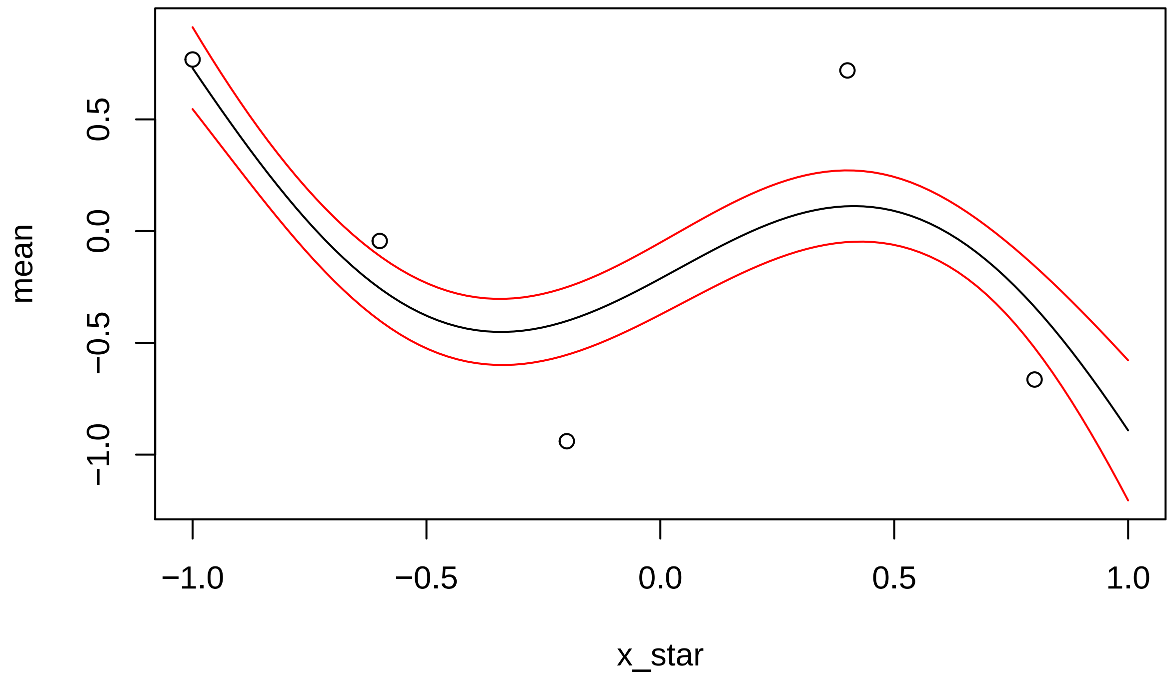
```r
kernel <- squared_exp_kernel(1, 0.3)
x_star <- seq(-1, 1, length=100)
x <- c(-1.0, -0.6, -0.2, 0.4, 0.8)
y <- c(0.768, -0.044, -0.940, 0.719, -0.664)
noise <- 0.1

pgp <- posterior_gp(x_star, x, y, noise, kernel)
```

```r
plot_gp(pgp, x_star)
points(x, y)
```



e)

```r
kernel <- squared_exp_kernel(1, 1)
x_star <- seq(-1, 1, length=100)
x <- c(-1.0, -0.6, -0.2, 0.4, 0.8)
y <- c(0.768, -0.044, -0.940, 0.719, -0.664)
noise <- 0.1

pgp <- posterior_gp(x_star, x, y, noise, kernel)

plot_gp(pgp, x_star)
points(x, y)
```



We can clearly see that the length scale impact the smoothness of the curve, that is, the higher the length the smoother the curve. Simply a way of controlling under/overfitting.

2)

```r
data <- read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/Code/TempTullinge.c
                 header=TRUE, sep=";")
data$time<- 1:nrow(data)
data$day <- 0:(nrow(data) - 1) %% 365 + 1

thinned_data <- data[(data$time - 1) %% 5 == 0, ]
```

```r
single_squared_exp_kernel <- function(sigma, l) {
    f <- function(x1, x2) {
        sigma^2 * exp(-0.5 * ((x1 - x2) / l)^2)
    }
    class(f) <- "kernel"
    f
}

single_periodic_kernel <- function(sigma, l1, l2, d) {
    f <- function(x1, x2) {
        sigma^2 *
            exp(-2 * (sin(pi * abs(x1 - x2) / d))^2 / l1^2) *
            exp(- (1 / 2) * ((x1 - x2) / l2)^2)
    }
    class(f) <- "kernel"
    f
}
```

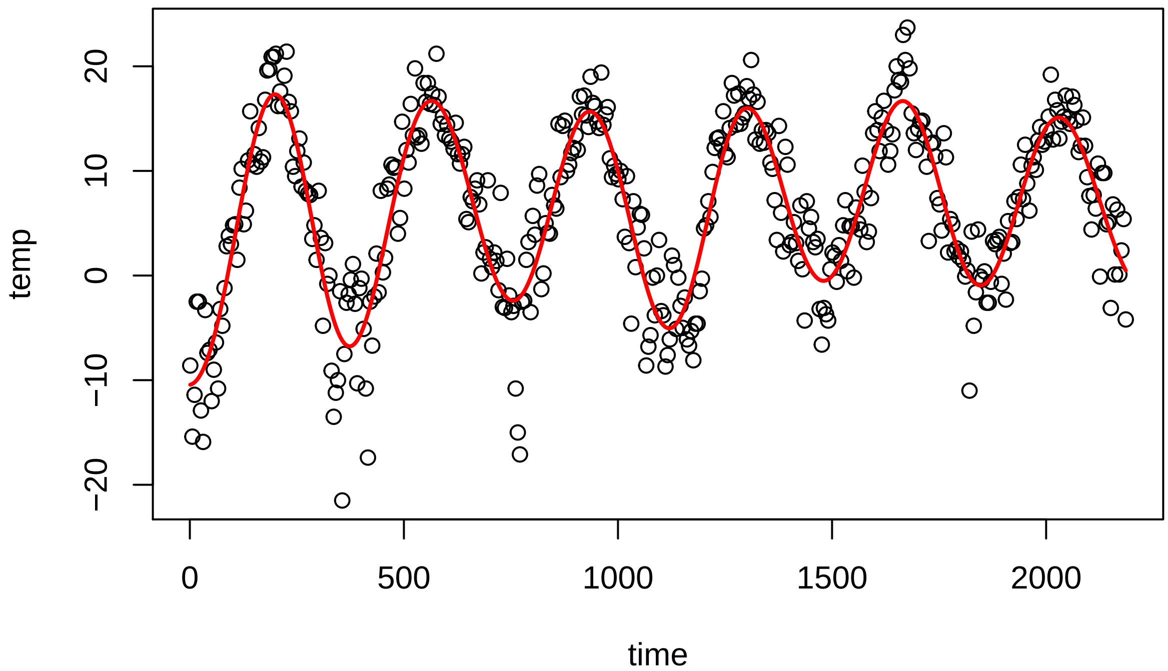
a)

```r
x <- c(1, 3, 4)
x_star <- c(2, 3, 4)

kernel <- single_squared_exp_kernel(1, 1)
kernelMatrix(kernel, x, x_star)
#> 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
```

b)

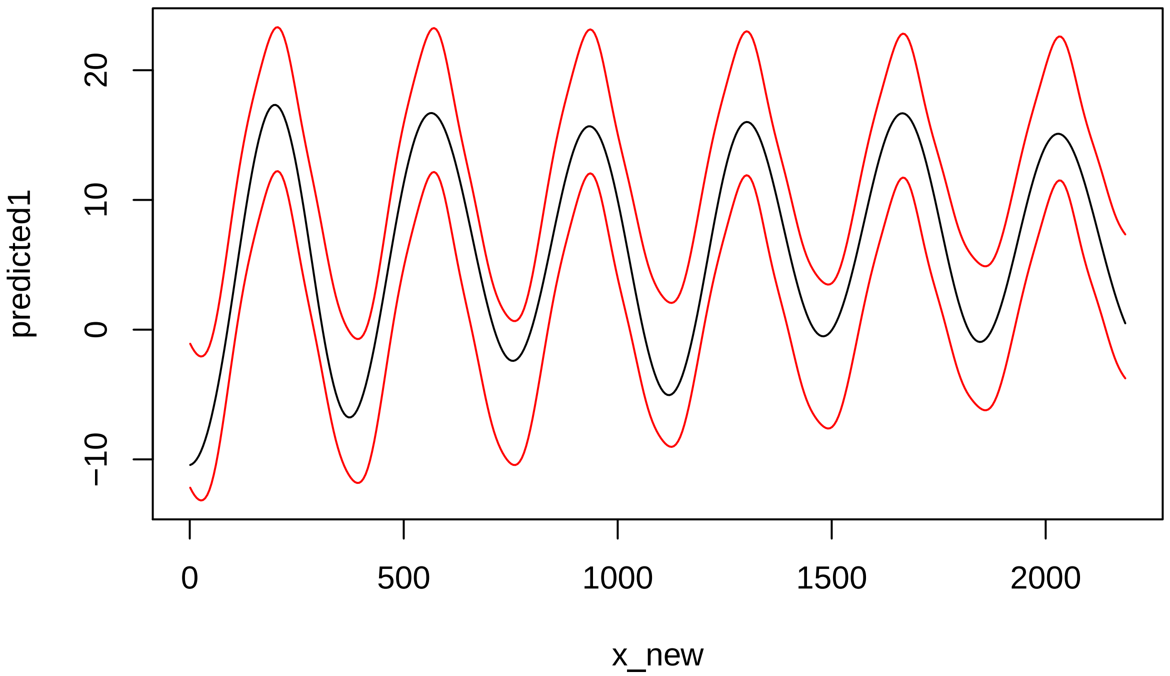
```r
kernel <- single_squared_exp_kernel(20, 0.2)

lm_fit <- lm(temp ~ poly(time, 2), thinned_data)
sigma <- sd(resid(lm_fit))

gp_fit1 <- gausspr(temp ~ time, thinned_data, kernel=kernel, var=sigma^2)
predicted1 <- predict(gp_fit1, thinned_data)
```

```r
plot(thinned_data$time, thinned_data$temp, type="p", xlab="time", ylab="temp")
lines(thinned_data$time, predicted1, col="red", lwd=2)
```



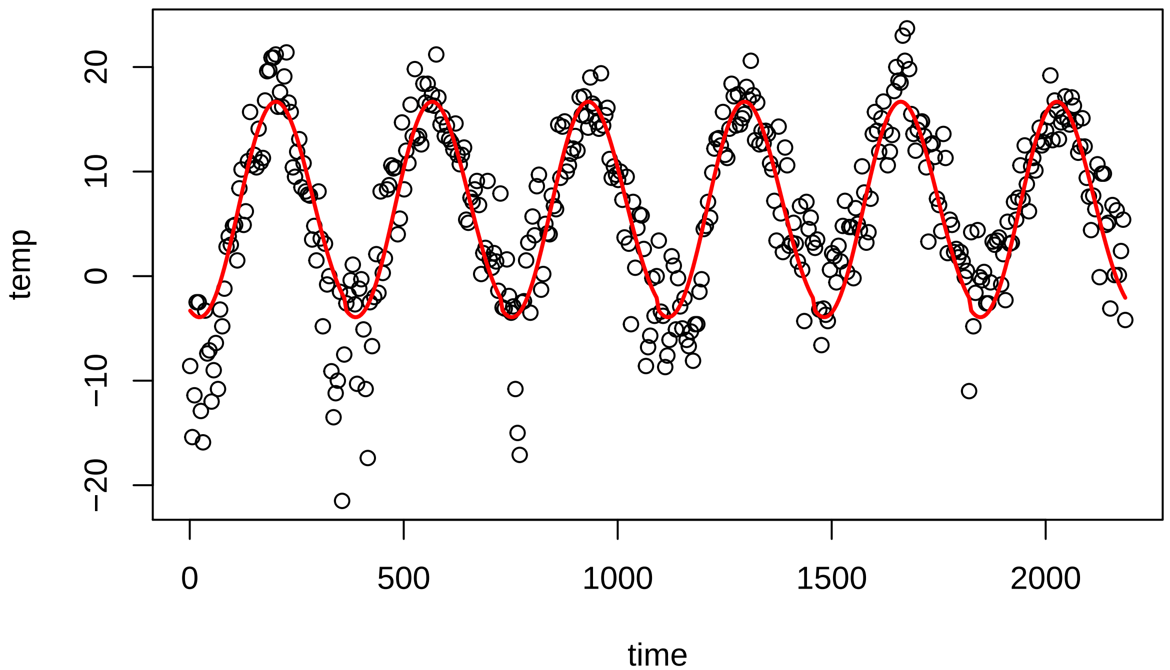
c)

```r
prediction <- function(x_new, x, y, kernel, noise) {
    K <- kernel(x_new, x)
    S <- solve(kernel(x, x) + diag(noise, length(x), length(x)))
    pred <- K %*% S %*% y
    sigma <- kernel(x_new, x_new) - K %*% S %*% t(K)
    list(pred=pred, variance=sigma)
}

kernel <- squared_exp_kernel(20, 0.2)
x_new <- thinned_data$time
x <- thinned_data$time
y <- thinned_data$temp

preds <- prediction(x_new, x, y, kernel, sigma)

mean <- predicted
lower_band <- mean - 1.96 * sqrt(diag(preds$variance))
upper_band <- mean + 1.96 * sqrt(diag(preds$variance))

plot(x_new, predicted1, ylim=c(min(lower_band), max(upper_band)), type="l")
lines(x_new, lower_band, col="red")
lines(x_new, upper_band, col="red")
```



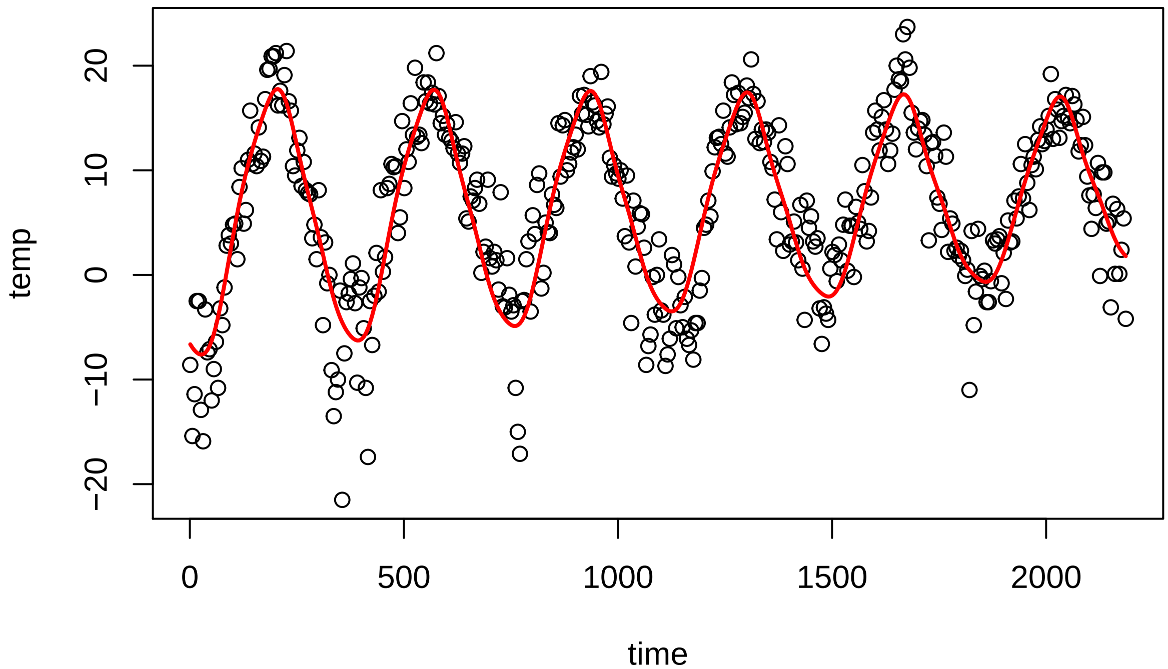
d)

```
kernel <- single_squared_exp_kernel(20, 1.2)

gp_fit2 <- gausspr(temp ~ day, thinned_data, kernel=kernel, var=sigma^2)
predicted2 <- predict(gp_fit2, thinned_data)

plot(thinned_data$time, thinned_data$temp, type="p", xlab="time", ylab="temp")
lines(thinned_data$time, predicted2, col="red", lwd=2)
```

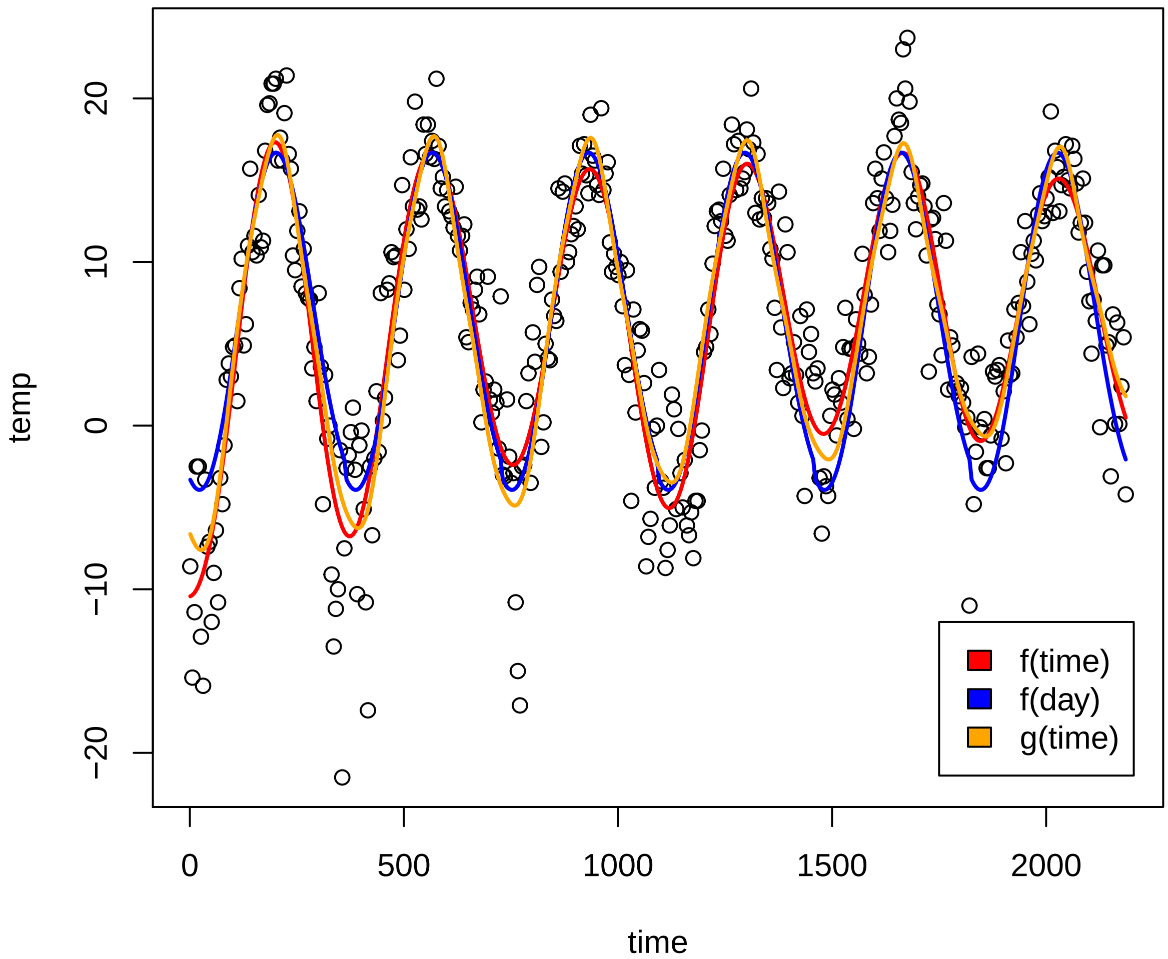


e)

```
kernel <- single_periodic_kernel(20, 1, 10, 365 / sd(thinned_data$time))

gp_fit3 <- gausspr(temp ~ time, thinned_data, kernel=kernel, var=sigma^2)
predicted3 <- predict(gp_fit3, thinned_data)

plot(thinned_data$time, thinned_data$temp, type="p", xlab="time", ylab="temp")
lines(thinned_data$time, predicted3, col="red", lwd=2)
```




```
plot(thinned_data$time, thinned_data$temp, type="p", xlab="time", ylab="temp")
lines(thinned_data$time, predicted1, col="red", lwd=2)
lines(thinned_data$time, predicted2, col="blue", lwd=2)
lines(thinned_data$time, predicted3, col="orange", lwd=2)
legend(1750, -12, legend=c("f(time)", "f(day)", "g(time)"), fill=c("red", "blue", "orange"))
```



We can see that all the curves are fairly similar and follow the data pretty well. From the data we can clearly see a seasonal pattern which is not really explicitly encoded in the time variable but is in the day variable. We can see that the model using the day variable, the blue line, is more stable and does not try to fit the noise. The model using the periodic kernel, the orange line, do look to follow the seasonal pattern very well but also is affected by the variations that are seen from season to season more so than the blue line. Finally the model that uses the time variable with the squared exponential kernel, the red line, does not really know about the seasonal pattern and just fits the data which it does rather well.

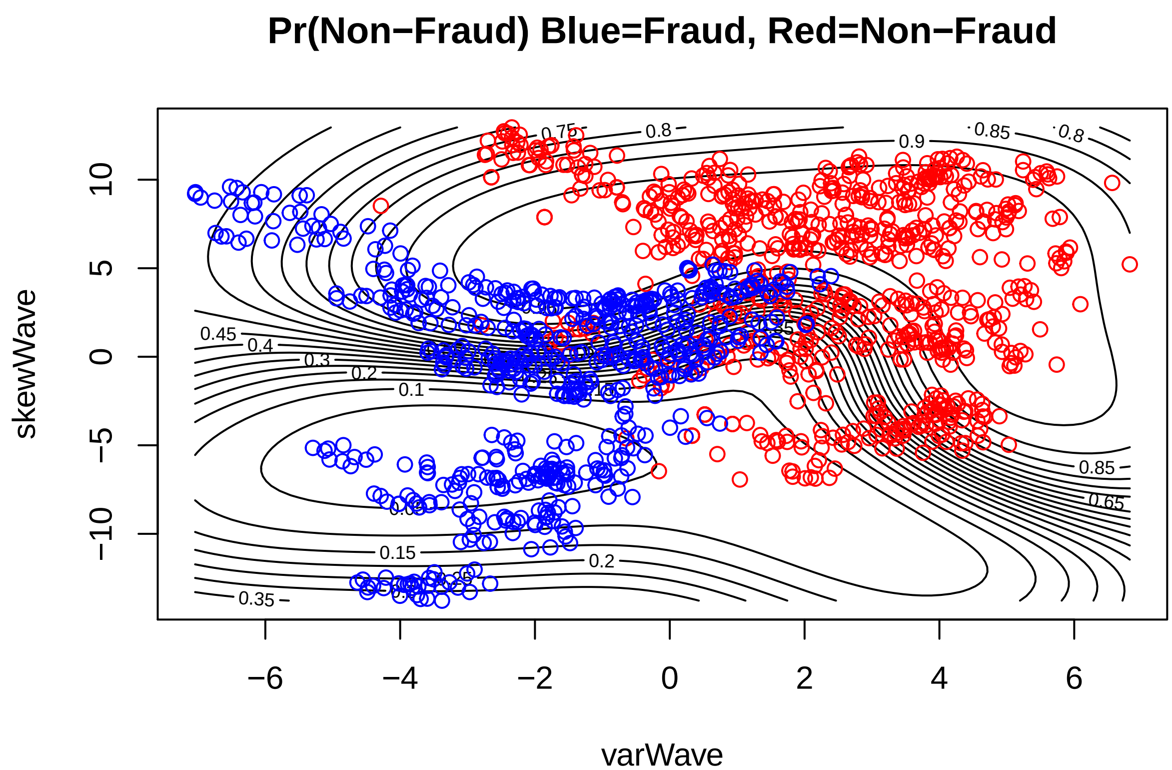
3)

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

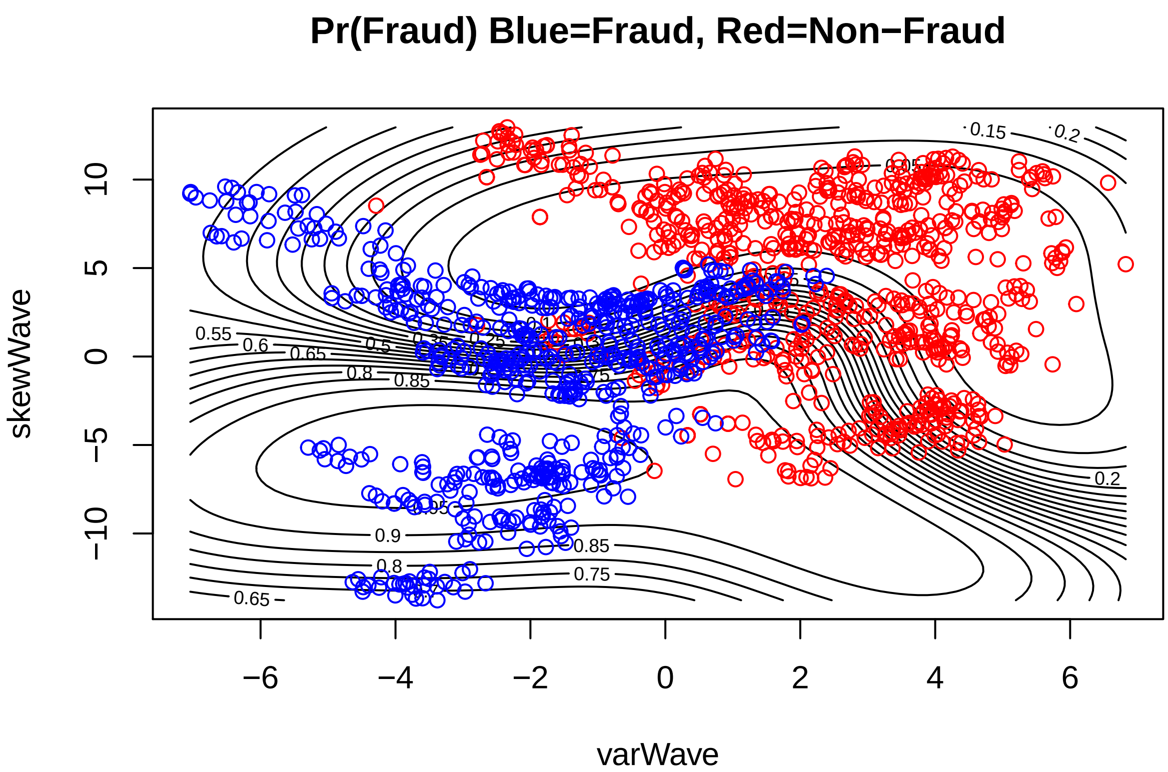
a)

```
gp_fit <- gausspr(fraud ~ varWave + skewWave, data=train)
#> Using automatic sigma estimation (sigest) for RBF or laplace kernel
train_predictions <- predict(gp_fit, train)
train_tbl <- table(train_predictions, train$fraud)
train_acc1 <- sum(diag(train_tbl)) / sum(train_tbl)
train_tbl
#>
#> train_predictions   0   1
#>                 0 512  24
#>                 1  44 420
train_acc1
#> [1] 0.932
```

```
x1 <- seq(min(data$varWave), max(data$varWave), length=100)
x2 <- seq(min(data$skewWave), max(data$skewWave), length=100)
grid_points <- meshgrid(x1, x2)
grid_points <- cbind(c(grid_points$x), c(grid_points$y))
grid_points <- data.frame(grid_points)
names(grid_points) <- c("varWave", "skewWave")
predicted_probs <- predict(gp_fit, grid_points, type="probabilities")

## Plotting for Prob(Non-Fraud)
contour(x1, x2, matrix(predicted_probs[, 1], 100), 20,
        xlab = "varWave", ylab="skewWave",
        main = 'Pr(Non-Fraud) Blue=Fraud, Red=Non-Fraud')
points(data$varWave[data$fraud == 0], data$skewWave[data$fraud == 0], col="red")
points(data$varWave[data$fraud == 1], data$skewWave[data$fraud == 1], col="blue")
```




```
## Plotting for Prob(Fraud)
contour(x1, x2, matrix(predicted_probs[, 2], 100), 20,
        xlab = "varWave", ylab="skewWave",
        main = 'Pr(Fraud) Blue=Fraud, Red=Non-Fraud')
points(data$varWave[data$fraud == 0], data$skewWave[data$fraud == 0], col="red")
points(data$varWave[data$fraud == 1], data$skewWave[data$fraud == 1], col="blue")
```



b)

```
test_predictions <- predict(gp_fit, test)
test_tbl <- table(test_predictions, test$fraud)
test_acc1 <- sum(diag(test_tbl)) / sum(test_tbl)
test_tbl
#>
#> test_predictions   0   1
#>                0 191   9
#>                1  15 157
test_acc1
#> [1] 0.9354839
```

c)

```
gp_fit <- gausspr(fraud ~ varWave + skewWave + kurtWave + entropyWave, data=train)
#> Using automatic sigma estimation (sigest) for RBF or laplace kernel
train_predictions <- predict(gp_fit, train)
train_tbl <- table(train_predictions, train$fraud)
train_acc2 <- sum(diag(train_tbl)) / sum(train_tbl)
train_tbl
#>
#> train_predictions   0   1
#>                 0 552   0
#>                 1   4 444
```

```
train_acc2
#> [1] 0.996
```

```
test_predictions <- predict(gp_fit, test)
test_tbl <- table(test_predictions, test$fraud)
test_acc2 <- sum(diag(test_tbl)) / sum(test_tbl)
test_tbl
#>
#> test_predictions   0   1
#>                0 205   0
#>                1   1 166
test_acc2
#> [1] 0.9973118
```

```
kdata <- data.frame(train_acc=c(train_acc1, train_acc2), test_acc=c(test_acc1, test_acc2))
rownames(kdata) <- c("two covariates", "four covariates")
kable(kdata)
```

	train_acc	test_acc
two covariates	0.932	0.9354839
four covariates	0.996	0.9973118

We can see that using more covariates do improve both train and test accuracy. Since the test accuracy is increased as well the model may not have overfitted the data.