732A96: Advanced Machine Learning

Computer Lab 4: Gaussian Processes

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October 11, 2019

Contents

Question 1: Implementing GP Regression

This first exercise will have you writing your own code for the Gaussian process regression model:

$$y = f(x) + \epsilon \quad \text{with} \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2) \quad \text{and} \quad f \sim \mathcal{GP}(0, k(x, x'))$$

You must implement Algorithm 2.1 on page 19 of Rasmussen and Willams' book. The algorithm uses the Cholesky decomposition (`chol` in `R`) to attain numerical stability. Note that L in the algorithm is a lower triangular matrix, whereas the R function returns an upper triangular matrix. So, you need to transpose the output of the R function. In the algorithm, the notation $\mathbf{A}\backslash\mathbf{b}$ means the vector x that solves the equation $\mathbf{Ax} = \mathbf{b}$ (see p. xvii in the book). This is implemented in R with the help of the function `solve`.

1.1 Function to compute GP Posterior

Question: Write your own code for simulating from the posterior distribution of f using the squared exponential kernel. The function (name it `posteriorGP`) should return a vector with the posterior mean and variance of f, both evaluated at a set of x-values ($X_\star$). You can assume that the prior mean of f is zero for all x. The function should have the following inputs:

- `X`: Vector of training inputs.
- `y`: Vector of training targets/outputs.
- `XStar`: Vector of inputs where the posterior distribution is evaluated, i.e. $X_\star$.
- `hyperParam`: Vector with two elements, σ_f and ℓ.
- `sigmaNoise`: Noise standard deviation, σ_n.

Hint: Write a separate function for the kernel (see the file `GaussianProcess.R` on the course web page).

Answer:

The following `squared_exp_kernel()` function computes the kernel matrix between `x1` and `x2` using the given `sigma_f` and `l` hyperparameters.

```r
# Kernel function - Squared exponential kernel
squared_exp_kernel = function(x1, x2, sigma_f = 1, l = 3){
  n1 = length(x1)
  n2 = length(x2)
  K = matrix(NA,n1,n2)

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

  return(K)
}
```

The `posteriorGP()` function computes the posterior mean, variance (matrix) and marginal log-likelihood for the given known data points `(X, y)`, new data points `XStar` and the given hyperparameters. Th function is created as per the given specifications.

1.2 GP Posterior with one observation

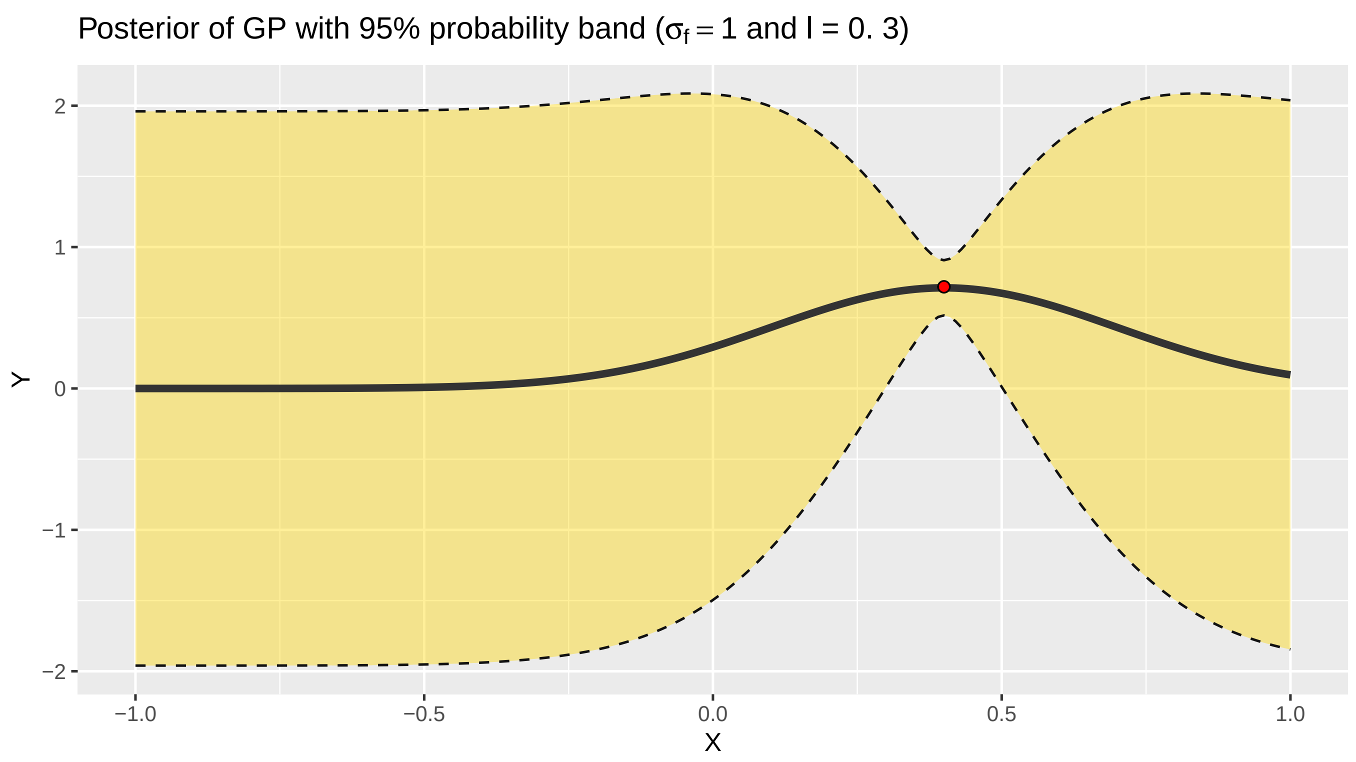
Question: Now, let the prior hyperparameters be $\sigma_f = 1$ and $\ell = 0.3$. Update this prior with a single observation: $(x, y) = (0.4,\ 0.719)$. Assume that $\sigma_n = 0.1$. Plot the posterior mean of f over the interval $x \in [-1, 1]$. Plot also 95 % probability (pointwise) bands for f.

Answer:

We use the given hyperparameters $\sigma_f = 1$ and $\ell = 0.3$ and update the prior with a single observation $(x, y) = (0.4,\ 0.719)$. We also use the given $\sigma_n = 0.1$. In this way, we compute the posterior GP function.

```
x = c(0.4)
y = c(0.719)
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 0.3

post_gp_2 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)
```

The following plot shows the posterior mean of f and the 95% probability bands of f after updating with the given single data point.



1.3 GP Posterior with two observations

Question: Update your posterior from (2) with another observation: $(x, y) = (-0.6, \ -0.044)$. Plot the posterior mean of f over the interval $x \in [-1, 1]$. Plot also 95 % probability (pointwise) bands for f.

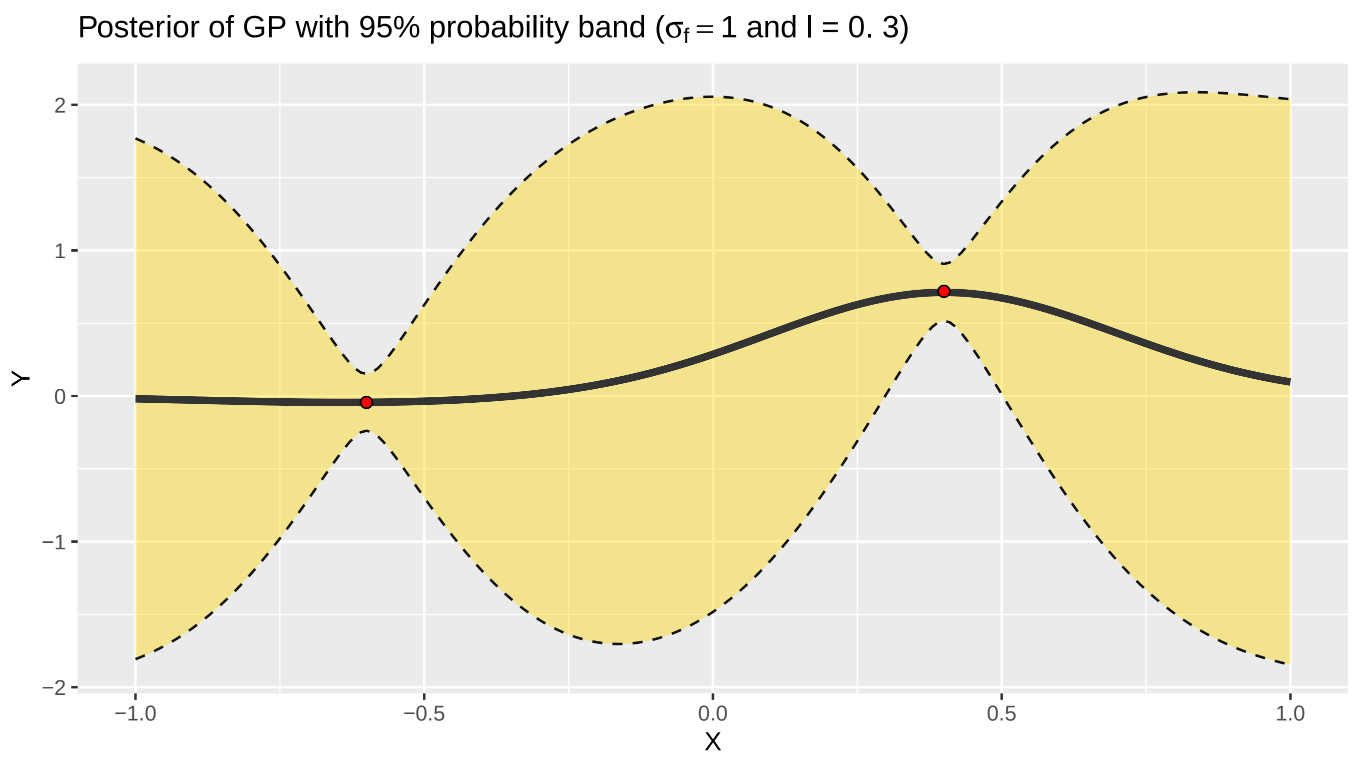
Hint: Updating the posterior after one observation with a new observation gives the same result as updating the prior directly with the two observations.

Answer:

In this task, we recompute the posterior function f by updating the prior with the 2 given data points.

```r
x = c(0.4, -0.6)
y = c(0.719, -0.044)
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 0.3

post_gp_3 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)
```

The following plot shows the posterior mean of f and the 95% probability bands of f after updating with the given 2 data points.



1.4 GP Posterior with five observations

Question: Compute the posterior distribution of f using all the five data points in the table below (note that the two previous observations are included in the table). Plot the posterior mean of f over the interval $x \in [-1, 1]$. Plot also 95 % probability (pointwise) bands for f.

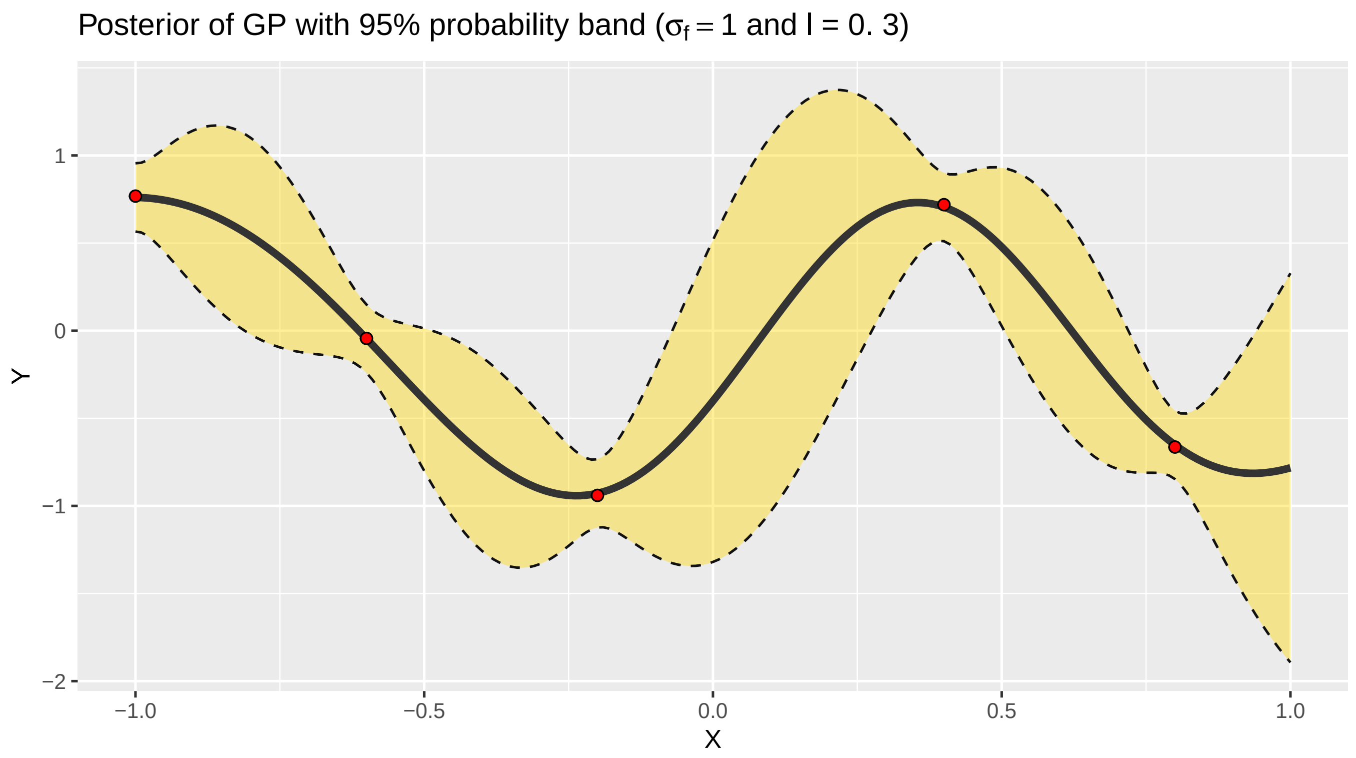
x	y
-1.0	0.768
-0.6	-0.044
-0.2	-0.940
0.2	0.719
0.6	-0.664

Answer:

In this task, we recompute the posterior function f by updating the prior with the 5 given data points.

```r
x = c(-1, -0.6, -0.2, 0.4, 0.8)
y = c(0.768, -0.044, -0.940, 0.719, -0.664)
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 0.3

post_gp_4 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)
```

The following plot shows the posterior mean of f and the 95% probability bands of f after updating with the given 5 data points.



1.5 GP Posterior with five observations, different hyperparameters

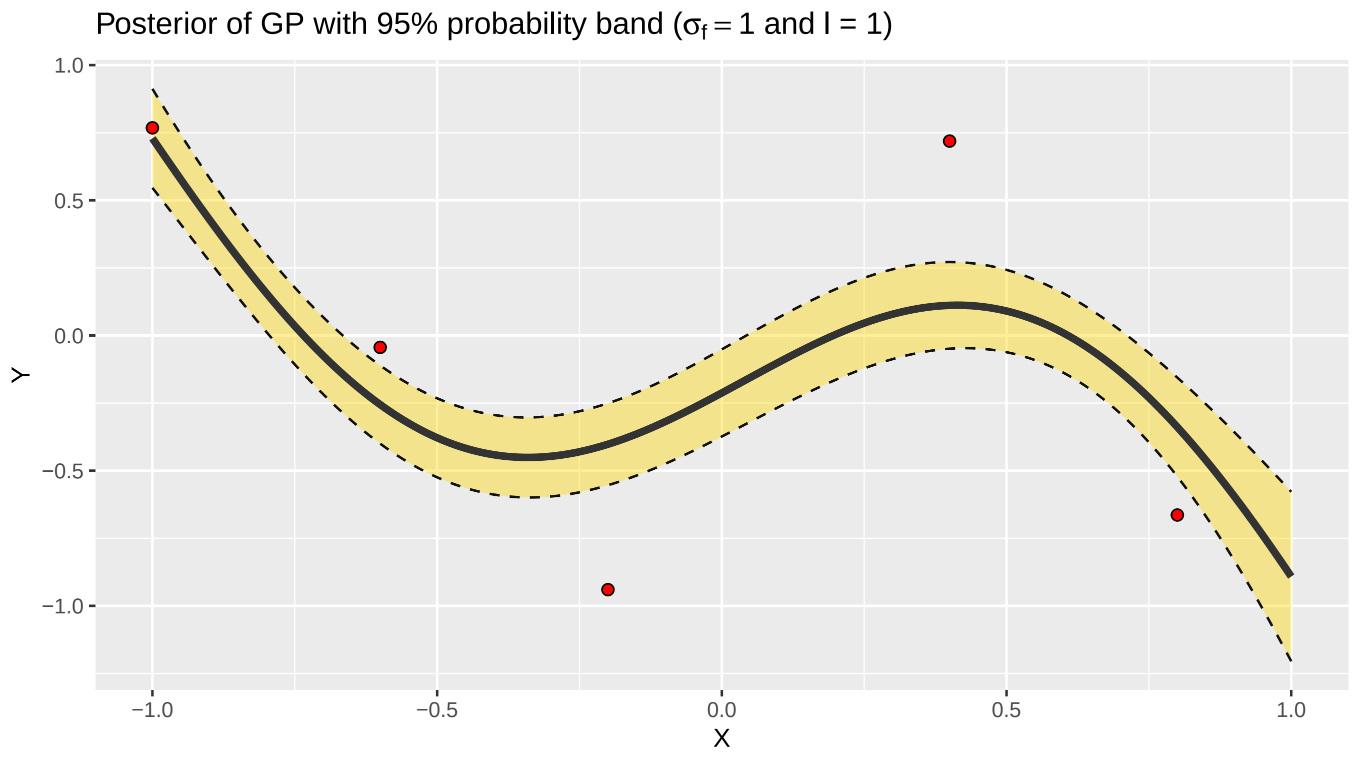
Question: Repeat (4), this time with hyperparameters $\sigma_f = 1$ and $\ell = 1$. Compare the results.

Answer:

In this task, we repeat the previous task but with hyperparameters $\sigma_f = 1$ and $\ell = 1$.

```r
x = c(-1, -0.6, -0.2, 0.4, 0.8)
y = c(0.768, -0.044, -0.940, 0.719, -0.664)
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 1

post_gp_5 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)
```

The following plot shows the posterior mean of f and the 95% probability bands of f after updating with the given 5 data points and using the new hyperparameters.



By comparing the plots obtained, we see that the posterior function gets too smooth when we use $\ell = 1$ compared to when we use $\ell = 0.3$. This is an expected behavior of the ℓ parameter of the squared exponential kernel that we have used. When $\ell = 0.3$, the posterior function mean perfectly passes through the data points that we used. Whereas when we used $\ell = 1$, we see that 4 out of the 5 data points do not even lie within the 95% probability band. So, using $\ell = 1$ leads to worse results compared to using $\ell = 0.3$ in this particular case.

Question 2: GP Regression with `kernlab`

In this exercise, you will work with the daily mean temperature in Stockholm (Tullinge) during the period January 1, 2010 - December 31, 2015. We have removed the leap year day February 29, 2012 to make things simpler. You can read the dataset with the command:

```
read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/GaussianProcess/
Code/TempTullinge.csv", header=TRUE, sep=";")
```

Create the variable `time` which records the day number since the start of the dataset (i.e., `time` = 1, 2, . . . , 365 x 6 = 2190). Also, create the variable `day` that records the day number since the start of each year (i.e., `day`= 1, 2, . . . , 365, 1, 2, . . . , 365). Estimating a GP on 2190 observations can take some time on slower computers, so let us subsample the data and use only every fifth observation. This means that your time and day variables are now time= 1, 6, 11, . . . , 2186 and day= 1, 6, 11, . . . , 361, 1, 6, 11, . . . , 361.

```r
temp_tullinge = read.csv2("TempTullinge.csv", stringsAsFactors = F)

temp_tullinge$temp = as.numeric(temp_tullinge$temp)
temp_tullinge$time = 1:nrow(temp_tullinge)
temp_tullinge$day = rep(1:365, 6)
temp_tullinge$date = NULL

temp_tullinge = temp_tullinge[temp_tullinge$time %% 5 == 1 , ]

kable(tail(temp_tullinge), booktabs = T) %>%
  kable_styling(latex_option = "striped")
```

	temp	time	day
2161	0.1	2161	336
2166	6.3	2166	341
2171	0.1	2171	346
2176	2.4	2176	351
2181	5.4	2181	356
2186	-4.2	2186	361

2.1 Function usage: `gausspr` and `kernelMatrix`

Question: Familiarize yourself with the functions `gausspr` and `kernelMatrix` in `kernlab`. Do `?gausspr` and read the input arguments and the output. Also, go through the file `KernLabDemo.R` available on the course website. You will need to understand it. Now, define your own square exponential kernel function (with parameters ℓ (`ell`) and σ_f (`sigmaf`)), evaluate it in the point $x = 1, x' = 2$, and use the `kernelMatrix` function to compute the covariance matrix $K(X, X_\star)$ for the input vectors $X = (1, 3, 4)^T$ and $X_\star = (2, 3, 4)^T$.

Answer:

We create a kernel function factory to create squared exponential kernel functions with given hyper-parameters `sigma_f` and `ell`.

```r
# Kernel function factory for a squared exponential kernel
# with given hyperparameters
get_SE_kernel = function(sigma_f, ell){
  kernel_func = function(x, x_star){
    (sigma_f^2) * exp(-((x - x_star)^2)/(2*(ell^2)))
  }

  class(kernel_func) = "kernel"

  return(kernel_func)
}

SE_kernel = get_SE_kernel(sigma_f = 1, ell = 1)
```

We evaluate the squared exponential kernel created above with parameters $\sigma_f = 1$ and $\ell = 1$ using $x = 1$ and $x' = 2$.

```r
cat("Kernel value = ", SE_kernel(1, 2))
```

```
## Kernel value =  0.6065307
```

Now, we use the `kernelMatrix()` function to compute the covariance matrix for given X and $X_\star$.

```r
x = matrix(c(1,3,4), ncol = 1)
x_star = matrix(c(2,3,4), ncol = 1)
K = kernelMatrix(kernel = SE_kernel, x = x, y = x_star)
```

```
## Kernel matrix:

## 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
```

2.2 GP Model `f(time)` with Squared Exponential kernel

Question: Consider first the following model:

$$\text{temp} = f(\text{time}) + \epsilon \quad \text{with } \epsilon \sim \mathcal{N}\left(0, \sigma_n^2\right) \text{ and } f \sim \mathcal{GP}\left(0, k\left(\text{time}, \text{time}'\right)\right)$$

Let σ_n^2 be the residual variance from a simple quadratic regression fit (using the `lm` function in R). Estimate the above Gaussian process regression model using the squared exponential function from

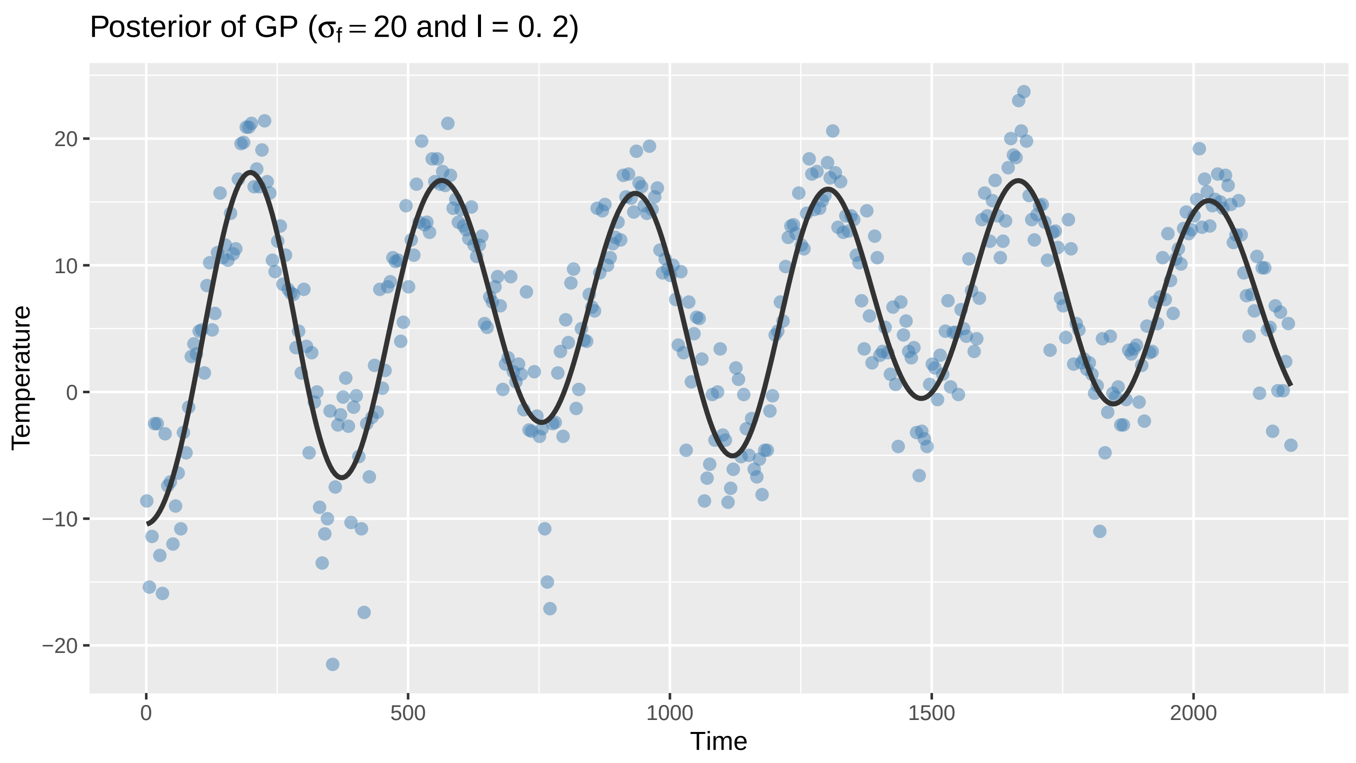
(1) with $\sigma_f = 20$ and $\ell = 0.2$. Use the `predict` function in R to compute the posterior mean at every data point in the training dataset. Make a scatterplot of the data and superimpose the posterior mean of f as a curve (use `type="l"` in the plot function). Play around with different values on σ_f and ℓ (no need to write this in the report though).

Answer:

We create the squared exponential kernel using the given hyperparameters. We compute σ_n^2 using a simple quadratic regression fit. Then, we use the `gausspr()` function to fit a Gaussian Process `temp ~ time`. We use this model to predict the temperature values for all the time values in the training data.

```r
SE_kernel = get_SE_kernel(sigma_f = 20, ell = 0.2)

# Compute sigma noise using a simple quadratic regression fit
lm_temp_time = lm(temp ~ time + I(time^2), data = temp_tullinge)
sigma_n_time = sd(lm_temp_time$residuals)

gp_time_fit = gausspr(temp_tullinge$time, temp_tullinge$temp,
                      kernel = get_SE_kernel,
                      kpar = list(sigma_f = 20, ell = 0.2),
                      var = sigma_n_time^2)

gp_time_pred = predict(gp_time_fit, temp_tullinge$time)
```

The following plot shows the GP mean of temperature predictions along with the true data points.



2.3 Computation of GP posterior variance

Question: `kernlab` can compute the posterior variance of f, but it seems to be a bug in the code. So, do your own computations for the posterior variance of f and plot the 95 % probability (pointwise) bands for f. Superimpose these bands on the figure with the posterior mean that you obtained in (2).

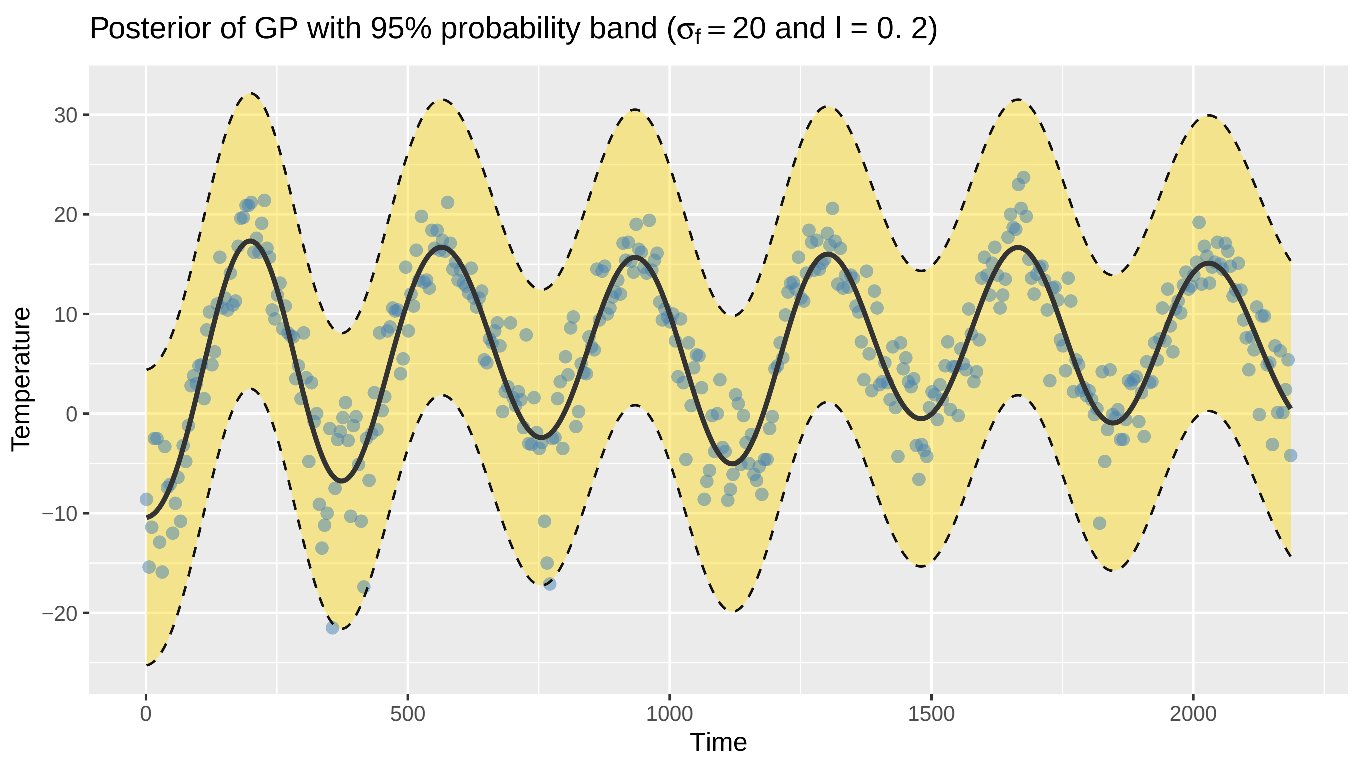
Hint: Note that Algorithm 2.1 on page 19 of Rasmussen and Willams' book already does the calculations required. Note also that `kernlab` scales the data by default to have zero mean and standard deviation one. So, the output of your implementation of Algorithm 2.1 will not coincide with the output of `kernlab` unless you scale the data first. For this, you may want to use the R function `scale`.

Answer:

In this task, we create our own function to calculate the variance of a GP for a given kernel function and pair of `X` vectors (train and test). We use this function to compute the posterior GP variance at different values of time.

```r
calc_variance = function(kernel, x, x_star, sigma_n){
  n = length(x)

  Kss = kernelMatrix(kernel = kernel, x = x_star, y = x_star)
  Kxx = kernelMatrix(kernel = kernel, x = x, y = x)
  Kxs = kernelMatrix(kernel = kernel, x = x, y = x_star)
  f_var = Kss-t(Kxs)%*%solve(Kxx + sigma_n^2*diag(n), Kxs)

  return(f_var)
}

gp_time_pred_var = calc_variance(SE_kernel, temp_tullinge$time,
                                 temp_tullinge$time, sigma_n_time)
```

The following plot shows the GP mean of temperature predictions and 95% probability bands along with the true data points.



2.4 GP Model `f(day)` with Squared Exponential kernel

Question: Consider now the following model:

$$temp = f(day) + \epsilon \quad \text{with} \quad \epsilon \sim \mathcal{N}\left(0, \sigma_n^2\right) \text{ and } f \sim \mathcal{GP}\left(0, k\left(day, day'\right)\right)$$

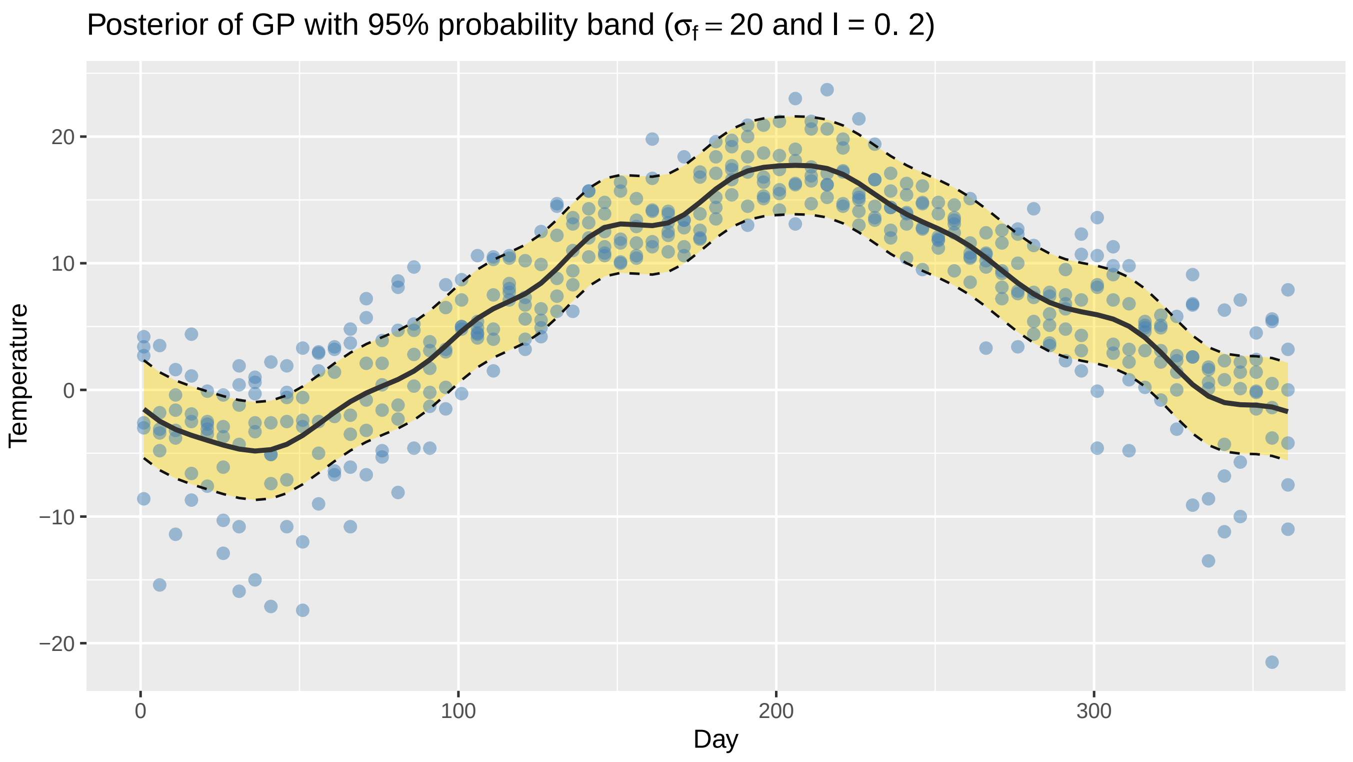
Estimate the model using the squared exponential function with $\sigma_f = 20$ and $\ell = 0.2$. Superimpose the posterior mean from this model on the posterior mean from the model in (2). Note that this plot should also have the time variable on the horizontal axis. Compare the results of both models. What are the pros and cons of each model?

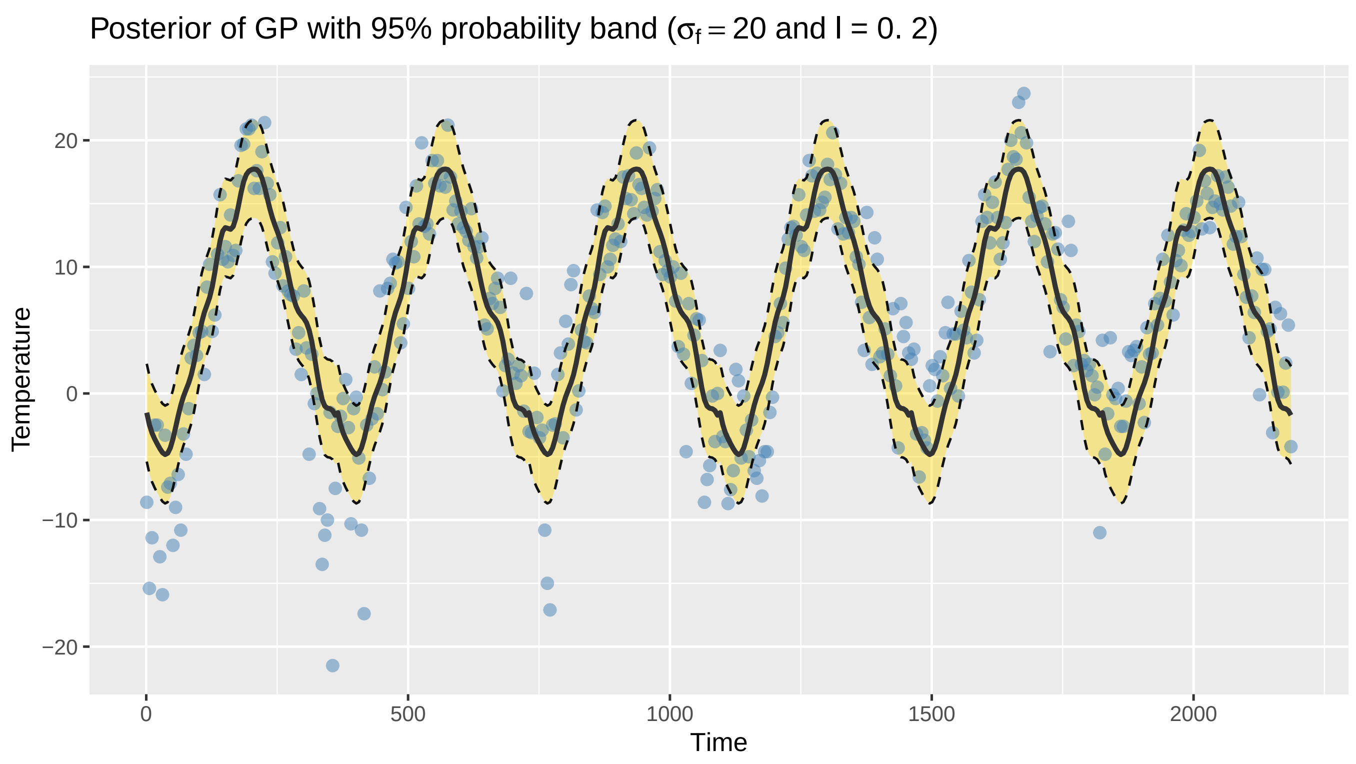
Answer:

Now, we repeat a similar GP model fit but now we model temperature as a function of day instead of a function of time.

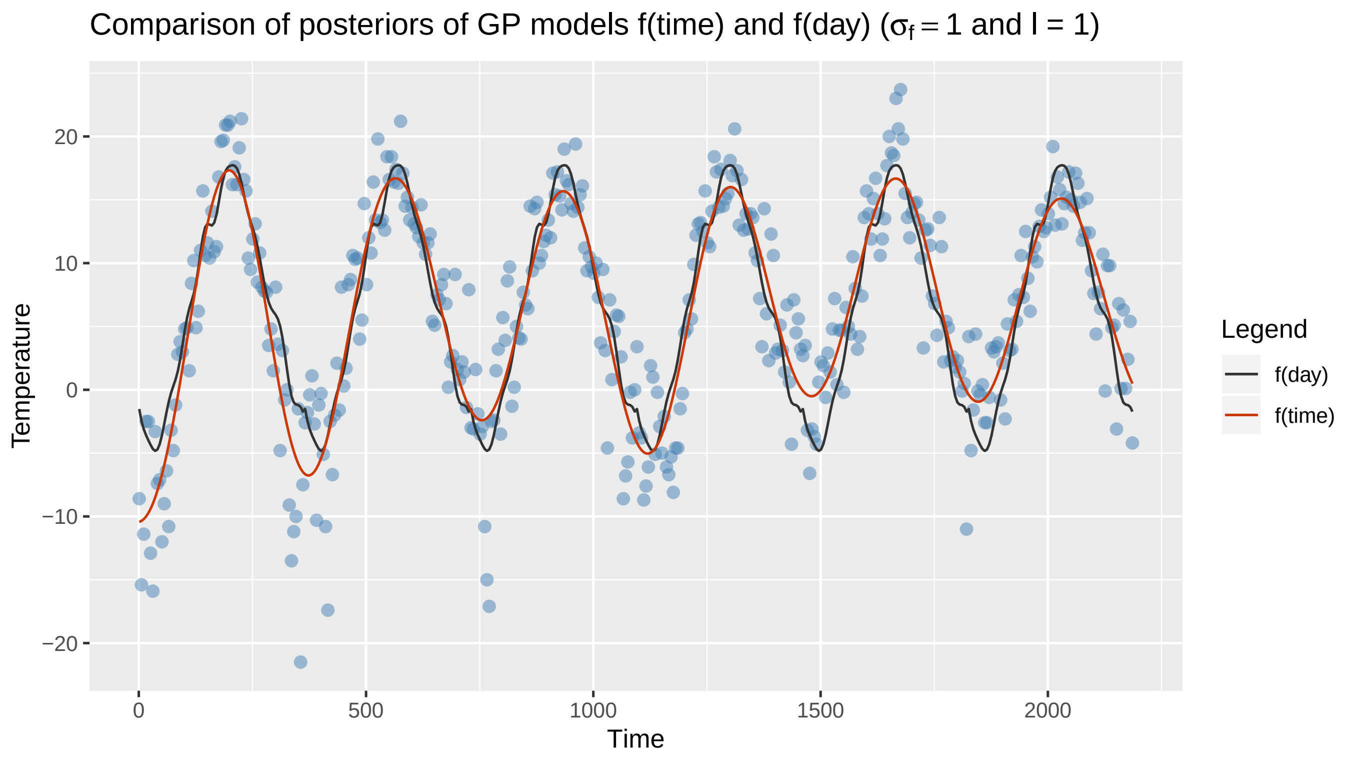
```r
# Compute sigma noise using a simple quadratic regression fit
lm_temp_day = lm(temp ~ day + I(day^2), data = temp_tullinge)
sigma_n_day = sd(lm_temp_day$residuals)

gp_day_fit = gausspr(temp_tullinge$day, temp_tullinge$temp,
                      kernel = get_SE_kernel,
                      kpar = list(sigma_f = 20, ell = 0.2),
                      var = sigma_n_day^2)

gp_day_pred = predict(gp_day_fit, temp_tullinge$day)

gp_day_pred_var = calc_variance(SE_kernel, temp_tullinge$day,
                                temp_tullinge$day, sigma_n_day)
```

The following plots show the posterior GP mean for temperature and the 95% probability bands along with the true data points.





The following plot shows a comparison between the posterior means of the GP models `f(time)` and `f(day)`.



Comparison of models:

- The `f(day)` model is based on day values in the range 1 to 365 only and it is repeated 6 times. So, we model the relationship between the day of the year and the temperature. This is exactly repeated 6 times. So, the model does not capture the trend occurring over years.

- The `f(time)` model is based on a continuous series of days in the range 1 to 6*365. So, the model captures the global trend and also the periodic aspect of temperature to some extent.
- The `f(day)` model looks more bumpy than the `f(time)` model. This is because we have more data points for each day but we have only 1 data point for each time. So, the `f(day)` model is a more closely fitting model as it is supported by more data points at each value of X and it captures the trends at different times of the year. This can be observed in the plot of the posterior GP function and days 1-365.

Pros and cons of models:

- The `f(time)` model is good at getting a generally good fit for the data but it does not capture the periodic aspect of the model that well.
- The `f(day)` model brings a periodic aspect to the model and captures the trends occurring within a year very well . But it does not capture any global trend that occurs across years (for example: global warming).

- The `f(day)` model is more robust to outliers as we have many data points for each day. So, the model is not easily influenced by a few extreme values.

2.5 GP Model `f(time)` with a periodic kernel

Question: Finally, implement a generalization of the periodic kernel given in the lectures:

$$k(x, x') = \sigma_f^2 \exp\left\{-\frac{2\sin^2(\pi|x-x'|/d)}{\ell_1^2}\right\} \exp\left\{-\frac{1}{2}\frac{|x-x'|^2}{\ell_2^2}\right\}$$

Note that we have two different length scales here, and ℓ_2 controls the correlation between the same day in different years. Estimate the GP model using the time variable with this kernel and hyperparameters $\sigma_f = 20$, $\ell_1 = 1$, $\ell_2 = 10$ and $d = 365/$`sd(time)`. The reason for the rather strange period here is that kernlab standardizes the inputs to have standard deviation of 1. Compare the fit to the previous two models (with $\sigma_f = 20$ and $\ell = 0.2$). Discuss the results.

Answer:

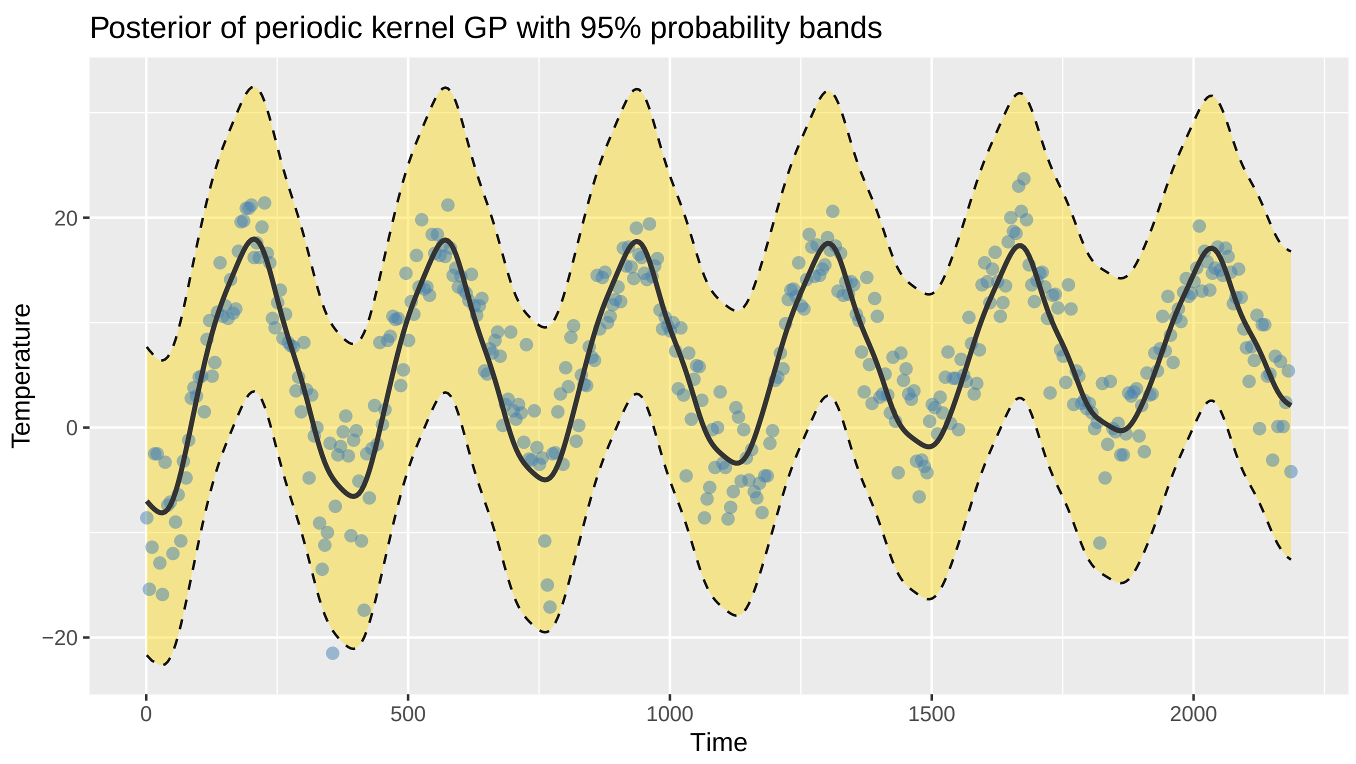
Now, we create a new periodic kernel that consists of 2 terms - one for modelling the general increasing/decreasing trend and another to model to yearly periodic aspect of temperature.

```r
# Function factory for periodic kernel
get_period_kernel = function(sigma_f, l1, l2, d){
  kernel_func = function(x, x_star){
    r = abs(x - x_star)
    (sigma_f^2) * exp(-(2*(sin(pi*r/d))^2)/(l1^2)) *
      exp(-(r^2)/(2*(l2^2)))
  }

  class(kernel_func) = "kernel"

  return(kernel_func)
}
```

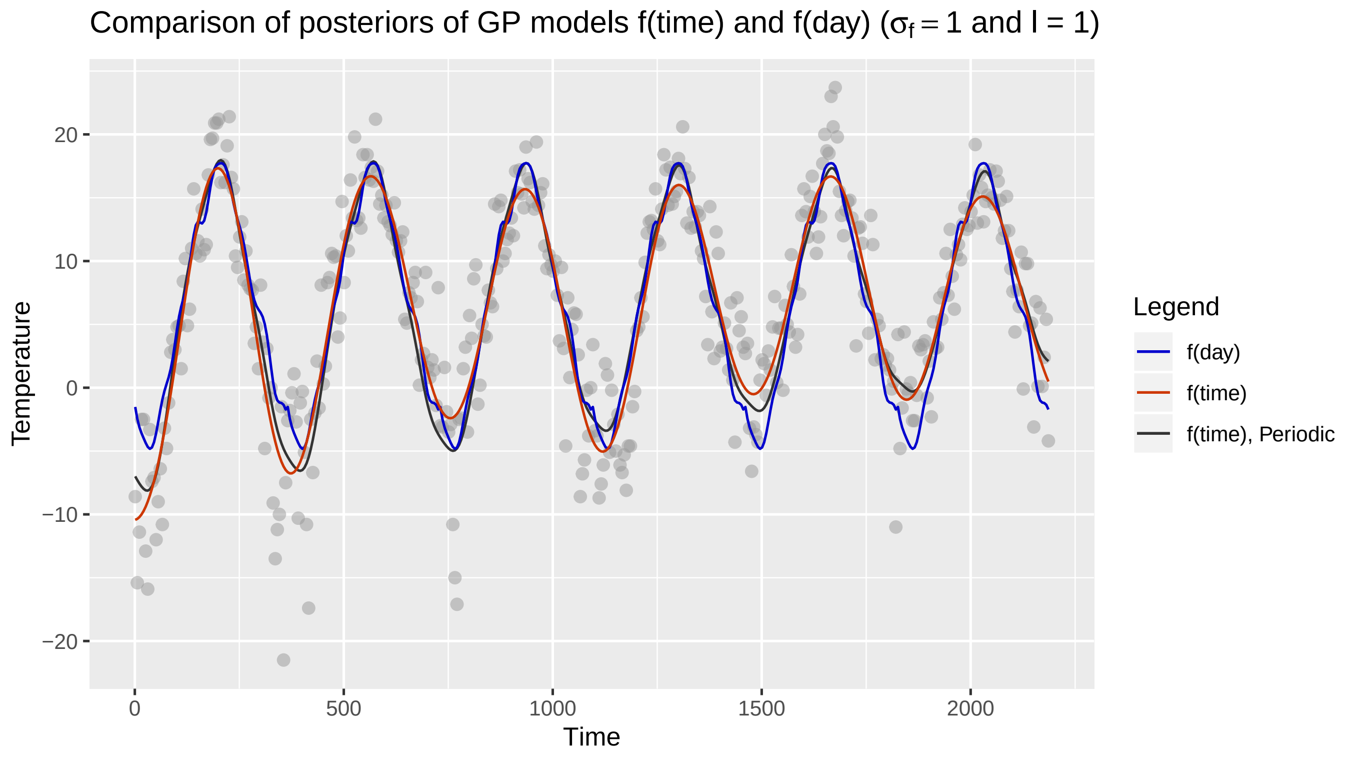
Using the above kernel, we fit a GP model and predict the posterior GP mean and compute its variance.

```r
kernel_params = list(sigma_f = 20, l1 = 1, l2 = 10, d = 365/sd(temp_tullinge$time))

gp_period_fit = gausspr(temp_tullinge$time, temp_tullinge$temp,
                        kernel = get_period_kernel,
                        kpar = kernel_params,
                        var = sigma_n_day^2)

gp_period_pred = predict(gp_period_fit, temp_tullinge$time)

period_kernel = get_period_kernel(sigma_f = 20, l1 = 1, l2 = 10,
                                  d = 365/sd(temp_tullinge$time))

gp_period_pred_var = calc_variance(period_kernel, temp_tullinge$time,
                                   temp_tullinge$time, sigma_n_time)
```

The following plot shows the posterior GP mean for temperature and the 95% probability bands along with the true data points.



The following plot shows a comparison between the posterior means of the GP models `f(time)`, `f(day)` and the periodic `f(time)`.

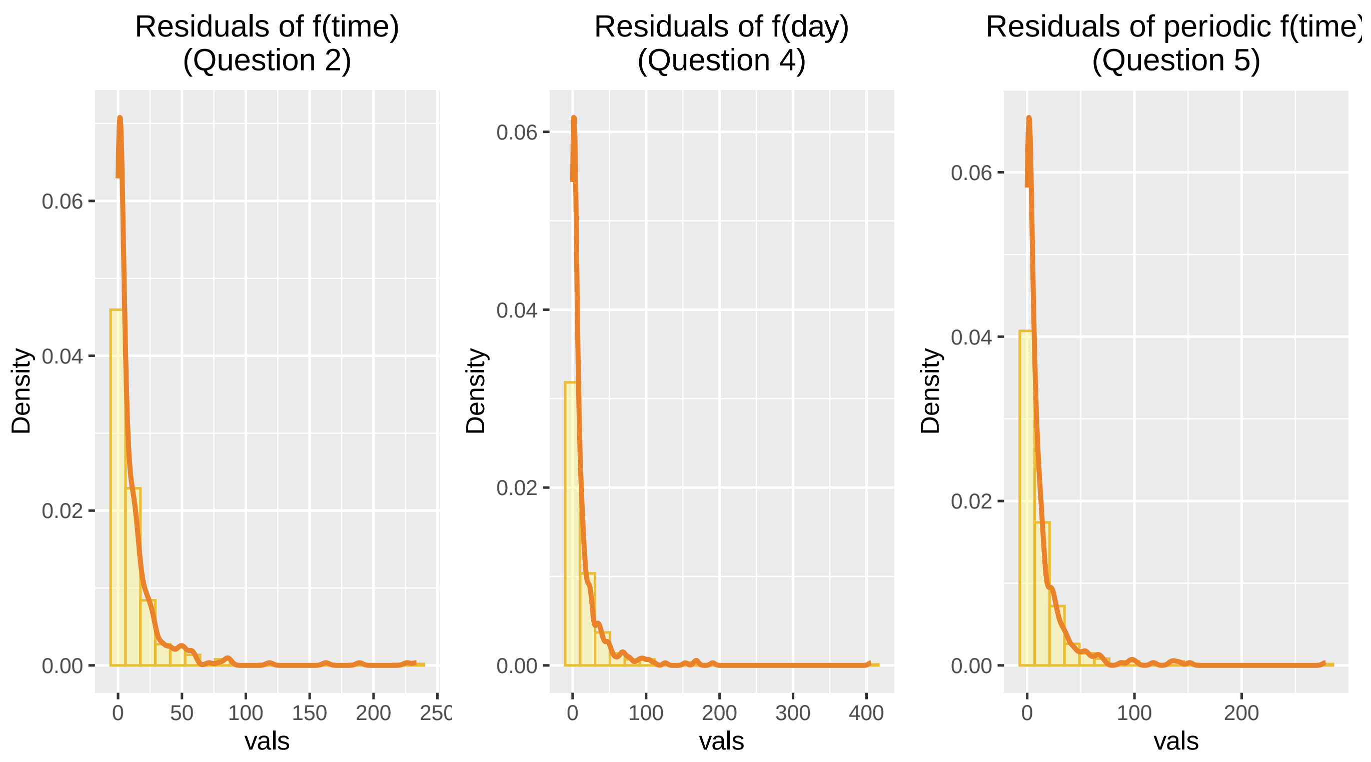


Now, we compute the residuals of the 3 models and plot their distribution. The mean residuals of each model is shown below.

Table 1: MSE of models

Gaussian Process	MSE
f(time)	12.50590
f(day)	15.44681
Periodic f(time)	13.30335

```r
# MSE of models
mse_ftime = (temp_tullinge$temp - gp_time_pred)^2
mse_fday = (temp_tullinge$temp - gp_day_pred)^2
mse_ftime_period = (temp_tullinge$temp - gp_period_pred)^2
```



Discussion of results:

The 3 models look very similar overall but there are some differences. The periodic `f(time)` model consists of a component to model the yearly periodic trend and another component to model the global trend.

- In the `periodic f(time)` model, there is a clear global trend which is increasing. In the `f(day)` model there was no global increasing/decreasing trend. In the `f(time)` model, the global trend increased and decreased depending on the data for each specific year.
- It appears like the `periodic f(time)` model is balancing between the global trend and the yearly periodic aspect of temperature.
- We observe that the `f(time)` model had the lowest MSE as it tries to fit the data best even if it gets influenced by outliers. The `f(day)` model is robust to outliers but does not capture the global trend and hence, has the lowest MSE. The `periodic f(time)` model has MSE between

the other 2 models and seems like a better generalization than the other 2 models as it balances the global trend and the yearly periodic aspect.

Question 3: GP Classification with `kernlab`

Download the banknote fraud data:

`data <- read.csv("https://github.com/STIMALiU/AdvMLCourse/raw/master/ GaussianProcess/Code/b`
`header=FALSE, sep=",")`

`names(data) <- c("varWave","skewWave","kurtWave","entropyWave","fraud")`

`data[,5] <- as.factor(data[,5])`

You can read about this dataset here. Choose 1000 observations as training data using the following command (i.e., use the vector `SelectTraining` to subset the training observations):

`set.seed(111); SelectTraining <- sample(1:dim(data)[1], size = 1000, replace = FALSE)`

```r
bn_data = read.csv("banknoteFraud.csv", header = F, sep=",")
names(bn_data) = c("varWave", "skewWave", "kurtWave", "entropyWave", "fraud")
bn_data[ , 5] = as.factor(bn_data[ , 5])

set.seed(111)
SelectTraining = sample(1:dim(bn_data)[1], size = 1000, replace = FALSE)
bn_train = bn_data[SelectTraining, ]
bn_test = bn_data[-SelectTraining, ]
```

	varWave	skewWave	kurtWave	entropyWave	fraud
814	-2.1333	1.5685	-0.084261	-1.74530	1
997	-2.3142	2.0838	-0.468130	-1.67670	1
508	4.6014	5.6264	-2.123500	0.19309	0
705	3.7022	6.9942	-1.851100	-0.12889	0
517	-2.3983	12.6060	2.946400	-5.78880	0
572	2.2517	-5.1422	4.291600	-1.24870	0

3.1 GP Classification Model with 2 covariates

Question: Use the R package `kernlab` to fit a Gaussian process classification model for fraud on the training data. Use the default kernel and hyperparameters. Start using only the covariates `varWave` and `skewWave` in the model. Plot contours of the prediction probabilities over a suitable grid of values for `varWave` and `skewWave`. Overlay the training data for fraud = 1 (as blue points) and fraud = 0 (as red points). You can reuse code from the file `KernLabDemo.R` available on the course website. Compute the confusion matrix for the classifier and its accuracy.

Answer:

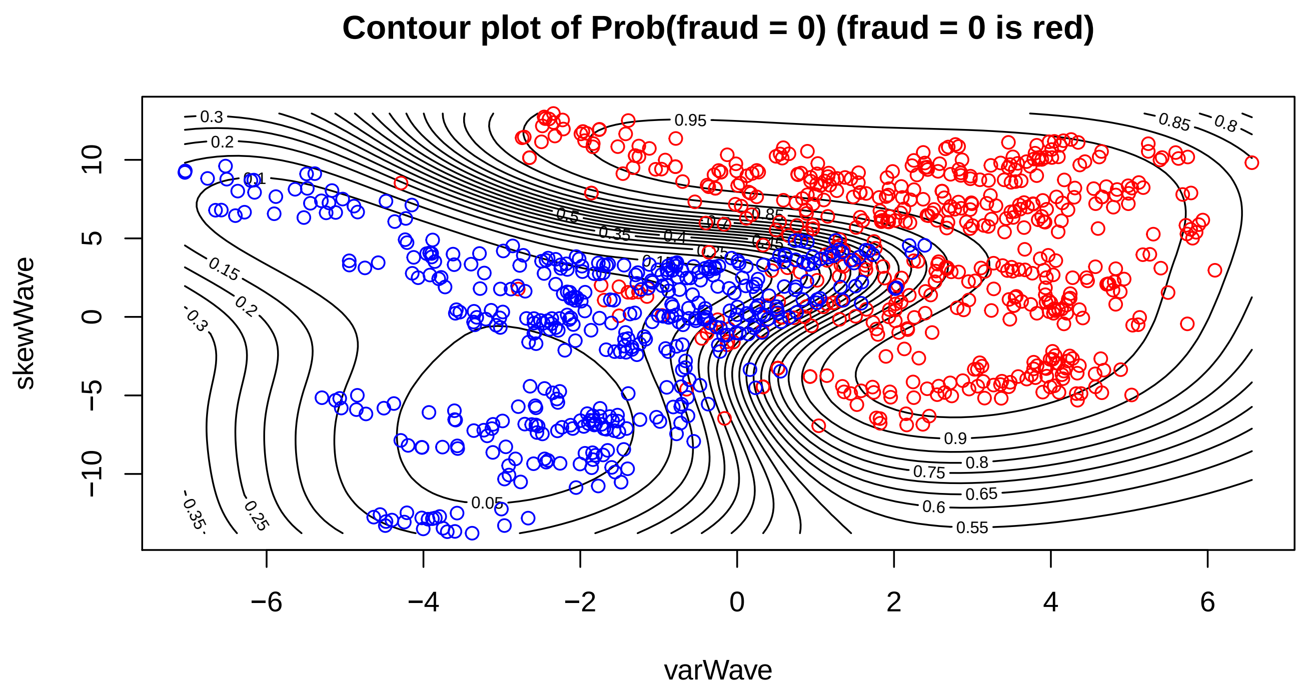
We create a GP classification model for fraud using the 2 covariates - `varWave` and `skewWave`. We use this model to make predictions for the training data.

```
# Fit GP model with only 2 covariates and predict for train data
bn_gp_fit = gausspr(fraud ~ varWave + skewWave, data = bn_train)
```

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

```
pred_train = predict(bn_gp_fit, bn_train)
```

The following contour plot shows the probabilities for fraud=0 and visualizes the regions in the 2-covariate space where the fraud will be predicted as 0 and 1.



The confusion matrix for the training data predictions are as follows.

```
confusionMatrix(pred_train, bn_train$fraud)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 512  24
##           1  44 420
##
##                Accuracy : 0.932
##                  95% CI : (0.9146, 0.9468)
##     No Information Rate : 0.556
##     P-Value [Acc > NIR] : < 0.0000000000000002
##
##                   Kappa : 0.8629
##
##  Mcnemar's Test P-Value : 0.02122
##
##             Sensitivity : 0.9209
##             Specificity : 0.9459
##          Pos Pred Value : 0.9552
##          Neg Pred Value : 0.9052
##              Prevalence : 0.5560
##          Detection Rate : 0.5120
##    Detection Prevalence : 0.5360
##       Balanced Accuracy : 0.9334
##
##        'Positive' Class : 0
##
```

3.2 Class predictions for test dataset

Question: Using the estimated model from (1), make predictions for the test set. Compute the accuracy.

Answer:

Now, we make predictions for the test data and the confusion matrix is as follows.

```r
# Use GP model with 2 covariates to predict for test data
pred_test = predict(bn_gp_fit, bn_test)
confusionMatrix(pred_test, bn_test$fraud)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 191   9
##          1  15 157
```

```
##
##                Accuracy : 0.9355
##                  95% CI : (0.9055, 0.9582)
##     No Information Rate : 0.5538
##     P-Value [Acc > NIR] : <0.0000000000000002
##
##                   Kappa : 0.8699
##
##  Mcnemar's Test P-Value : 0.3074
##
##             Sensitivity : 0.9272
##             Specificity : 0.9458
##          Pos Pred Value : 0.9550
##          Neg Pred Value : 0.9128
##              Prevalence : 0.5538
##          Detection Rate : 0.5134
##    Detection Prevalence : 0.5376
##       Balanced Accuracy : 0.9365
##
##        'Positive' Class : 0
##
```

3.3 GP Classification Model with all 4 covariates

Question: Train a model using all four covariates. Make predictions on the test set and compare the accuracy to the model with only two covariates.

Answer:

In this task, we use all the 4 covariates which are available to create the classification GP model. Then, we make predictions for training and test data. The confusion matrix shown below corresponds to the predictions for the test data.

```
# Fit GP model with all covariates and predict for train and test data
bn_gp_all_fit = gausspr(fraud ~ ., data = bn_train)
```

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

```
pred_all_train = predict(bn_gp_all_fit, bn_train)
pred_all_test = predict(bn_gp_all_fit, bn_test)

confusionMatrix(pred_all_test, bn_test$fraud)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 205   0
##          1   1 166
##
##                Accuracy : 0.9973
##                  95% CI : (0.9851, 0.9999)
##     No Information Rate : 0.5538
##     P-Value [Acc > NIR] : <0.0000000000000002
##
##                   Kappa : 0.9946
##
##  Mcnemar's Test P-Value : 1
##
##             Sensitivity : 0.9951
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.9940
##              Prevalence : 0.5538
##          Detection Rate : 0.5511
##    Detection Prevalence : 0.5511
##       Balanced Accuracy : 0.9976
##
##        'Positive' Class : 0
##
```

```r
# Calculate model accuracies
acc_2_cov_train = mean(pred_train == bn_train$fraud)
acc_2_cov_test = mean(pred_test == bn_test$fraud)
acc_all_cov_train = mean(pred_all_train == bn_train$fraud)
acc_all_cov_test = mean(pred_all_test == bn_test$fraud)
```

The following table shows the accuracies of the GP models trained using 2 covariates and all covariates for the training and test data.

Table 2: Model Accuracies

Covariates	Train	Test
varWave, skewWave	0.932	0.9354839
All	0.996	0.9973118

By looking at the accuracies, we see that the GP model trained using all the covariates clearly performs better than the GP model trained using only 2 covariates.

Appendix

```r
# Set up general options

knitr::opts_chunk$set(echo = FALSE, warning = FALSE, message = FALSE, fig.width=8)

set.seed(123456)

library(ggplot2)
options(kableExtra.latex.load_packages = FALSE)
library(kableExtra)
library(caret)
library(gridExtra)
library(kernlab)
library(mvtnorm)
library(latex2exp)
library(AtmRay)

options(scipen=999)

# Function to plot histogram and density of a sample
hist_plt = function(vals){
  n_bins = ceiling(sqrt(length(vals)))
  plt = qplot(vals, geom = 'blank') +
    geom_histogram(aes(y = ..density..), alpha = 0.4,
                   bins = n_bins, color = "#EBBC36", fill = "#FFF57D") +
    geom_line(aes(y = ..density.., color = 'Empirical Density'),
              stat = 'density', size = 1, color = "#E8822B") +
    theme(plot.title = element_text(hjust = 0.5),
          plot.subtitle = element_text(hjust = 0.5)) + ylab("Density")

  return(plt)
}

# Function to plot posterior of Gaussian Process
# Use when the number of data points are few
post_gp_plot = function(x, y, x_star, y_star, variance, pred_conf,
                        sigma_f, l, axis_titles = c("X", "Y")){
  bw = qnorm(p = pred_conf + ((1-pred_conf)/2))
  y_min = y_star - bw*sqrt(diag(variance))
  y_max = y_star + bw*sqrt(diag(variance))

  ggplot() +
    geom_ribbon(aes(x = x_star, ymin = y_min, ymax = y_max),
                fill = "gold", alpha = 0.4) +
    geom_line(aes(x = x_star, y = y_star),
              color = "#333333", size = 1.5) +
    geom_line(aes(x = x_star, y = y_min),
              color = "#111111", linetype = "dashed") +
    geom_line(aes(x = x_star, y = y_max),
              color = "#111111", linetype = "dashed") +
    geom_point(aes(x = x, y = y), shape = 21, fill = "red", size = 2) +
    labs(x = axis_titles[1], y = axis_titles[2]) +
    ggtitle(TeX(paste0("Posterior of GP with ", round(100*pred_conf, 1),
                       "% probability band ($\\sigma_f = ",
                       sigma_f, "$ and l = ", l, ")")))

}

# Function to plot posterior of Gaussian Process
# Use when the number of data points are many
post_gp_scatterplot = function(x, y, x_star, y_star, variance,
                               pred_conf, sigma_f, l,
                               axis_titles = c("X", "Y")){
  plt = NA

  # Check whether to plot the prediction bands
  if(is.na(variance)){
    plt = ggplot() +
      geom_point(aes(x = x, y = y),
                 color = "steelblue", alpha = 0.5, size = 2) +
      geom_line(aes(x = x_star, y = y_star),
                color = "#333333", size = 1) +
      labs(x = axis_titles[1], y = axis_titles[2]) +
      ggtitle(TeX(paste0("Posterior of GP ($\\sigma_f = ",
                         sigma_f, "$ and l = ", l, ")")))
  }
  else{
    bw = qnorm(p = pred_conf + ((1-pred_conf)/2))
    y_min = y_star - bw*sqrt(diag(variance))
    y_max = y_star + bw*sqrt(diag(variance))

    plt = ggplot() +
      geom_ribbon(aes(x = x_star, ymin = y_min, ymax = y_max),
                  fill = "gold", alpha = 0.4) +
      geom_point(aes(x = x, y = y),
                 color = "steelblue", alpha = 0.5, size = 2) +
      geom_line(aes(x = x_star, y = y_star),
                color = "#333333", size = 1) +
      geom_line(aes(x = x_star, y = y_min),
                color = "#111111", linetype = "dashed") +
      geom_line(aes(x = x_star, y = y_max),
                color = "#111111", linetype = "dashed") +
      labs(x = axis_titles[1], y = axis_titles[2]) +
      ggtitle(TeX(paste0("Posterior of GP with ", round(100*pred_conf, 1),
                         "% probability band ($\\sigma_f = ",
                         sigma_f, "$ and l = ", l, ")")))
  }

  return(plt)
}




# ---------------------------------------------------------------------------------
# Question 1.1
# ---------------------------------------------------------------------------------

# Kernel function - Squared exponential kernel
squared_exp_kernel = function(x1, x2, sigma_f = 1, l = 3){
  n1 = length(x1)
  n2 = length(x2)
  K = matrix(NA,n1,n2)

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

  return(K)
}

# Function to compute posterior GP function mean, variance
# and marginal log-likelihood
posteriorGP = function(X, y, XStar, hyperParam, sigmaNoise){
  sigma_f = hyperParam[1]
  ell = hyperParam[2]
  n = length(X)

  K = squared_exp_kernel(X, X, sigma_f = sigma_f, l = ell)
  K_star = squared_exp_kernel(X, XStar, sigma_f = sigma_f, l = ell)

  L = t(chol(K + (sigmaNoise^2) * diag(x = 1, nrow = n)))
  alpha = solve(t(L), (solve(L, y, drop = F)), drop = F)
  f_star = t(K_star) %*% alpha
  v = solve(L, K_star)

  Var_f_star = squared_exp_kernel(XStar, XStar,
                                  sigma_f = sigma_f,
                                  l = ell) - (t(v) %*% v)

  log_ml = -0.5*t(y)%*%alpha - sum(diag(L)) - n*log(2*pi)/2
  return(list(mean = f_star, variance = Var_f_star, log_ml = log_ml))
}


# ------------------------------------------------------------------------------
# Question 1.2
# ------------------------------------------------------------------------------

x = c(0.4)
y = c(0.719)
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 0.3

post_gp_2 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)

post_gp_plot(x, y, x_star, post_gp_2$mean, post_gp_2$variance, 0.95, sigma_f, l)


# ------------------------------------------------------------------------------
# Question 1.3
# ------------------------------------------------------------------------------

x = c(0.4, -0.6)
y = c(0.719, -0.044)
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 0.3

post_gp_3 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)

post_gp_plot(x, y, x_star, post_gp_3$mean, post_gp_3$variance, 0.95, sigma_f, l)

kable(data.frame(x = seq(-1, 0.8, 0.4),
                 y = c(0.768, -0.044, -0.940, 0.719, -0.664)))


# ------------------------------------------------------------------------------
# Question 1.4
# ------------------------------------------------------------------------------

x = c(-1, -0.6, -0.2, 0.4, 0.8)
y = c(0.768, -0.044, -0.940, 0.719, -0.664)
```

```r
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 0.3

post_gp_4 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)

post_gp_plot(x, y, x_star, post_gp_4$mean, post_gp_4$variance, 0.95, sigma_f, l)


# ---------------------------------------------------------------------------
# Question 1.5
# ---------------------------------------------------------------------------

x = c(-1, -0.6, -0.2, 0.4, 0.8)
y = c(0.768, -0.044, -0.940, 0.719, -0.664)
x_star = seq(-1, 1, 0.01)
sigma_f = 1
l = 1

post_gp_5 = posteriorGP(X = x, y = y, XStar = x_star,
                        hyperParam = c(sigma_f = sigma_f, l = l),
                        sigmaNoise = 0.1)

post_gp_plot(x, y, x_star, post_gp_5$mean, post_gp_5$variance, 0.95, sigma_f, l)

temp_tullinge = read.csv2("TempTullinge.csv", stringsAsFactors = F)

temp_tullinge$temp = as.numeric(temp_tullinge$temp)
temp_tullinge$time = 1:nrow(temp_tullinge)
temp_tullinge$day = rep(1:365, 6)
temp_tullinge$date = NULL

temp_tullinge = temp_tullinge[temp_tullinge$time %% 5 == 1 , ]

kable(tail(temp_tullinge), booktabs = T) %>%
  kable_styling(latex_option = "striped")

# ---------------------------------------------------------------------------
# Question 2.1
# ---------------------------------------------------------------------------

# Kernel function factory for a squared exponential kernel
# with given hyperparameters
get_SE_kernel = function(sigma_f, ell){
  kernel_func = function(x, x_star){
    (sigma_f^2) * exp(-((x - x_star)^2)/(2*(ell^2)))
  }

  class(kernel_func) = "kernel"

  return(kernel_func)
}

SE_kernel = get_SE_kernel(sigma_f = 1, ell = 1)

cat("Kernel value = ", SE_kernel(1, 2))

x = matrix(c(1,3,4), ncol = 1)
x_star = matrix(c(2,3,4), ncol = 1)
K = kernelMatrix(kernel = SE_kernel, x = x, y = x_star)

cat("Kernel matrix: ")
print(K)


# -----------------------------------------------------------------------------
# Question 2.2
# -----------------------------------------------------------------------------

SE_kernel = get_SE_kernel(sigma_f = 20, ell = 0.2)

# Compute sigma noise using a simple quadratic regression fit
lm_temp_time = lm(temp ~ time + I(time^2), data = temp_tullinge)
sigma_n_time = sd(lm_temp_time$residuals)

gp_time_fit = gausspr(temp_tullinge$time, temp_tullinge$temp,
                      kernel = get_SE_kernel,
                      kpar = list(sigma_f = 20, ell = 0.2),
                      var = sigma_n_time^2)

gp_time_pred = predict(gp_time_fit, temp_tullinge$time)

post_gp_scatterplot(temp_tullinge$time, temp_tullinge$temp, temp_tullinge$time,
                    gp_time_pred, NA, NA, 20, 0.2,
                    axis_titles = c("Time", "Temperature"))


# -----------------------------------------------------------------------------
# Question 2.3
# -----------------------------------------------------------------------------

calc_variance = function(kernel, x, x_star, sigma_n){
```

```r
  n = length(x)

  Kss = kernelMatrix(kernel = kernel, x = x_star, y = x_star)
  Kxx = kernelMatrix(kernel = kernel, x = x, y = x)
  Kxs = kernelMatrix(kernel = kernel, x = x, y = x_star)
  f_var = Kss-t(Kxs)%*%solve(Kxx + sigma_n^2*diag(n), Kxs)

  return(f_var)
}

gp_time_pred_var = calc_variance(SE_kernel, temp_tullinge$time,
                                 temp_tullinge$time, sigma_n_time)

post_gp_scatterplot(temp_tullinge$time, temp_tullinge$temp, temp_tullinge$time,
                    gp_time_pred, gp_time_pred_var, 0.95, 20, 0.2,
                    axis_titles = c("Time", "Temperature"))


# ---------------------------------------------------------------------------
# Question 2.4
# ---------------------------------------------------------------------------

# Compute sigma noise using a simple quadratic regression fit
lm_temp_day = lm(temp ~ day + I(day^2), data = temp_tullinge)
sigma_n_day = sd(lm_temp_day$residuals)

gp_day_fit = gausspr(temp_tullinge$day, temp_tullinge$temp,
                     kernel = get_SE_kernel,
                     kpar = list(sigma_f = 20, ell = 0.2),
                     var = sigma_n_day^2)

gp_day_pred = predict(gp_day_fit, temp_tullinge$day)

gp_day_pred_var = calc_variance(SE_kernel, temp_tullinge$day,
                                temp_tullinge$day, sigma_n_day)

post_gp_scatterplot(temp_tullinge$day, temp_tullinge$temp, temp_tullinge$day,
                    gp_day_pred, gp_day_pred_var, 0.95, 20, 0.2,
                    axis_titles = c("Day", "Temperature"))

post_gp_scatterplot(temp_tullinge$time, temp_tullinge$temp, temp_tullinge$time,
                    gp_day_pred, gp_day_pred_var, 0.95, 20, 0.2,
                    axis_titles = c("Time", "Temperature"))

ggplot() +
  geom_point(aes(x = time, y = temp), data = temp_tullinge,
             color = "steelblue", alpha = 0.5, size = 2) +
  geom_line(aes(x = time, y = gp_day_pred, color = "f(day)"),
            data = temp_tullinge) +
  geom_line(aes(x = time, y = gp_time_pred, color = "f(time)"),
            data = temp_tullinge) +
  labs(x = "Time", y = "Temperature", color = "Legend") +
  scale_color_manual(values = c("f(time)" = "orangered3",
                                "f(day)" = "#333333")) +
  ggtitle(TeX(paste0("Comparison of posteriors of GP models f(time) and f(day) ",
                     "($\\sigma_f = ", sigma_f, "$ and l = ", l, ")")))


# ------------------------------------------------------------------------------
# Question 2.5
# ------------------------------------------------------------------------------

# Function factory for periodic kernel
get_period_kernel = function(sigma_f, l1, l2, d){
  kernel_func = function(x, x_star){
    r = abs(x - x_star)

    (sigma_f^2) * exp(-(2*(sin(pi*r/d))^2)/(l1^2)) *
      exp(-(r^2)/(2*(l2^2)))
  }

  class(kernel_func) = "kernel"

  return(kernel_func)
}

kernel_params = list(sigma_f = 20, l1 = 1, l2 = 10, d = 365/sd(temp_tullinge$time))

gp_period_fit = gausspr(temp_tullinge$time, temp_tullinge$temp,
                        kernel = get_period_kernel,
                        kpar = kernel_params,
                        var = sigma_n_day^2)

gp_period_pred = predict(gp_period_fit, temp_tullinge$time)

period_kernel = get_period_kernel(sigma_f = 20, l1 = 1, l2 = 10,
                                  d = 365/sd(temp_tullinge$time))

gp_period_pred_var = calc_variance(period_kernel, temp_tullinge$time,
                                   temp_tullinge$time, sigma_n_time)

post_gp_scatterplot(temp_tullinge$time, temp_tullinge$temp, temp_tullinge$time,
                    gp_period_pred, gp_period_pred_var, 0.95, 20, 0.2,
                    axis_titles = c("Time", "Temperature")) +
  ggtitle("Posterior of periodic kernel GP with 95% probability bands")

ggplot() +
  geom_point(aes(x = time, y = temp), data = temp_tullinge,
             color = "#999999", alpha = 0.5, size = 2) +
  geom_line(aes(x = time, y = gp_period_pred,
                color = "f(time), Periodic"), data = temp_tullinge) +
  geom_line(aes(x = time, y = gp_day_pred,
                color = "f(day)"), data = temp_tullinge) +
  geom_line(aes(x = time, y = gp_time_pred,
                color = "f(time)"), data = temp_tullinge) +
  labs(x = "Time", y = "Temperature", color = "Legend") +
  scale_color_manual(values = c("f(time)" = "orangered3",
                                "f(day)" = "mediumblue",
                                "f(time), Periodic" = "#333333")) +
  ggtitle(TeX(paste0("Comparison of posteriors of GP models f(time) and f(day) ",
                     "($\\sigma_f = ", sigma_f, "$ and l = ", l, ")")))

# MSE of models
mse_ftime = (temp_tullinge$temp - gp_time_pred)^2
mse_fday = (temp_tullinge$temp - gp_day_pred)^2
mse_ftime_period = (temp_tullinge$temp - gp_period_pred)^2

hplt_1 = hist_plt(mse_ftime) +
  ggtitle("Residuals of f(time)\n(Question 2)")

hplt_2 = hist_plt(mse_fday) +
  ggtitle("Residuals of f(day)\n(Question 4)")

hplt_3 = hist_plt(mse_ftime_period) +
  ggtitle("Residuals of periodic f(time)\n(Question 5)")

grid.arrange(hplt_1, hplt_2, hplt_3, nrow = 1)

res_df = data.frame(gp = c("f(time)", "f(day)", "Periodic f(time)"),
                    mean_res = c(mean(mse_ftime), mean(mse_fday),
                                 mean(mse_ftime_period)))

kable(res_df, booktabs = T, col.names = c("Gaussian Process",
                                          "MSE"),
      caption = "MSE of models") %>%
  kable_styling(latex_option = "striped")

bn_data = read.csv("banknoteFraud.csv", header = F, sep=",")
names(bn_data) = c("varWave", "skewWave", "kurtWave", "entropyWave", "fraud")
bn_data[ , 5] = as.factor(bn_data[ , 5])
```

```r
set.seed(111)
SelectTraining = sample(1:dim(bn_data)[1], size = 1000, replace = FALSE)
bn_train = bn_data[SelectTraining, ]
bn_test = bn_data[-SelectTraining, ]

kable(head(bn_train), booktabs = T) %>%
  kable_styling(latex_option = "striped")

# ------------------------------------------------------------------------------
# Question 3.1
# ------------------------------------------------------------------------------

# Fit GP model with only 2 covariates and predict for train data
bn_gp_fit = gausspr(fraud ~ varWave + skewWave, data = bn_train)
pred_train = predict(bn_gp_fit, bn_train)

# Code to make contour plot
x1 = seq(min(bn_train$varWave), max(bn_train$varWave), length = 100)
x2 = seq(min(bn_train$skewWave), max(bn_train$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")
grid_probs = predict(bn_gp_fit, grid_points, type = "probabilities")

contour(x1, x2, matrix(grid_probs[, 1], 100, byrow = TRUE),
        20, xlab = "varWave",
        ylab = "skewWave",
        main = "Contour plot of Prob(fraud = 0) (fraud = 0 is red)")

points(bn_train[bn_train$fraud == 0, "varWave"],
       bn_train[bn_train$fraud == 0, "skewWave"], col="red")
points(bn_train[bn_train$fraud == 1, "varWave"],
       bn_train[bn_train$fraud == 1, "skewWave"], col="blue")

# End of code to make contour plot

confusionMatrix(pred_train, bn_train$fraud)


# ------------------------------------------------------------------------------
# Question 3.2
# ------------------------------------------------------------------------------

# Use GP model with 2 covariates to predict for test data
```

```r
pred_test = predict(bn_gp_fit, bn_test)
confusionMatrix(pred_test, bn_test$fraud)


# ---------------------------------------------------------------------------------
# Question 3.3
# ---------------------------------------------------------------------------------

# Fit GP model with all covariates and predict for train and test data
bn_gp_all_fit = gausspr(fraud ~ ., data = bn_train)
pred_all_train = predict(bn_gp_all_fit, bn_train)
pred_all_test = predict(bn_gp_all_fit, bn_test)

confusionMatrix(pred_all_test, bn_test$fraud)

# Calculate model accuracies
acc_2_cov_train = mean(pred_train == bn_train$fraud)
acc_2_cov_test = mean(pred_test == bn_test$fraud)
acc_all_cov_train = mean(pred_all_train == bn_train$fraud)
acc_all_cov_test = mean(pred_all_test == bn_test$fraud)

acc_df = data.frame(Covariates = c("varWave, skewWave", "All"),
                    Train = c(acc_2_cov_train, acc_all_cov_train),
                    Test = c(acc_2_cov_test, acc_all_cov_test))

kable(acc_df, booktabs = T, longtable = T, caption = "Model Accuracies") %>%
  kable_styling(latex_option = "striped")
```