Introduction to Machine Learning - Lab 6

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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. The two formulas used for calculating this are presented below:

$$\bar{f}_* = K(x_*, x)[K(x, x) + \sigma^2 l]^{-1} y$$

$$cov(\bar{f}_*) = K(x_*, x_*) - K(x_*, x)[K(x, x) + \sigma^2 l]^{-1} K(x, x_*)$$

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

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

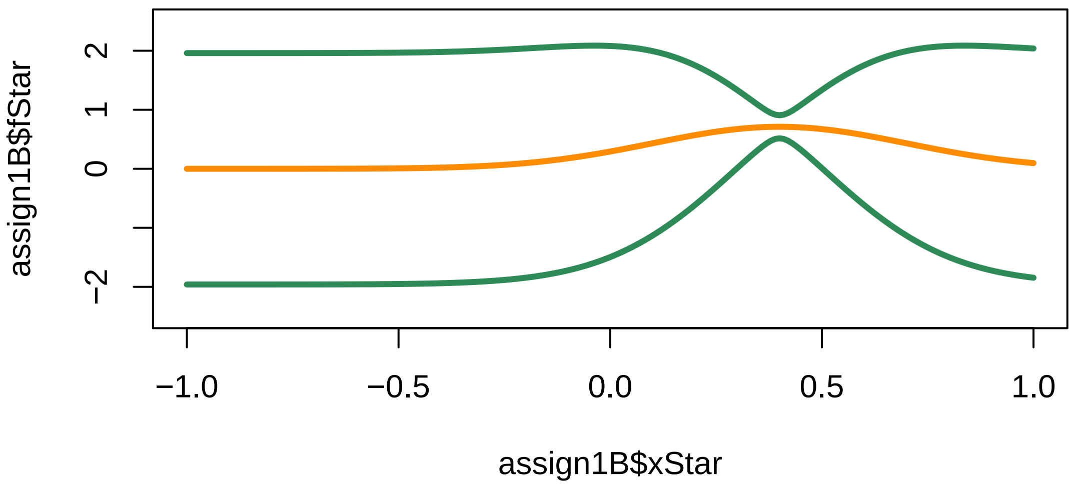
$$f(x) \sim GP(0, K(x, x'))$$

Then, the posterior guassian distribution looks as following:

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

(b)

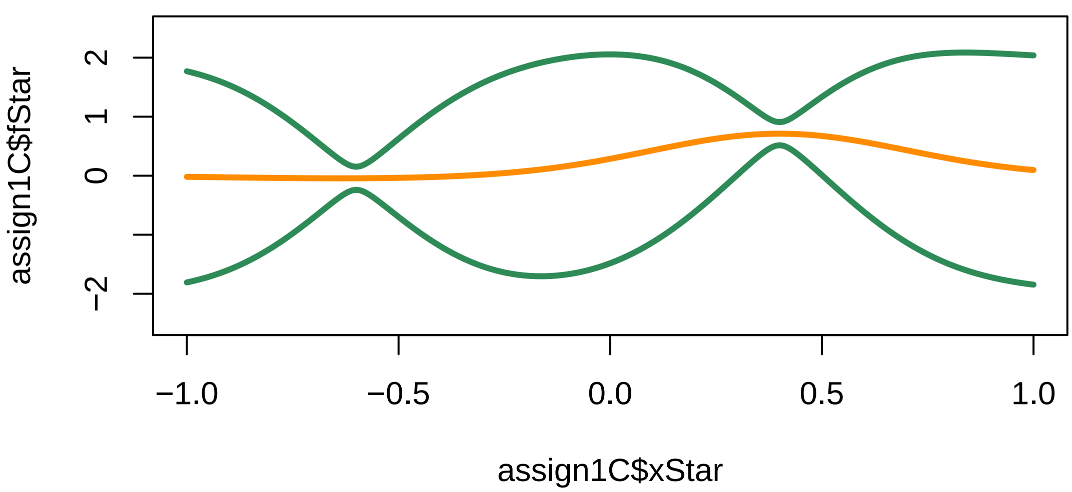
Since the noise standard deviation is assumed to be known the parameter σ_n is set to 0.1. The prior hyperparameter σ_f is set to 1 and the second prior hyperparameter ι is set to 0.3. Furthermore the prior is updated with one observation, *(x,y)*=(0.4, 0.719). A plot over the posterior mean of f over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



The probability bands are more narrow around the observed value.

(c)

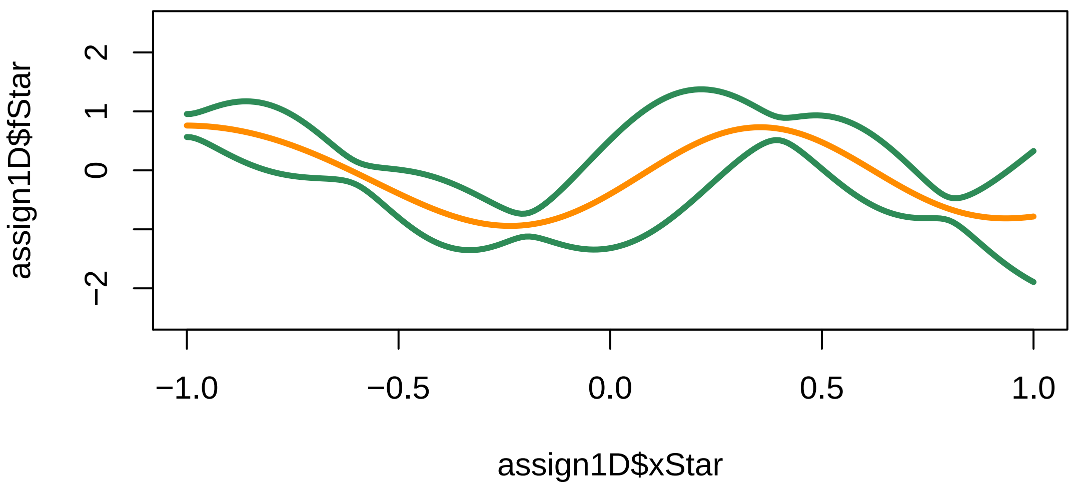
The posterior from *b)* is updated with another observation, *(x,y)*=(-0.6, -0.044).



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)

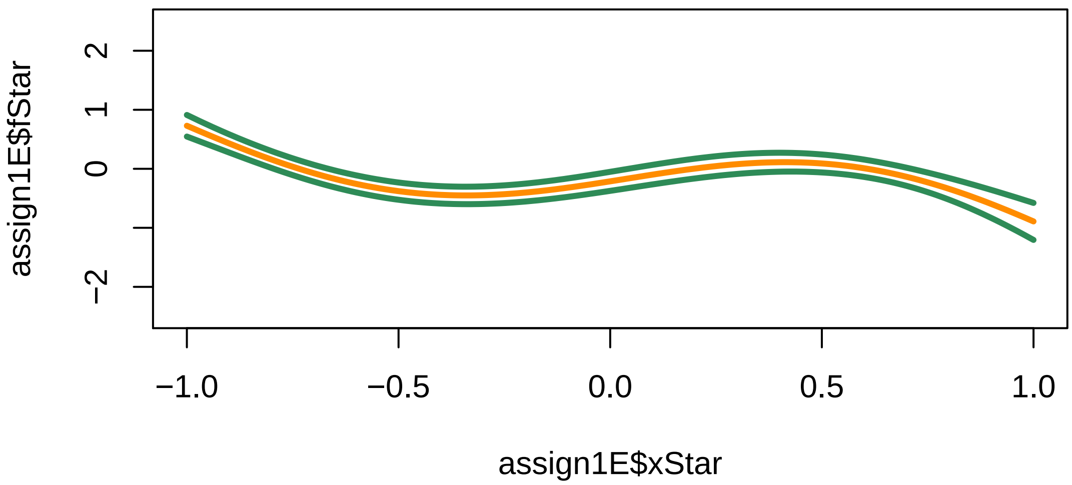
In *d)* the number of observations rises to five, resulting in the following plot over the posterior mean of f and its 95 % probability intervals.



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.

(e)

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

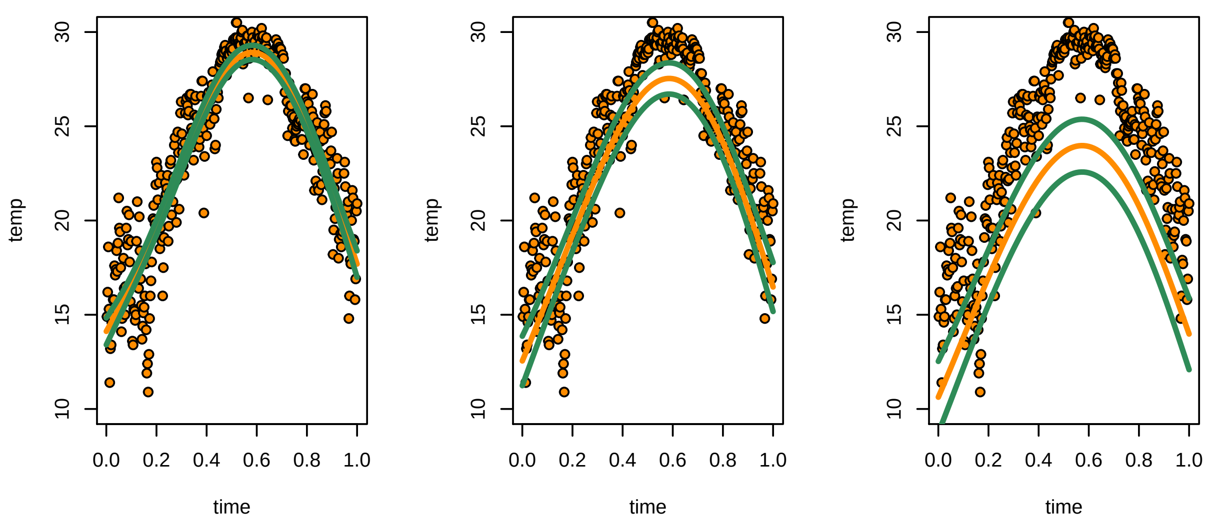


Compared to the plot in *d)*, the probability bands obtained with ι set to 1 looks much smoother and lies much closer to the curve for the posterior mean of *f*.

Assignment 2

The implemented functions in assignment 1 are now tested on the data set *JapanTemp*. This data set contains information about the daily temperatures during a year for some place in Japan. What that is mainly investigated in this assignment is the effect on the posterior for different values of the parameters σ_n, σ_f, and ι.

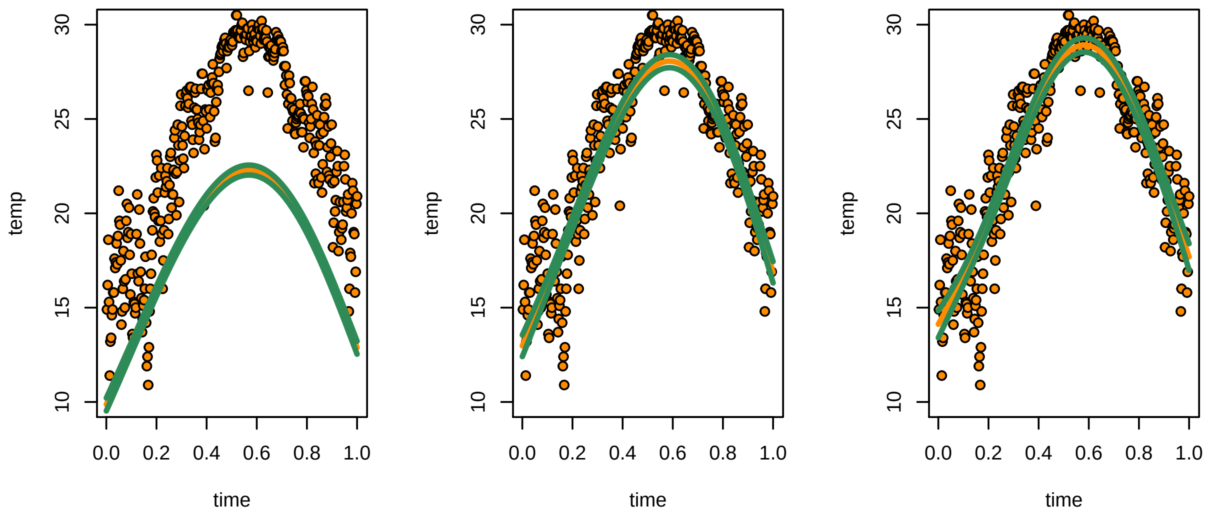
First the effect of changing the value for σ_n is investigated. The tested values for σ_n are 2, 5 and 10. The prior hyperparameters are fixed with σ_f set to 1.5 and ι set to 0.3.



It can be seen that better fits are given for lower values of σ_n. A lower noise standard deviation gives better results, both a better fit and narrower probability bands.

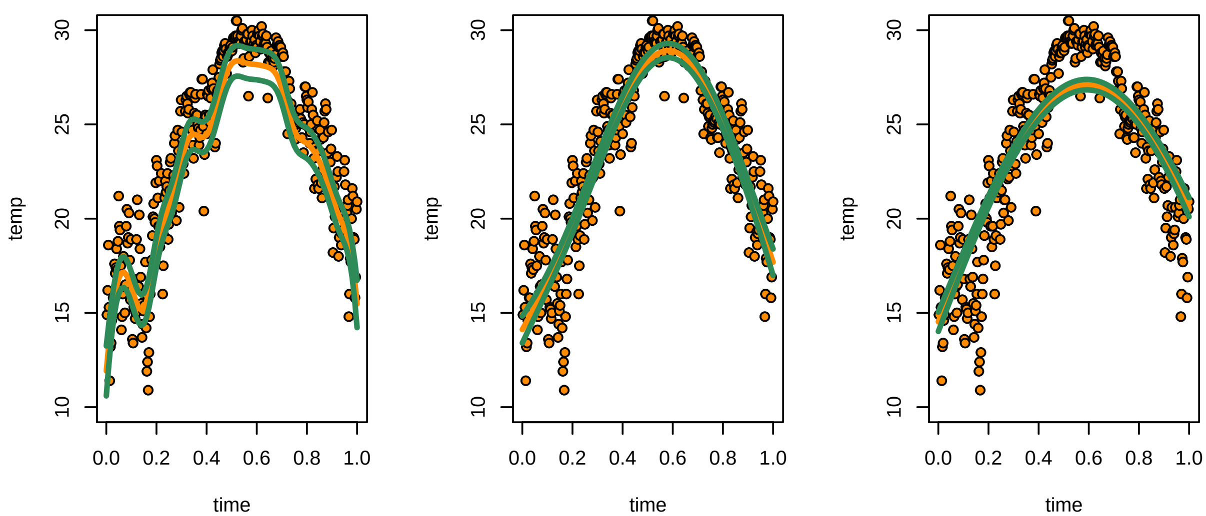
A bad fit for the highest value, a little bit better when equal to 5 and a quite good fit when σ_n is equal to 2. What exactly is it that σ_n affects? Is it flexibility/smoothness, larger variance affects certainty?

The effect of changing the value for σ_f is examined by setting the parameter equal to 0.25, 0.75 or 1.5 whilst the other parameters are fixed (σ_n=2 and ι=0.3).



The effect of changing the value of σ_f looks quite similar to the effect of changing the value of σ_n with the difference that the probability bands remains practically unchanged. Also higher values of σ_f seem to give a better fit, compared to σ_n where lower values resulted in better fits.

Finally, the effect on the posterior when changing the value for the prior hyperparameter ι is examined. The tested values for ι are 0.05, 0.30 and 0.75 while the other parameters are fixed (σ_n=2 and σ_f=1.5).



For a ι value of 0.05 the obtained curve is too flexible, it follows the observd values too well. For a little higher value, 0.30, the curve is more smooth and seem to be a quite good fit. When a even higher value is tested, 0.75, the curve instead becomes to unflexible.

Appendix

R-code

```
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
  fStar <- SqExpKernel(xStar, x, hyperParam) %*% solve(SqExpKernel(x, x, hyperParam)+
                                        sigmaNoise^2*diag(length(x))) %*% y
  # Calculates cov f star
  cov_fStar <- SqExpKernel(xStar, xStar, hyperParam) - SqExpKernel(xStar, x, hyperParam)%*%
    solve(SqExpKernel(x, x, hyperParam)+sigmaNoise^2*diag(length(x))) %*%
    SqExpKernel(x, xStar, hyperParam)

  # Store all values in a list
  val_list <- list(fStar=fStar, 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)
Upper1B <- assign1B$fStar + 1.96 * sqrt(diag(assign1B$cov_fStar))
Lower1B <- assign1B$fStar - 1.96 * sqrt(diag(assign1B$cov_fStar))

plot(y=assign1B$fStar, assign1B$xStar, ylim=c(-2.5,2.5), type="l", lwd=3, col="darkorange")
lines(y=Upper1B, assign1B$xStar, col="seagreen", lwd=3)
lines(y=Lower1B, assign1B$xStar, col="seagreen", lwd=3)
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)
Upper1C <- assign1C$fStar + 1.96 * sqrt(diag(assign1C$cov_fStar))
Lower1C <- assign1C$fStar - 1.96 * sqrt(diag(assign1C$cov_fStar))

plot(y=assign1C$fStar, assign1C$xStar, ylim=c(-2.5,2.5), type="l", lwd=3, col="darkorange")
lines(y=Upper1C, assign1C$xStar, col="seagreen", lwd=3)
lines(y=Lower1C, assign1C$xStar, col="seagreen", lwd=3)
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=s
                        hyperParam=c(1, 0.3),sigmaNoise=0.1)
Upper1D <- assign1D$fStar + 1.96 * sqrt(diag(assign1D$cov_fStar))
Lower1D <- assign1D$fStar - 1.96 * sqrt(diag(assign1D$cov_fStar))

plot(y=assign1D$fStar, assign1D$xStar, ylim=c(-2.5,2.5),type="l", lwd=3, col="darkorange")
lines(y=Upper1D, assign1D$xStar, col="seagreen", lwd=3)
```

```
lines(y=Lower1D, assign1D$xStar, col="seagreen", lwd=3)
assign1E <- PosteriorGP(x=c(0.8, 0.4, -0.2, -0.6, -1), y=c(-0.664, 0.719, -0.94, -0.044, 0.768), xStar=s
                        hyperParam=c(1, 1),sigmaNoise=0.1)
Upper1E <- assign1E$fStar + 1.96 * sqrt(diag(assign1E$cov_fStar))
Lower1E <- assign1E$fStar - 1.96 * sqrt(diag(assign1E$cov_fStar))

plot(y=assign1E$fStar, assign1E$xStar, ylim=c(-2.5,2.5), type="l", lwd=3, col="darkorange")
lines(y=Upper1E, assign1E$xStar, col="seagreen", lwd=3)
lines(y=Lower1E, assign1E$xStar, col="seagreen", lwd=3)
JapanTemp <- read.delim("C:/Users/Gustav/Documents/Machine-Learning/Lab 6/JapanTemp.dat", sep="", heade
par(mfrow=c(1,3))
SigmaVal <- c(2, 5, 10)
for(i in SigmaVal){
  Assign2 <- PosteriorGP(x=JapanTemp$time, y=JapanTemp$temp, xStar=seq(0,1, 0.01),
                       hyperParam=c(1.5, 0.3),sigmaNoise=i)
Upper2 <- Assign2$fStar + 1.96 * sqrt(diag(Assign2$cov_fStar))
Lower2 <- Assign2$fStar - 1.96 * sqrt(diag(Assign2$cov_fStar))

plot(JapanTemp, ylim=c(10,30), pch=21, bg="darkorange")
lines(y=Assign2$fStar, Assign2$xStar, type="l", lwd=3, col="darkorange")
lines(y=Upper2, Assign2$xStar, col="seagreen", lwd=3)
lines(y=Lower2, Assign2$xStar, col="seagreen", lwd=3)
}
par(mfrow=c(1,1))
par(mfrow=c(1,3))
Sigma_fVal <- c(0.25, 0.75, 1.5)
for(i in Sigma_fVal){
Assign2 <- PosteriorGP(x=JapanTemp$time, y=JapanTemp$temp, xStar=seq(0,1, 0.01),
                       hyperParam=c(i, 0.3),sigmaNoise=2)
Upper2 <- Assign2$fStar + 1.96 * sqrt(diag(Assign2$cov_fStar))
Lower2 <- Assign2$fStar - 1.96 * sqrt(diag(Assign2$cov_fStar))

plot(JapanTemp, ylim=c(10,30), pch=21, bg="darkorange")
lines(y=Assign2$fStar, Assign2$xStar, type="l", lwd=3, col="darkorange")
lines(y=Upper2, Assign2$xStar, col="seagreen", lwd=3)
lines(y=Lower2, Assign2$xStar, col="seagreen", lwd=3)
}
par(mfrow=c(1,1))
par(mfrow=c(1,3))
iota <- c(0.05, 0.3, 0.75)
for(i in iota){
Assign2 <- PosteriorGP(x=JapanTemp$time, y=JapanTemp$temp, xStar=seq(0,1, 0.01),
                       hyperParam=c(1.5, i),sigmaNoise=2)
Upper2 <- Assign2$fStar + 1.96 * sqrt(diag(Assign2$cov_fStar))
Lower2 <- Assign2$fStar - 1.96 * sqrt(diag(Assign2$cov_fStar))

plot(JapanTemp, ylim=c(10,30), pch=21, bg="darkorange")
lines(y=Assign2$fStar, Assign2$xStar, type="l", lwd=3, col="darkorange")
lines(y=Upper2, Assign2$xStar, col="seagreen", lwd=3)
lines(y=Lower2, Assign2$xStar, col="seagreen", lwd=3)
}
par(mfrow=c(1,1))
##
```