Profiling Gaussian Processes

Mathematical Formulas

The derivation of Gaussian Process regression formulas are beyond the scope of this portfolio, however formulas are replicated here to aid understanding.

Implementations

Data Generation and Problem Settings

Import the necessary packages. The library `provfis` is a stochastic profiler and can be used to profile our code.

```
library(profvis)
library(tidyverse)
library(MASS)
library(microbenchmark)
```

First, let's decide some parameters and settings such as the amount of training and testing data.

```
# Number of data points for plotting & Bandwidth squared of the RBF kernel
ntest <- 500
# Characteristic Length-scale for kernel
sigmasq <- 1.0
# Number of training points, standard deviation of additive noise
ntrain <- 10
sigma_n <- 0.5
# Define number of samples for prior gp mvn and posterior gp mvn to take
nprior_samples <- 5
npost_samples <- 5
```

Define some helper functions. In particular, the kernel function is a squared exponential. The bandwidth is computed as the median of all pairwise distances. We also define a matrix that applies the squared exponential to rows of two matrices, i.e. it computes the kernel matrix $K(X, Y)$. for two matrices X and Y. Finally, we also have a regression function which represents the true structure of the data. This is just a quintic polynomial for simplicity, but can be replaced by more complicated functions.

```
squared_exponential <- function(x, c, sigmasq){
  return(exp(-0.5*sum((x - c)^2) / sigmasq))
}
kernel_matrix <- function(X, Xstar, sigmasq){
  # compute the kernel matrix
  K <- apply(
    X=Xstar,
    MARGIN=1,
    FUN=function(xstar_row) apply(
      X=X,
      MARGIN=1,
      FUN=squared_exponential,
```

```
      xstar_row,
      sigmasq
      )
    )
  return(K)
}
regression_function <- function(x){
    val <- (x+5)*(x+2)*(x)*(x-4)*(x-3)/10 + 2
  return(val)
}
```

Now let's actually generate some data

```
# training data
xtrain <- matrix(runif(ntrain, min=-5, max=5))
ytrain <- regression_function(xtrain) + matrix(rnorm(ntrain, sd=sigma_n))
# testing data
xtest <- matrix(seq(-5,5, len=ntest))
```

Naive Vectorized Implementation

The firt implementation that we look at is naive in the sense that it basically blindly copies the operations. This means that we invert $K + \sigma_n^2 I$ directly.

```
source("gp_naive.R", keep.source = TRUE)
profvis(result <- gp_naive(xtrain, ytrain, xtest, sigma_n, sigmasq))
```

Smart Implementation

This implementation can also be used *online*. It is recommended in the "Gaussian Processes for Machine Learning" book.

```
source("gp_online.R", keep.source = TRUE)
profvis(result_online <- gp_online(xtrain, ytrain, xtest, sigma_n, sigmasq))
```

Implementation using a vectorized kernel matrix

We can see that most of the time is spent computing the kernel matrix. We can therefore find a faster way to compute it as follows

```
kernel_matrix_vectorized <- function(X, sigmasq, Y=NULL){
  if (is.null(Y)){
    Y <- X
  }
  n <- nrow(X)
  m <- nrow(Y)
  # Find three matrices above
  Xnorm <- matrix(apply(X^2, 1, sum), n, m)
  Ynorm <- matrix(apply(Y^2, 1, sum), n, m, byrow=TRUE)
  XY <- tcrossprod(X, Y)
  return(exp(-(Xnorm - 2*XY + Ynorm) / (2*sigmasq)))
}
```

using this, we get

```
source("gp_online_vect.R", keep.source = TRUE)
profvis(gp_online_vect(xtrain, ytrain, xtest, sigma_n, sigmasq))
```

We can see that this implementation uses much less memory and it's much faster.

Completely vectorized implementation

We can combine these ideas to obtain a much faster implementation.

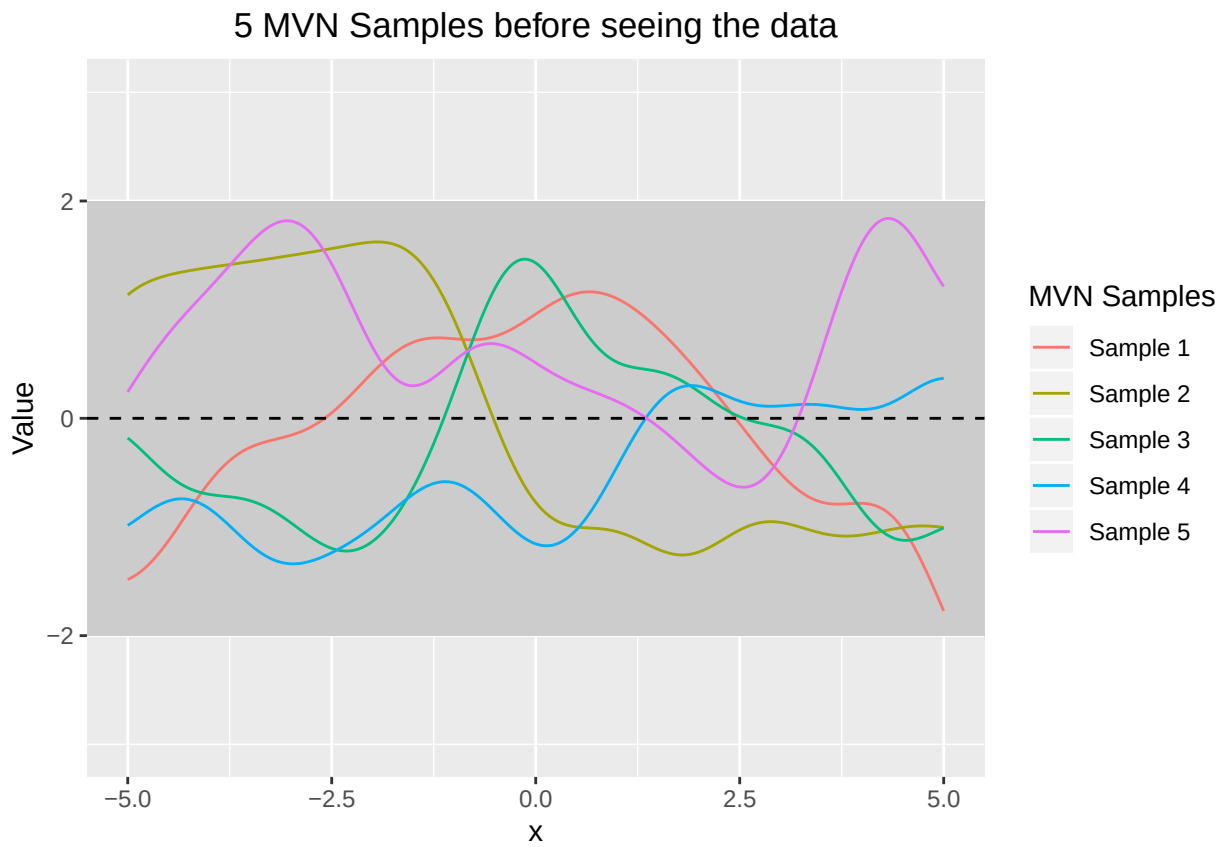
```
source("gp_completely_vectorized.R", keep.source = TRUE)
profvis(gp_completely_vectorized(xtrain, ytrain, xtest, sigma_n, sigmasq), interval=0.005)
```

Visualizations

Before seeing training data

Before seeing the training data we only have the test data. The Gaussian Process will therefore predict random (smooth) functions with mean zero.

```
Kss <- kernel_matrix_vectorized(xtest, sigmasq)
# Sample nprior_samples Multivariate Normals with mean zero and variance-covariance
# being the kernel matrix
data.frame(x=xtest, t(mvrnorm(nprior_samples, rep(0, length=ntest), Kss))) %>%
  setNames(c("x", sprintf("Sample %s", 1:nprior_samples))) %>%
  gather("MVN Samples", "Value", -x) %>%
  ggplot(aes(x=x, y=Value)) +
    # Because diag(Kss) are all 1s. We use mean +\- 2*standard deviation
    geom_rect(xmin=-Inf, xmax=Inf, ymin=-2, ymax=2, fill="grey80") +
    geom_line(aes(color=`MVN Samples`)) +
    geom_abline(slope=0.0, intercept=0.0, lty=2) +
    scale_y_continuous(lim=c(-3, 3)) +
    labs(title=paste(nprior_samples, "MVN Samples before seeing the data")) +
    theme(plot.title=element_text(hjust=0.5))
```



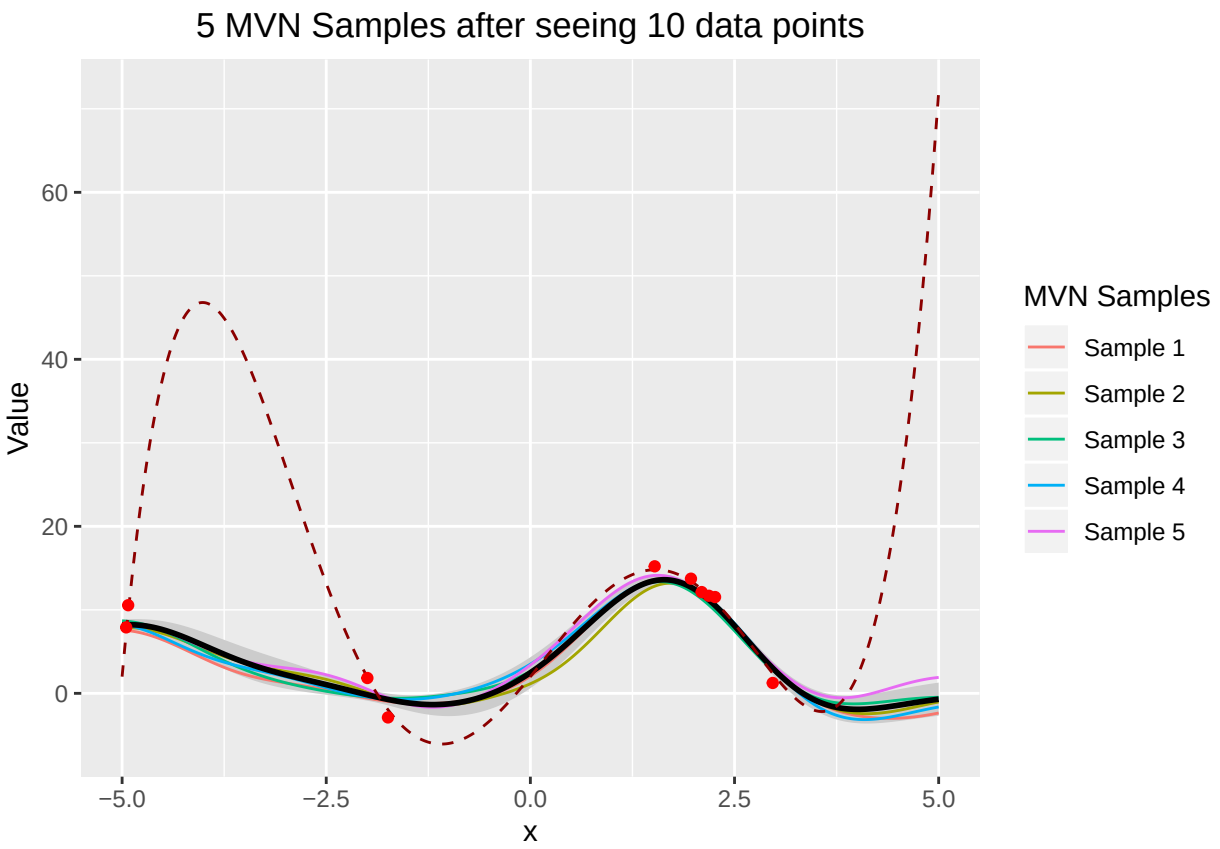
After seeing training data

We only need to find the predicted mean and the predicted variance.

```
# Get predicitons. To predict noisy data just add sigma_n^2*diag(ncol(xtest)) to the covariance matrix
# as implemented in the script `gp_completely_vectorized_noisy.R`.
results <- gp_completely_vectorized(xtrain, ytrain, xtest, sigma_n, sigmasq)

gpmean <- results[[1]]
gpvcov <- results[[2]]
# for plotting
dftrain = data.frame(xtrain=xtrain, ytrain=ytrain)
# Plot
data.frame(x=xtest, t(mvrnorm(npost_samples, gpmean, gpvcov))) %>%
  setNames(c("x", sprintf("Sample %s", 1:npost_samples))) %>%
  mutate(ymin=gpmean-2*sqrt(diag(gpvcov)), ymax=gpmean+2*sqrt(diag(gpvcov)),
         gpmean=gpmean, ytrue=regression_function(xtest)) %>%
  gather("MVN Samples", "Value", -x, -ymin, -ymax, -gpmean, -ytrue) %>%
  ggplot(aes(x=x, y=Value)) +
    geom_ribbon(aes(ymin=ymin, ymax=ymax), fill="grey80") +
    geom_line(aes(color=`MVN Samples`)) +
    geom_line(aes(y=gpmean), size=1) +
    geom_line(aes(y=ytrue), color="darkred", lty=2) +
    geom_point(data=dftrain, aes(x=xtrain, y=ytrain), color="red") +
    ggtitle(paste(npost_samples, "MVN Samples after seeing", ntrain, "data points")) +
```

```
    theme(plot.title=element_text(hjust=0.5))
```



Note on Vectorized Kernel Matrix

One might wonder why in the function `kernel_matrix_vectorized()` we fill the matrix `Ynorm` by row. Afterall `R` works with column-major storage so this should be inefficient. One can compare filling in a matrix by row versus filling it by column and then taking the transpose in different cases:

- Number of rows $<$ Number of columns

```
nrows <- 100
ncols <- 1000
microbenchmark(
  matrix(0, nrows, ncols, byrow=TRUE),
  t(matrix(0, nrows, ncols))
  )
```

- Number of rows $=$ Number of columns

```
nrows <- 1000
ncols <- 1000
microbenchmark(
```

```
  matrix(0, nrows, ncols, byrow=TRUE),
  t(matrix(0, nrows, ncols))
  )
```

- Number of rows > Number of columns

```
nrows <- 1000
ncols <- 100
microbenchmark(
  matrix(0, nrows, ncols, byrow=TRUE),
  t(matrix(0, nrows, ncols))
  )
```

Generally, `byrow=TRUE` is faster, except when the number of rows is smaller than the number of columns. One could see if implementing an if-statement checking for `n<m` and then using `t()` rather than `byrow=TRUE` would lead to serious performance improvement.