

# Assessment\_2

2023-03-15

## Kernel Methods For Regression

### Part 1

#### Question 1

The Gaussian kernel is an example of a kernel for which the model is identifiable. The model is unidentifiable for the kernel:  $k(x, y) = 1$  for  $x, y \in \mathbb{R}^p$ . This kernel is positive semi-definite and by the Moore-Aronszajn theorem there exists a unique RKHS for which  $k$  is the reproducing kernel. In this RKHS all the functions are constant, let's pick two functions  $f_1, f_2 \in H_k$  where  $f_1(x) = c, f_2(x) = d$  for all  $x \in \mathcal{X}$ . Then if we let the  $\alpha$  we use with  $f_2$ ,  $\alpha_2 = \alpha_1 - d + c$ , where  $\alpha_1$  is the  $\alpha$  we use with  $f_1$ , then these are the same model. Hence our model is unidentifiable.

#### Question 2

We have for some  $f \in H_k$ :  $f = f_1 + f_2$ , for some  $f_1 \in \tilde{H}, f_2 \in \tilde{H}^\perp$ . By orthogonality:

$$\|f_1 + f_2\|^2 = \|f_1\|^2 + \|f_2\|^2$$

And by the reproducing property:

$$\begin{aligned} & \frac{1}{2n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + (f_1 + f_2)(x_i^0)), \phi) \\ &= \frac{1}{2n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + f_1(x_i^0)), \phi) \end{aligned}$$

Combining the above,

$$\begin{aligned} & \frac{1}{2n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + (f_1 + f_2)(x_i^0)), \phi) - \lambda \|f_1 + f_2\|^2 \\ &= \frac{1}{2n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + f_1(x_i^0)), \phi) - \lambda \|f_1\|^2 + \lambda \|f_2\|^2 \\ &\geq \frac{1}{2n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + f_1(x_i^0)), \phi) - \lambda \|f_1\|^2 \end{aligned}$$

Hence, we have that  $\hat{f}_\lambda \in \tilde{H}$  and therefore can write  $\hat{f}_\lambda$  as a linear combination of  $k(x_1^0, \cdot), \dots, k(x_n^0, \cdot)$  therefore we can write:

$$\hat{f}_\lambda = \sum_{i=1}^n \hat{\beta}_{\lambda, i} k(x_i^0, \cdot)$$

### Question 3

We have that,

$$\begin{aligned}
-\lambda \|f\|_{H_k}^2 &= -\lambda \left\| \sum_{i=1}^n \beta_{\lambda,i} k(x_i^0, \cdot) \right\|_{H_k}^2 \\
&= -\lambda \left\langle \sum_{i=1}^n \beta_{\lambda,i} k(x_i^0, \cdot), \sum_{j=1}^n \beta_{\lambda,j} k(x_j^0, \cdot) \right\rangle_k \\
&= -\lambda \sum_{i=1}^n \beta_{\lambda,i} \left\langle k(x_i^0, \cdot), \sum_{j=1}^n \beta_{\lambda,j} k(x_j^0, \cdot) \right\rangle_k \\
&= -\lambda \sum_{i=1}^n \sum_{j=1}^n \beta_{\lambda,i} \beta_{\lambda,j} \left\langle k(x_i^0, \cdot), k(x_j^0, \cdot) \right\rangle_k \\
&= -\lambda \sum_{i=1}^n \sum_{j=1}^n \beta_{\lambda,i} \beta_{\lambda,j} k(x_i^0, x_j^0) \\
&= -\lambda \beta_{\lambda}^T K \beta_{\lambda}
\end{aligned}$$

Where  $K = [k(x_i^0, x_j^0)]_{i,j}$ . Hence we can rewrite (2) as:

$$\frac{1}{2n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + \beta_{\lambda}^T \cdot K^{(i)}), \phi) - \lambda \beta_{\lambda}^T K \beta_{\lambda}$$

### Question 4

Let  $m < n + 2$ , consider the optimization problem posed in the previous question, the Nyronstrom method involves reducing the dimension of the gram matrix,  $K$ , hence reducing the dimensionality of the optimization problem. We will approximate the kernel,  $k$ , by  $\tilde{k}^{(m)}$  such that the matrix  $\tilde{K}^{(m)}$  obtained by replacing  $k$  with  $\tilde{k}^{(m)}$  has rank  $\leq m$ . We will let,

$$\tilde{k}^{(m)}(x, x') = k_m(x)^T (K_m)^{-1} k_m(x')$$

where  $K_m$  is the first  $m$  rows and columns of  $K$  and

$$k_m(x) = (k(x_1^0, x), \dots, k(x_m^0, x))$$

Let's now rewrite  $f$  using our new kernel:

$$\begin{aligned}
f_{\lambda}(x) &\approx \beta_{\lambda}^T \tilde{k}^{(m)}(x) \\
&= \beta_{\lambda}^T K(X_{1:m}, X)^T (K_m^0)^{-1} K(X_{1:m}, x) \\
&= \gamma^T (K_m^0)^{-1} K(X_{1:m}, x)
\end{aligned}$$

where  $K(A, B) = [k(a_i, b_j)]_{i,j}$ ,  $X$  is our data matrix where  $X_{1:m}$  means the data matrix including only the first  $m$  datapoints and we let  $\gamma^T = \beta_{\lambda}^T K(X_{1:m}, X)^T$ . Let's now rewrite the penalty:

$$\begin{aligned}
-\lambda \beta_{\lambda}^T K \beta_{\lambda} &\approx -\lambda \beta_{\lambda}^T \tilde{K}^{(m)} \beta_{\lambda} \\
&= -\lambda \beta_{\lambda}^T K(X_{1:m}, X)^T (K_m^0)^{-1} K(X_{1:m}, X) \beta_{\lambda} \\
&= -\lambda \gamma^T (K_m^0)^{-1} \gamma
\end{aligned}$$

This leaves us with the following optimization problem,

$$\arg \max_{\alpha \in \mathbb{R}, \phi \in (0, \inf), \gamma \in \mathbb{R}^m} \frac{1}{2n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + \gamma^T (K_m^0)^{-1} K(X_{1:m}, x_i^0)), \phi) - \lambda \gamma^T (K_m^0)^{-1} \gamma$$

## Question 5

Let's first find the spectral decomposition of  $(K_m^0)^{-1}$ ,

$$(K_m^0)^{-1} = S\Lambda S^{-1}$$

Then we can write,

$$\gamma^T (K_m^0)^{-1} \gamma = \gamma^T S^{-T} \Lambda S^{-1} \gamma = \|\Lambda^{\frac{1}{2}} S^{-1} \gamma\|_2^2$$

Glmnet estimates parameters that minimize the following (if using the ridge penalty):

$$-\frac{1}{n} \sum_{i=1}^n \log f(y_i; g^{-1}(\alpha + \gamma^T X_i), \phi) + \frac{\lambda}{2} \|\gamma_{glm}\|_2^2$$

which is the same as maximizing optimization problem as ours, except for if we instead try to find the minimum of the negative of our optimization problem, a factor of two and if we substitute for  $\gamma_{glm}$ . We have that,

$$\begin{aligned} \gamma_{glm} &= \Lambda^{\frac{1}{2}} S \gamma \\ \Rightarrow \gamma &= S^{-1} \Lambda^{-\frac{1}{2}} \gamma_{glm} \end{aligned}$$

Therefore we can find our value for  $\gamma$  using the estimate we get from glmnet where for  $X_i$  we use  $(K_m^0)^{-1} K(X_{1:m}, x_i^0)$ .

## Part 2

We are going to use the wesdr dataset:

```
library(gss)
data(wesdr)
head(wesdr)
```

```
##      dur  gly  bmi  ret
## 1 10.3 13.7 23.8    0
## 2  9.9 13.5 23.5    0
## 3 15.6 13.8 24.8    0
## 4 26.0 13.0 21.6    1
## 5 13.8 11.1 24.6    1
## 6 31.1 11.3 24.6    1
```

Let's now split it into a testing and training set:

```
n.test <- round(0.15 * nrow(wesdr))
test_ind <- sample(seq_len(nrow(wesdr)), size = n.test)

train <- wesdr[-test_ind, ]
test <- wesdr[test_ind, ]
```

## Question 6

We are going to use a binomial distribution as we are modelling a response variable that is either 0 or 1, we are going to set  $\alpha = 0$  so that we are using the ridge penalty and we will use the radial basis kernel function for which the model is identifiable.

```
library(glmnet)
```

```
## Loading required package: Matrix
## Loaded glmnet 4.1-6
```

```

library(kernlab)

gaussian_kernel <- function(x, y, sigma) {
  exp(-sum((x - y)^2) / (2*sigma^2))
}

fit_model <- function(X, y, lambda, sigma, m){
  n <- nrow(X)
  rbf <- rbfdot(sigma = sigma)
  K <- kernelMatrix(rbf, X)
  K_m_inverse <- solve(K[1:m, 1:m])
  K_mn <- matrix(0, m, n)
  X_m <- X[1:m,]
  for (i in 1:m) {
    for (j in 1:n) {
      K_mn[i,j] <- gaussian_kernel(X_m[i,], X[j,], sigma)
    }
  }
  input <- t(K_m_inverse %*% K_mn)
  results <- glmnet(input, y, family = "binomial", alpha = 0, lambda = lambda)
  gamma_glm <- results$beta

  eig <- eigen(K_m_inverse)
  S <- eig$vectors
  L <- diag(eig$values)

  gamma <- solve(S) %*% sqrt(solve(L)) %*% gamma_glm
  list(gamma = gamma, results= results)
}

X <- as.matrix(train[,-4])
y <- train[,4]
head(fit_model(X, y, 0.1, 1, 50))

## $gamma
## 50 x 1 Matrix of class "dgeMatrix"
##           s0
## [1,] -1.60440236
## [2,]  1.91049004
## [3,]  1.20842762
## [4,]  0.06052861
## [5,]  0.66606875
## [6,] -0.46944090
## [7,]  2.01952518
## [8,] -0.31374185
## [9,] -2.74610904
## [10,]  1.08667732
## [11,]  0.87790162
## [12,] -0.33901408
## [13,] -0.26918396
## [14,]  0.37501646
## [15,]  0.32290458
## [16,]  0.03496745
## [17,] -1.80486805

```

```
## [18,] 0.63346531
## [19,] 2.02958252
## [20,] 0.77003666
## [21,] 1.07216753
## [22,] -1.36466366
## [23,] 1.75448879
## [24,] -2.80198283
## [25,] 3.11027165
## [26,] 0.53932317
## [27,] 0.86212862
## [28,] 2.60839961
## [29,] -1.29322286
## [30,] -0.25718187
## [31,] -2.01565360
## [32,] -1.64046870
## [33,] 1.61240689
## [34,] -2.80782100
## [35,] -1.69175051
## [36,] -0.08286890
## [37,] 0.61514286
## [38,] -1.07512878
## [39,] 0.18112783
## [40,] -0.19490723
## [41,] 2.56773697
## [42,] -0.41486552
## [43,] 0.56424404
## [44,] 1.31427989
## [45,] 2.72301774
## [46,] 0.48488163
## [47,] 1.20385634
## [48,] -0.45302684
## [49,] 1.57948177
## [50,] -3.12751456
##
## $results
##
## Call: glmnet(x = input, y = y, family = "binomial", alpha = 0, lambda = lambda)
##
##      Df    %Dev Lambda
## 1 50 12.37    0.1
```

## Question 7

Let's fit our model using a grid of parameters to see for which parameters it works and doesn't and to identify which (if any) parameters lead to errors.

```
# Define the parameter values to search over
lambda_range <- c(0.001, 0.01, 0.1, 0.5, 1.0, 2, 5, 10, 100, 1000, 10000)
sigma_range <- c(0.01, 0.1, 1.0)
m_range <- c(2, 5, 10, 20, 100, 400)

# Generate all combinations of parameters
param_combinations <- expand.grid(lambda_range, sigma_range, m_range)

# Loop through each parameter combination and calculate the score
```

```

for (i in 1:nrow(param_combinations)) {
  lambda_val <- param_combinations[i, 1]
  sigma_val <- param_combinations[i, 2]
  m_val <- param_combinations[i, 3]
  cat("Current parameters: lambda=", lambda_val, ", sigma=", sigma_val, ", m=", m_val, "\n")
  # Call function to calculate score using the current parameters
  gamma <- fit_model(X, y, lambda_val, sigma_val, m_val)
}

```

```

## Current parameters: lambda= 0.001 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.01 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.1 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.5 , sigma= 0.01 , m= 2
## Current parameters: lambda= 1 , sigma= 0.01 , m= 2
## Current parameters: lambda= 2 , sigma= 0.01 , m= 2
## Current parameters: lambda= 5 , sigma= 0.01 , m= 2
## Current parameters: lambda= 10 , sigma= 0.01 , m= 2
## Current parameters: lambda= 100 , sigma= 0.01 , m= 2
## Current parameters: lambda= 1000 , sigma= 0.01 , m= 2
## Current parameters: lambda= 10000 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.001 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.01 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.1 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.5 , sigma= 0.1 , m= 2
## Current parameters: lambda= 1 , sigma= 0.1 , m= 2
## Current parameters: lambda= 2 , sigma= 0.1 , m= 2
## Current parameters: lambda= 5 , sigma= 0.1 , m= 2
## Current parameters: lambda= 10 , sigma= 0.1 , m= 2
## Current parameters: lambda= 100 , sigma= 0.1 , m= 2
## Current parameters: lambda= 1000 , sigma= 0.1 , m= 2
## Current parameters: lambda= 10000 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.001 , sigma= 1 , m= 2
## Current parameters: lambda= 0.01 , sigma= 1 , m= 2
## Current parameters: lambda= 0.1 , sigma= 1 , m= 2
## Current parameters: lambda= 0.5 , sigma= 1 , m= 2
## Current parameters: lambda= 1 , sigma= 1 , m= 2
## Current parameters: lambda= 2 , sigma= 1 , m= 2
## Current parameters: lambda= 5 , sigma= 1 , m= 2
## Current parameters: lambda= 10 , sigma= 1 , m= 2
## Current parameters: lambda= 100 , sigma= 1 , m= 2
## Current parameters: lambda= 1000 , sigma= 1 , m= 2
## Current parameters: lambda= 10000 , sigma= 1 , m= 2
## Current parameters: lambda= 0.001 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.01 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.1 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.5 , sigma= 0.01 , m= 5
## Current parameters: lambda= 1 , sigma= 0.01 , m= 5
## Current parameters: lambda= 2 , sigma= 0.01 , m= 5
## Current parameters: lambda= 5 , sigma= 0.01 , m= 5
## Current parameters: lambda= 10 , sigma= 0.01 , m= 5
## Current parameters: lambda= 100 , sigma= 0.01 , m= 5
## Current parameters: lambda= 1000 , sigma= 0.01 , m= 5
## Current parameters: lambda= 10000 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.001 , sigma= 0.1 , m= 5

```



[illegible]



```
## Current parameters: lambda= 10000 , sigma= 0.1 , m= 100
## Current parameters: lambda= 0.001 , sigma= 1 , m= 100
## Current parameters: lambda= 0.01 , sigma= 1 , m= 100
## Current parameters: lambda= 0.1 , sigma= 1 , m= 100
## Current parameters: lambda= 0.5 , sigma= 1 , m= 100
## Current parameters: lambda= 1 , sigma= 1 , m= 100
## Current parameters: lambda= 2 , sigma= 1 , m= 100
## Current parameters: lambda= 5 , sigma= 1 , m= 100
## Current parameters: lambda= 10 , sigma= 1 , m= 100
## Current parameters: lambda= 100 , sigma= 1 , m= 100
## Current parameters: lambda= 1000 , sigma= 1 , m= 100
## Current parameters: lambda= 10000 , sigma= 1 , m= 100
## Current parameters: lambda= 0.001 , sigma= 0.01 , m= 400
```

```
## Error in solve.default(K[1:m, 1:m]): system is computationally singular: reciprocal condition number
```

From the above we see that it works for a large range of values for lambda and sigma, however, when m get's too large we are getting an error. This is happening when we try and invert our matrix  $K_m$ , we can fix this by adding some small  $\epsilon$  to the diagonal of this matrix, let's modify our function to include this:

```
fit_model <- function(X, y, lambda, sigma, m, eps=0.0001){
  n <- nrow(X)
  rbf <- rbfdot(sigma = sigma)
  K <- kernelMatrix(rbf, X)
  K_m_inverse <- solve(K[1:m, 1:m] + diag(m) * eps)
  K_mn <- matrix(0, m, n)
  X_m <- X[1:m,]
  for (i in 1:m) {
    for (j in 1:n) {
      K_mn[i,j] <- gaussian_kernel(X_m[i,], X[j,], sigma)
    }
  }
  input <- t(K_m_inverse %*% K_mn)
  results <- glmnet(input, y, family = "binomial" , alpha = 0, lambda = lambda)
  gamma_glm <- results$beta

  eig <- eigen(K_m_inverse)
  S <- eig$vectors
  L <- diag(eig$values)

  gamma <- solve(S) %*% sqrt(solve(L)) %*% gamma_glm
  list(gamma = gamma, results= results)
}
```

Let's now try our grid search to see if our function now works for large values of m:

```
# Define the parameter values to search over
lambda_range <- c(0.001, 0.01, 0.1, 0.5, 1.0, 2, 5, 10, 100, 1000, 10000)
sigma_range <- c(0.01, 0.1, 1.0)
m_range <- c(2, 5, 10, 20, 100, 400)

# Generate all combinations of parameters
param_combinations <- expand.grid(lambda_range, sigma_range, m_range)

# Loop through each parameter combination and calculate the score
for (i in 1:nrow(param_combinations)) {
```

```

lambda_val <- param_combinations[i, 1]
sigma_val <- param_combinations[i, 2]
m_val <- param_combinations[i, 3]
cat("Current parameters: lambda=", lambda_val, ", sigma=", sigma_val, ", m=", m_val, "\n")
# Call function to calculate score using the current parameters
gamma <- fit_model(X, y, lambda_val, sigma_val, m_val)
}

## Current parameters: lambda= 0.001 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.01 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.1 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.5 , sigma= 0.01 , m= 2
## Current parameters: lambda= 1 , sigma= 0.01 , m= 2
## Current parameters: lambda= 2 , sigma= 0.01 , m= 2
## Current parameters: lambda= 5 , sigma= 0.01 , m= 2
## Current parameters: lambda= 10 , sigma= 0.01 , m= 2
## Current parameters: lambda= 100 , sigma= 0.01 , m= 2
## Current parameters: lambda= 1000 , sigma= 0.01 , m= 2
## Current parameters: lambda= 10000 , sigma= 0.01 , m= 2
## Current parameters: lambda= 0.001 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.01 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.1 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.5 , sigma= 0.1 , m= 2
## Current parameters: lambda= 1 , sigma= 0.1 , m= 2
## Current parameters: lambda= 2 , sigma= 0.1 , m= 2
## Current parameters: lambda= 5 , sigma= 0.1 , m= 2
## Current parameters: lambda= 10 , sigma= 0.1 , m= 2
## Current parameters: lambda= 100 , sigma= 0.1 , m= 2
## Current parameters: lambda= 1000 , sigma= 0.1 , m= 2
## Current parameters: lambda= 10000 , sigma= 0.1 , m= 2
## Current parameters: lambda= 0.001 , sigma= 1 , m= 2
## Current parameters: lambda= 0.01 , sigma= 1 , m= 2
## Current parameters: lambda= 0.1 , sigma= 1 , m= 2
## Current parameters: lambda= 0.5 , sigma= 1 , m= 2
## Current parameters: lambda= 1 , sigma= 1 , m= 2
## Current parameters: lambda= 2 , sigma= 1 , m= 2
## Current parameters: lambda= 5 , sigma= 1 , m= 2
## Current parameters: lambda= 10 , sigma= 1 , m= 2
## Current parameters: lambda= 100 , sigma= 1 , m= 2
## Current parameters: lambda= 1000 , sigma= 1 , m= 2
## Current parameters: lambda= 10000 , sigma= 1 , m= 2
## Current parameters: lambda= 0.001 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.01 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.1 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.5 , sigma= 0.01 , m= 5
## Current parameters: lambda= 1 , sigma= 0.01 , m= 5
## Current parameters: lambda= 2 , sigma= 0.01 , m= 5
## Current parameters: lambda= 5 , sigma= 0.01 , m= 5
## Current parameters: lambda= 10 , sigma= 0.01 , m= 5
## Current parameters: lambda= 100 , sigma= 0.01 , m= 5
## Current parameters: lambda= 1000 , sigma= 0.01 , m= 5
## Current parameters: lambda= 10000 , sigma= 0.01 , m= 5
## Current parameters: lambda= 0.001 , sigma= 0.1 , m= 5
## Current parameters: lambda= 0.01 , sigma= 0.1 , m= 5

```



[illegible]

```

## Current parameters: lambda= 0.001 , sigma= 1 , m= 100
## Current parameters: lambda= 0.01 , sigma= 1 , m= 100
## Current parameters: lambda= 0.1 , sigma= 1 , m= 100
## Current parameters: lambda= 0.5 , sigma= 1 , m= 100
## Current parameters: lambda= 1 , sigma= 1 , m= 100
## Current parameters: lambda= 2 , sigma= 1 , m= 100
## Current parameters: lambda= 5 , sigma= 1 , m= 100
## Current parameters: lambda= 10 , sigma= 1 , m= 100
## Current parameters: lambda= 100 , sigma= 1 , m= 100
## Current parameters: lambda= 1000 , sigma= 1 , m= 100
## Current parameters: lambda= 10000 , sigma= 1 , m= 100
## Current parameters: lambda= 0.001 , sigma= 0.01 , m= 400
## Current parameters: lambda= 0.01 , sigma= 0.01 , m= 400
## Current parameters: lambda= 0.1 , sigma= 0.01 , m= 400
## Current parameters: lambda= 0.5 , sigma= 0.01 , m= 400
## Current parameters: lambda= 1 , sigma= 0.01 , m= 400
## Current parameters: lambda= 2 , sigma= 0.01 , m= 400
## Current parameters: lambda= 5 , sigma= 0.01 , m= 400
## Current parameters: lambda= 10 , sigma= 0.01 , m= 400
## Current parameters: lambda= 100 , sigma= 0.01 , m= 400
## Current parameters: lambda= 1000 , sigma= 0.01 , m= 400
## Current parameters: lambda= 10000 , sigma= 0.01 , m= 400
## Current parameters: lambda= 0.001 , sigma= 0.1 , m= 400
## Current parameters: lambda= 0.01 , sigma= 0.1 , m= 400
## Current parameters: lambda= 0.1 , sigma= 0.1 , m= 400
## Current parameters: lambda= 0.5 , sigma= 0.1 , m= 400
## Current parameters: lambda= 1 , sigma= 0.1 , m= 400
## Current parameters: lambda= 2 , sigma= 0.1 , m= 400
## Current parameters: lambda= 5 , sigma= 0.1 , m= 400
## Current parameters: lambda= 10 , sigma= 0.1 , m= 400
## Current parameters: lambda= 100 , sigma= 0.1 , m= 400
## Current parameters: lambda= 1000 , sigma= 0.1 , m= 400
## Current parameters: lambda= 10000 , sigma= 0.1 , m= 400
## Current parameters: lambda= 0.001 , sigma= 1 , m= 400
## Current parameters: lambda= 0.01 , sigma= 1 , m= 400
## Current parameters: lambda= 0.1 , sigma= 1 , m= 400
## Current parameters: lambda= 0.5 , sigma= 1 , m= 400
## Current parameters: lambda= 1 , sigma= 1 , m= 400
## Current parameters: lambda= 2 , sigma= 1 , m= 400
## Current parameters: lambda= 5 , sigma= 1 , m= 400
## Current parameters: lambda= 10 , sigma= 1 , m= 400
## Current parameters: lambda= 100 , sigma= 1 , m= 400
## Current parameters: lambda= 1000 , sigma= 1 , m= 400
## Current parameters: lambda= 10000 , sigma= 1 , m= 400

```

It does! we have solved our problem.

## Question 8

This function will compute the approximate solution to (2) for any  $c \in C$  and integer  $m \leq n + 2$  where lambda is chosen using 10-fold cross validation using the missclassification error, here is the function and it ran on an example so we can check it works:

```

fit_model_cv_1 <- function(X, y, sigma, m, eps=0.0001){
  n <- nrow(X)

```

```

rbf <- rbfdot(sigma = sigma)
K <- kernelMatrix(rbf, X)
K_m_inverse <- solve(K[1:m, 1:m] + diag(m) * eps)
K_mn <- matrix(0, m, n)
X_m <- X[1:m,]
for (i in 1:m) {
  for (j in 1:n) {
    K_mn[i,j] <- gaussian_kernel(X_m[i,], X[j,], sigma)
  }
}
input <- t(K_m_inverse %*% K_mn)
cv <- cv.glmnet(input, y, family = "binomial", alpha = 0)
lambda <- cv$lambda.min
fit_model(X, y, lambda, sigma, m)
}

X <- as.matrix(train[,-4])
y <- train[,4]
head(fit_model_cv_1(X, y, 1, 50))

```

```

## $gamma
## 50 x 1 Matrix of class "dgeMatrix"
##           s0
## [1,] -0.462820836
## [2,]  0.544547657
## [3,]  0.425338129
## [4,] -0.028036385
## [5,]  0.157677908
## [6,] -0.016263649
## [7,]  0.587411472
## [8,] -0.104811440
## [9,] -0.759762262
## [10,] 0.310796763
## [11,] 0.305467560
## [12,] -0.082385046
## [13,] 0.073586168
## [14,] 0.192698613
## [15,] 0.152727165
## [16,] 0.096630815
## [17,] -0.560821716
## [18,] 0.227131256
## [19,] 0.652098766
## [20,] 0.266057458
## [21,] 0.375983270
## [22,] -0.464892968
## [23,] -0.520344105
## [24,] -0.888896221
## [25,] 0.795010099
## [26,] -0.319793781
## [27,] 0.346037199
## [28,] -0.094992874
## [29,] 1.020163420
## [30,] -0.103809474
## [31,] -0.687727390

```

```
## [32,] -0.531075087
## [33,]  0.559736015
## [34,] -0.876601438
## [35,] -0.617213273
## [36,] -0.002724833
## [37,]  0.150899788
## [38,] -0.384154937
## [39,] -0.089217641
## [40,]  0.079449029
## [41,] -0.812630340
## [42,]  0.134488197
## [43,]  0.204006779
## [44,]  0.527285532
## [45,] -1.030757128
## [46,]  0.219829510
## [47,]  0.490800236
## [48,] -0.114128234
## [49,]  0.614800959
## [50,] -1.107081754
##
## $results
##
## Call:  glmnet(x = input, y = y, family = "binomial", alpha = 0, lambda = lambda)
##
##      Df %Dev Lambda
## 1 50 5.71 0.7098
```

## Question 9

Let's now make it so that sigma is also chosen by cross-validation, here is the function:

```
predict_our_model <- function(fit, train_X, test_X, sigma, m, eps=0.0001){
  n <- nrow(test_X)
  rbf <- rbfdot(sigma = sigma)
  K <- kernelMatrix(rbf, train_X)
  K_m_inverse <- solve(K[1:m, 1:m] + diag(m) * eps)
  K_mn <- matrix(0, m, n)
  X_m <- train_X[1:m,]
  for (i in 1:m) {
    for (j in 1:n) {
      K_mn[i,j] <- gaussian_kernel(X_m[i,], test_X[j,], sigma)
    }
  }
  input <- t(K_m_inverse %*% K_mn)

  out <- predict(fit$results, newx=input)
  ifelse(out>0.5, 1, 0)
}

fit_model_cv_l_sigma <- function(X, y, m, sigma_list=c(0.01, 0.1, 1.0)) {

  # initialize variables to store the best parameter and misclassification error
  best_param <- NULL
  best_error <- Inf
  best_fit <- NULL
```

```

# loop over the parameter values
for (i in 1:length(sigma_list)) {

  # set the parameter value
  sigma <- sigma_list[i]

  # carry out cross-validation using the misclassification error
  folds <- cut(seq(1,nrow(X)), breaks=10, labels=FALSE)
  misclass_error <- rep(NA, 10)
  for (j in 1:10) {
    test_idx <- which(folds == j)
    train_idx <- which(folds != j)
    train_data <- X[train_idx, ]
    test_data <- X[test_idx, ]
    train_y <- y[train_idx]
    test_y <- y[test_idx]
    fit <- fit_model_cv_l(train_data, train_y, sigma, m)
    pred <- predict_our_model(fit, X, test_data, sigma, m)
    misclass_error[j] <- mean(pred != test_y)
  }
  mean_misclass_error <- mean(misclass_error)

  # check if the current parameter gives a lower mean misclassification error than the previous best
  if (mean_misclass_error < best_error) {
    best_param <- sigma_list[i]
    best_error <- mean_misclass_error
    best_fit <- fit
  }
}

# return the best parameter value and misclassification error as a list
best_fit[["sigma"]] = best_param
best_fit[["MisclassificationError"]] = best_error
return(best_fit)
}

X <- as.matrix(train[,-4])
y <- train[,4]
head(fit_model_cv_l_sigma(X, y, 50))

```

```

## $gamma
## 50 x 1 Matrix of class "dgeMatrix"
##           s0
## [1,] -2.251361e-06
## [2,]  3.976049e-06
## [3,]  5.603991e-06
## [4,]  1.684639e-06
## [5,]  1.397109e-06
## [6,]  7.483336e-06
## [7,]  1.310969e-06
## [8,]  3.186262e-06
## [9,]  2.609344e-06
## [10,] 1.877686e-06

```



```

## [11,] 1.113746e-06
## [12,] 5.556009e-06
## [13,] 1.510892e-05
## [14,] 1.193626e-06
## [15,] 1.586852e-05
## [16,] -8.665329e-07
## [17,] 7.255815e-06
## [18,] 5.815453e-06
## [19,] 2.039161e-05
## [20,] 1.783108e-05
## [21,] -3.533980e-05
## [22,] -1.473606e-06
## [23,] -1.163293e-05
## [24,] 5.975308e-06
## [25,] -1.547631e-05
## [26,] -5.089571e-08
## [27,] 3.753316e-05
## [28,] -2.036002e-05
## [29,] -3.605203e-05
## [30,] 2.130693e-05
## [31,] -4.685337e-06
## [32,] -1.437389e-05
## [33,] 5.401744e-05
## [34,] -7.215700e-05
## [35,] 2.640436e-06
## [36,] -1.614215e-05
## [37,] -7.187167e-05
## [38,] 5.119470e-05
## [39,] -1.545914e-05
## [40,] 1.258507e-05
## [41,] 2.557927e-05
## [42,] -2.951897e-05
## [43,] -7.769601e-06
## [44,] 3.702747e-06
## [45,] 3.261114e-05
## [46,] 1.881216e-05
## [47,] 1.731062e-05
## [48,] 1.938809e-06
## [49,] -6.834239e-06
## [50,] 1.545074e-06
##
## $results
##
## Call: glmnet(x = input, y = y, family = "binomial", alpha = 0, lambda = lambda)
##
## Df %Dev Lambda
## 1 50 0.04 40.12
##
## $sigma
## [1] 0.01
##
## $MisclassificationError
## [1] 0.4078947

```

Again we run it on an example to check it works.

### Question 10

Let's now fit our model for different values of  $m$  and calculate the error on the test set:

```
X_test <- as.matrix(test[,-4])
y_test <- test[,4]
```

```
m_list <- c(10, 25, 50, 100, 200, 400)
misclass_error <- rep(NA, length(m_list))
for(i in 1:length(m_list)){
  m <- m_list[i]
  results <- fit_model_cv_l_sigma(X, y, m)
  pred <- predict_our_model(results, X, X_test, results$sigma, m)
  misclass_error[i] <- mean(pred != y_test)
}
```

```
## Error in solve(S) %*% sqrt(solve(L)) %*% gamma_glm: invalid class 'NA' to dup_mMatrix_as_dgeMatrix
m_list
```

```
## [1] 10 25 50 100 200 400
```

```
misclass_error
```

```
## [1] 0.46 0.46 0.46 0.46 0.46 NA
```

We see that for different values of  $m$  we are getting similar values for the missclassification error (basically the same), also note that this missclassification error is not particularly small. This suggests that if  $\lambda$  and  $\sigma$  are chosen well, then the choice of  $m$  is not particularly important. Which means we should set  $m$  small when trying to fit our model as we will achieve similar performance as if we use a large  $m$  but with less computation needed.

### Question 11

Let's now find the GAM estimate of model (1), where we will choose the penalty parameters,  $\{\lambda_j\}_{j=1}^p$ , using Generalized Cross Validation (GCV) which is the method gam uses by default:

```
library(mgcv)
```

```
## Loading required package: nlme
```

```
## This is mgcv 1.8-42. For overview type 'help("mgcv-package")'.
```

```
fit <- gam(ret~s(dur)+s(gly)+s(bmi), data = train)
preds <- predict(fit, newdata = test[,-4])
preds <- ifelse(preds > 0.5, 1, 0)
misclass_error <- mean(pred != test[,4])
misclass_error
```

```
## [1] 0.46
```

This missclassification error is the same as that achieved by our model, with much less computation involved partly down to the smaller number of hyper-parameters, which are chosen by cross validation (which is costly).