

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 α we use with f_2 , $\alpha_2 = \alpha_1 - d + c$, where α_1 is the α 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}_λ 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:

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

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 $\gamma = \beta_\lambda^T K(X_{1:m}, X)^T$. Let's now rewrite the penalty:

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

This leaves us with the following optimization problem,

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

Question 5

#TODO: change K_m^0 to inverse? Let's first find the spectral decomposition of K_m^0 ,

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

Then we can write,

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

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

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

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 γ_{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 γ 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,]  1.43659775
## [2,]  1.45609816
## [3,] -0.92103688
## [4,] -2.83875234
## [5,]  0.55973131
## [6,]  0.75289553
## [7,]  1.53109427
## [8,]  1.49939757
## [9,] -0.51240431
## [10,] -0.57453986
## [11,] -0.92069255
## [12,] -0.88165692
## [13,] -0.03653516
## [14,]  0.82783378
## [15,] -0.46607982
## [16,] -0.87322300
## [17,] -1.43433370

```

```
## [18,] -0.82793977
## [19,] -0.58558211
## [20,] -1.12625321
## [21,] -1.41233673
## [22,]  3.19435712
## [23,] -3.32929251
## [24,] -1.19123124
## [25,]  3.23637901
## [26,] -0.46396414
## [27,] -1.42531056
## [28,]  3.00418970
## [29,]  0.33771252
## [30,] -0.66218331
## [31,] -0.96544826
## [32,]  2.17660428
## [33,]  2.25770448
## [34,] -1.93957640
## [35,]  1.28459765
## [36,] -0.70099127
## [37,] -1.57979006
## [38,] -3.20271838
## [39,]  0.06948153
## [40,]  0.85833650
## [41,] -2.15451449
## [42,] -1.71858500
## [43,] -2.90334411
## [44,]  0.07820479
## [45,] -1.03935502
## [46,] -1.15885596
## [47,]  1.22657475
## [48,]  0.88847202
## [49,] -2.25968299
## [50,] -3.03396113
##
## $results
##
## Call:  glmnet(x = input, y = y, family = "binomial", alpha = 0, lambda = lambda)
##
##      Df    %Dev Lambda
## 1 50 13.76    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]

[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 ϵ 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]

[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,]  0.65645607
## [2,]  0.68160129
## [3,] -0.50743271
## [4,] -1.22837711
## [5,]  0.31072940
## [6,]  0.49733992
## [7,]  0.78307911
## [8,] -0.59573578
## [9,] -0.19855383
## [10,] -0.22282967
## [11,] -0.44417850
## [12,] -0.43310506
## [13,] -0.01739477
## [14,] -0.61182629
## [15,]  0.17587337
## [16,] -0.46536274
## [17,]  0.74145635
## [18,] -0.45580510
## [19,]  0.32417823
## [20,]  0.63052165
## [21,] -0.74413164
## [22,]  1.57950390
## [23,] -1.76148661
## [24,]  0.67230522
## [25,]  1.87386007
## [26,] -0.25030847
## [27,]  0.66277274
## [28,] -0.92765512
## [29,]  1.19986664
## [30,]  0.10856541
## [31,] -0.33432751

```

```
## [32,] -0.83144776
## [33,]  1.07155423
## [34,] -1.00539546
## [35,]  0.68147054
## [36,] -0.33737044
## [37,] -0.87675913
## [38,] -1.75643034
## [39,]  0.04047828
## [40,]  0.52743931
## [41,]  1.22061893
## [42,] -1.04919397
## [43,] -1.61660969
## [44,]  0.09292736
## [45,]  0.53928117
## [46,] -0.72922809
## [47,]  0.60192452
## [48,]  0.38193206
## [49,] -1.32221001
## [50,] -1.66136450
##
## $results
##
## Call:  glmnet(x = input, y = y, family = "binomial", alpha = 0, lambda = lambda)
##
##      Df %Dev Lambda
## 1 50 9.32 0.3513
```

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, X, 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)

  predict(fit$results, newx=input)
}

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, 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[["MisclassError"]] = 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,] 1.591237e-07
## [2,] 2.704329e-06
## [3,] -2.091028e-06
## [4,] -1.577493e-06
## [5,] 8.016742e-07
## [6,] -7.568510e-06
## [7,] 7.549181e-06
## [8,] -8.930431e-06
## [9,] 1.499799e-06
## [10,] -3.429631e-06
## [11,] -2.371041e-06

```



```

## [12,] -1.784042e-06
## [13,] -5.815656e-06
## [14,] -6.992650e-06
## [15,] -5.463789e-06
## [16,] -1.015994e-05
## [17,] -4.930184e-07
## [18,] 8.026546e-06
## [19,] -2.761578e-05
## [20,] -5.139168e-08
## [21,] 7.584227e-06
## [22,] 3.691202e-05
## [23,] -1.223511e-05
## [24,] 3.255395e-05
## [25,] -1.315822e-05
## [26,] 1.687449e-05
## [27,] -3.461956e-05
## [28,] 2.048075e-06
## [29,] -7.075795e-05
## [30,] 8.161573e-06
## [31,] 3.550068e-05
## [32,] -1.019103e-04
## [33,] 5.603571e-05
## [34,] -4.318271e-05
## [35,] -7.207591e-05
## [36,] 1.035485e-05
## [37,] -1.142273e-05
## [38,] 1.207901e-04
## [39,] 2.618963e-05
## [40,] -1.780179e-04
## [41,] -6.847141e-05
## [42,] -3.575141e-05
## [43,] -6.037151e-05
## [44,] 6.173354e-05
## [45,] -6.926709e-05
## [46,] 1.051831e-04
## [47,] -6.757526e-05
## [48,] 9.467387e-06
## [49,] 3.629619e-05
## [50,] -2.677580e-05
##
## $results
##
## Call:  glmnet(x = input, y = y, family = "binomial", alpha = 0, lambda = lambda)
##
##      Df %Dev Lambda
## 1 50 0.06 44.74
##
## $sigma
## [1] 0.01
##
## $Misclassification
## [1] 1

```

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(10,20,40,50)
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_test, results$sigma, m)
  misclass_error[i] <- mean(pred != y_test)
}
misclass_error

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

For some reason the fit of the model I am getting is very bad, but I couldn't find what was wrong before hand in time! #TODO: check misclassification error being computed correctly, also maybe change how error calculated? cross entropy? #TODO: actually, think I just need to round outputs to 0 or 1 ### 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
```

```
##          660          594          400          15          352          265
## 0.84557203 0.89987895 0.51826874 0.47185790 0.25171539 0.84035581
##          617           7          277           92          130          113
## 0.18735172 0.49790462 0.37773306 0.62088208 0.43452359 0.45967168
##          608          573          443          554          553          288
## 0.52518342 0.63518518 0.62884116 0.39549360 0.47248689 0.53083731
##          506          193          474          620          235          220
## 0.43923342 0.54527300 0.67021078 0.54577900 0.55168150 0.84633996
##          374           2          569          223          527          633
## 0.62218385 0.62208485 0.18858137 0.37036637 0.12876051 0.33817046
##          418           59          485          225          460          110
## 0.56701730 0.24589565 0.37529626 0.38226361 0.22932672 0.68535825
##          162          169          232          175          236          187
## 0.86855899 0.11010091 0.38058503 0.37500173 0.16362101 0.26717942
##          337          470          401          246          119          256
## 0.06450848 0.47597721 0.58911223 0.41495047 0.61214736 0.50954571
##          177          259          204          372          616          322
## 0.42059140 0.57588881 0.44932311 0.36178209 0.43718046 0.68563424
##          466          522          449          545          599          442
## 0.38417351 -0.11001244 0.89716298 0.11707847 0.50335096 0.27260351
##           1          578           43          646          316          341
## 0.64584009 0.30391500 0.01648494 0.60954475 0.41528791 0.06076037
##          483          317          144          181          622          19
```

```
## 0.68588905 0.66876502 0.33671924 0.61183965 0.45338530 0.26146188
##      568      58      48      298      402      406
## 0.17468929 0.54796214 -0.03405138 0.50692253 0.28907921 0.34967889
##      254      191      3      493      508      612
## 0.25054383 0.86600597 0.64506544 0.52389705 0.30997653 0.27300856
##      212      104      127      97      134      419
## 0.01110583 0.13993147 0.26100169 0.78527810 0.94354354 0.21542257
##      199      240      518      136      74      472
## 0.74014219 0.22953552 0.25656138 0.52560448 0.35342443 0.60543104
##      488      392      75      38
## 0.63622267 0.54609077 0.29537715 0.32865677
```

```
test[,4]
```

```
## [1] 0 1 1 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 1 0 1 0 1 0 0 0 0 1 0 0 0 0 0 0
## [38] 0 0 0 0 0 0 1 1 0 1 1 0 1 1 1 0 0 1 0 0 0 0 0 0 1 0 1 0 0 1 1 0 1 0 0 0 0
## [75] 0 0 1 1 0 0 0 0 0 1 0 1 0 1 1 0 1 1 0 1 0 0 1 1 0 0
```

```
misclass_error <- mean(pred != test[,4])
misclass_error
```

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

#TODO: comment on this result after fiddling with error calc.