SVM

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Linearly Separable SVM using Quadratic Programming

Install the `quadprog` package (there are similar ones in Python too) and utilize the function `solve.QP` to solve SVM (dual problem). The `solve.QP` function is trying to perform the minimization problem:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\boldsymbol{\beta}^T \mathbf{D}\boldsymbol{\beta} - d^T\boldsymbol{\beta} \\ \text{subject to} \quad & \mathbf{A}^T\boldsymbol{\beta} \geq a \end{aligned}$$

For more details, read the document file of the `quadprog` package on CRAN. Investigate the dual optimization problem of the seperable SVM formulation, and write the problem into the above form by properly defining $\mathbf{D}$, d, A and a.

Note: The package requires $\mathbf{D}$ to be positive definite, while it may not be true in our problem. A workaround is to add a "ridge," e.g., $10^{-5}\mathbf{I}$, to the $\mathbf{D}$ matrix, making it invertible. This may affect your later results, so figure out a way to fix them.

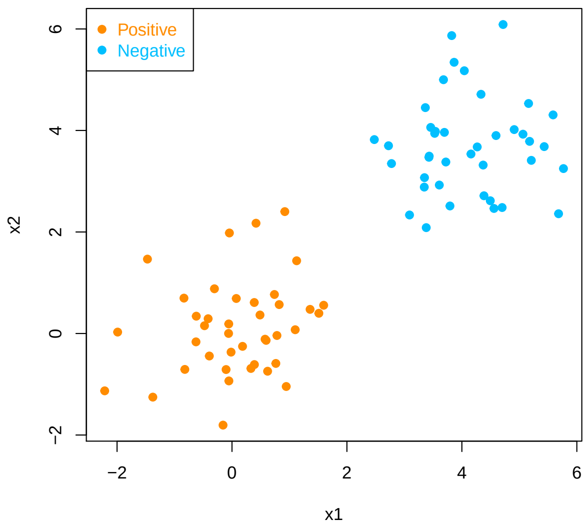
You should generate the data using the following code (or write a similar code in Python). After solving the quadratic programming problem, perform the following:

- Convert the solution into β and β_0, which can be used to define the classification rule
- Plot all data and the decision line
- Add the two separation margin lines to the plot
- Add the support vectors to the plot

```r
set.seed(1)
n <- 40
p <- 2
xpos <- matrix(rnorm(n * p, mean = 0, sd = 1), n, p)
xneg <- matrix(rnorm(n * p, mean = 4, sd = 1), n, p)
x <- rbind(xpos, xneg)
y <- matrix(c(rep(1, n), rep(-1, n)))

plot(
  x,
  col = ifelse(y > 0, "darkorange", "deepskyblue"),
  pch = 19,
  xlab = "x1",
  ylab = "x2"
)
legend(
  "topleft",
  c("Positive", "Negative"),
  col = c("darkorange", "deepskyblue"),
  pch = c(19, 19),
```

```
  text.col = c("darkorange", "deepskyblue")
)
```




```
#Implementing dual problem
Q <- sapply(1:nrow(x), function(i) y[i]*t(x)[,i])
D <- t(Q)%*%Q
I <- diag(10 ^ -5, nrow(x))
Dmat <- D + I
d <- matrix(1, nrow = nrow(x), ncol = 1)
A <- cbind(matrix(y, nrow=nrow(x), ncol=1), diag(nrow=nrow(x)))
b0 <- rbind( matrix(0, nrow=1, ncol=1) , matrix(0, nrow=nrow(x), ncol=1) )

#using quadprog
library(quadprog)
sol <- solve.QP(Dmat, dvec = d, Amat = A, b0, meq = 1)

#calculate beta = sum(alpha_i*y_i*x_i)
beta <- matrix(0, ncol = 2, nrow = 1)
for (i in 1:nrow(x)) {
  beta <- beta + sol$solution[i] * y[i] * x[i, ]
}
beta
```

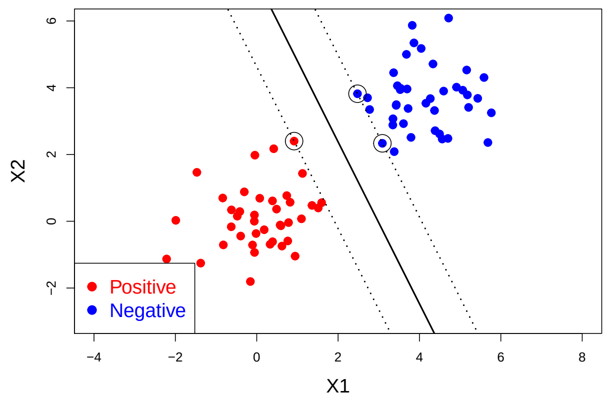
```
##             [,1]      [,2]
## [1,] -0.933426 -0.384982
```

```
#calculating beta zero as given in class
beta_zero <-
  -(max(x[y == -1,] %*% t(beta)) + min(x[y == 1,] %*% t(beta))) / 2
beta_zero
```

```
## [1] 2.782373
```

```r
b <- beta
b0 <- beta_zero

# plot on the data
plot(
  x,
  col = ifelse(y > 0, "red", "blue"),
  pch = 19,
  cex = 1.2,
  lwd = 2,
  xlab = "X1",
  ylab = "X2",
  cex.lab = 1.5,
  xlim = c(-4, 8),
  ylim = c(-3, 6),
)
legend(
  "bottomleft",
  c("Positive", "Negative"),
  col = c("red", "blue"),
  pch = c(19, 19),
  text.col = c("red", "blue"),
  cex = 1.5
)
#Decision Boundary
abline(
  a = -b0 / b[1, 2],
  b = -b[1, 1] / b[1, 2],
  col = "black",
  lty = 1,
  lwd = 2
)
# the two margin lines
abline(
  a = (-b0 - 1) / b[1, 2],
  b = -b[1, 1] / b[1, 2],
  col = "black",
  lty = 3,
  lwd = 2
)
abline(
  a = (-b0 + 1) / b[1, 2],
  b = -b[1, 1] / b[1, 2],
  col = "black",
  lty = 3,
  lwd = 2
)
#add support vectors
points(x[abs(sol$solution) > 5*10^-5, ], col="black", cex=3)
```



Linearly Non-seperable SVM using Penalized Loss

We also introduced an alternative method to solve SVM. Consider a logistic loss function

$$L(y, f(x)) = \log(1 + e^{-yf(x)})$$

and solve the penalized loss for a linear SVM

$$\arg\min_{\beta_0, \beta} \sum_{i=1}^{n} L(y_i, \beta_0 + x^T \beta) + \lambda \|\beta\|^2$$

The rest of the job is to solve this optimization problem. To do this, we will utilize a general-purpose optimization package/function. For example, in `R`, you can use the `optim` function. Read the documentation of this function (or equivalent ones in Python) and set up the objective function properly to solve for the parameters. If you need an example of how to use the `optim` function, read the corresponding part in the example file provide on our course website here (Section 10). You should generate the data using the following code (or write a similar code in Python). Perform the following:

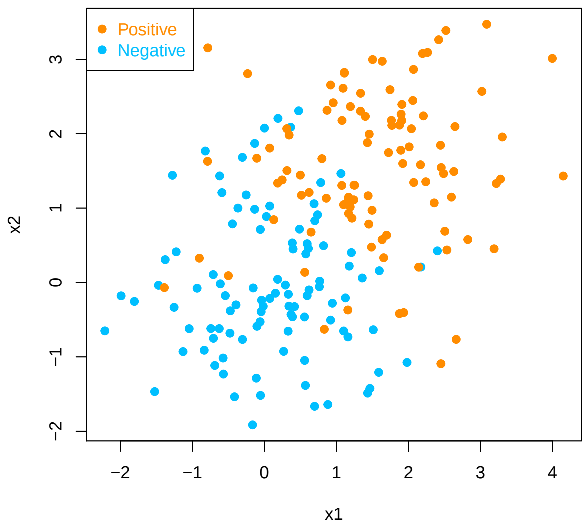
- Write a function to define the objective function (penalized loss). The algorithm may run faster if you further define the gradient function.
- Choose a reasonable λ value so that your optimization can run properly. In addition, I recommend using the `BFGS` method in the optimization.
- After solving the optimization problem, plot all data and the decision line
- If needed, modify your λ so that the model fits reasonably well (you do not have to optimize this tuning), and re-plot

```r
set.seed(1)
n = 100 # number of data points for each class
p = 2 # dimension

# Generate the positive and negative examples
xpos <- matrix(rnorm(n * p, mean = 0, sd = 1), n, p)
xneg <- matrix(rnorm(n * p, mean = 1.5, sd = 1), n, p)
x <- rbind(xpos, xneg)
y <- c(rep(-1, n), rep(1, n))

plot(
```

```
  x,
  col = ifelse(y > 0, "darkorange", "deepskyblue"),
  pch = 19,
  xlab = "x1",
  ylab = "x2"
)
legend(
  "topleft",
  c("Positive", "Negative"),
  col = c("darkorange", "deepskyblue"),
  pch = c(19, 19),
  text.col = c("darkorange", "deepskyblue")
)
```




```
#create a loss function
loss <- function(x, y, beta, lambda)
{
  sum = 0
  power <- x %*% beta
  for (i in 1:length(y)) {
    sum = sum + log(1 + exp(-y[i] * (power[i])))
  }
  beta_norm <- sqrt(sum(beta ^ 2))
  return(sum + lambda * beta_norm)
}

#using optim function to optimize with lambda = 0.5
solution = optim(
  matrix(rep(0, 3)),
  loss,
  x = cbind(1, x),
  y = y,
  lambda = 0.5,
```

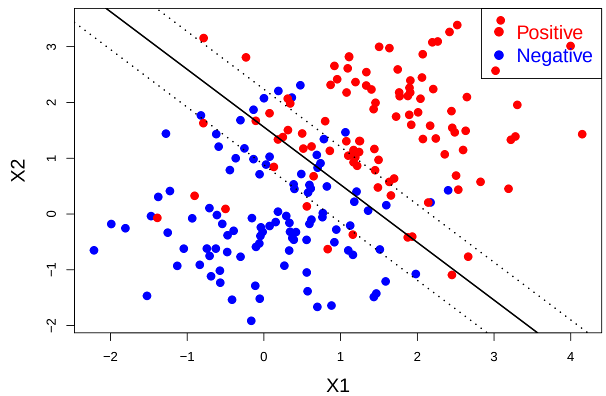
```r
  method = "BFGS"
)
solution$par
```

```
##            [,1]
## [1,] -2.298452
## [2,]  1.524495
## [3,]  1.474166
```

```r
#plot the results
plot(
  x,
  col = ifelse(y > 0, "red", "blue"),
  pch = 19,
  cex = 1.2,
  lwd = 2,
  xlab = "X1",
  ylab = "X2",
  cex.lab = 1.5
)
legend(
  "topright",
  c("Positive", "Negative"),
  col = c("red", "blue"),
  pch = c(19, 19),
  text.col = c("red", "blue"),
  cex = 1.5
)

b <- matrix(solution$par[2:length(solution$par)], ncol = 2)
b0 <- solution$par[1]
#decision boundary
abline(
  a = -b0 / b[1, 2],
  b = -b[1, 1] / b[1, 2],
  col = "black",
  lty = 1,
  lwd = 2
)
#plotting the margin
abline(
  a = (-b0 - 1) / b[1, 2],
  b = -b[1, 1] / b[1, 2],
  col = "black",
  lty = 3,
  lwd = 2
)
abline(
  a = (-b0 + 1) / b[1, 2],
  b = -b[1, 1] / b[1, 2],
  col = "black",
  lty = 3,
  lwd = 2
```

```
)
```



Nonlinear and Non-seperable SVM using Penalized Loss

We can further use the kernel trick to solve for a nonlinear decision rule. The optimization becomes

$$\sum_{i=1}^{n} L(y_i, K_i^T \beta) + \lambda \beta^T K \beta$$

where K_i is the ith column of the $n \times n$ kernel matrix K. For this problem, we consider the Gaussian kernel (you do not need an intercept). Again, we can use the logistic loss.

You should generate the data using the following code (or write a similar code in Python). Perform the following:

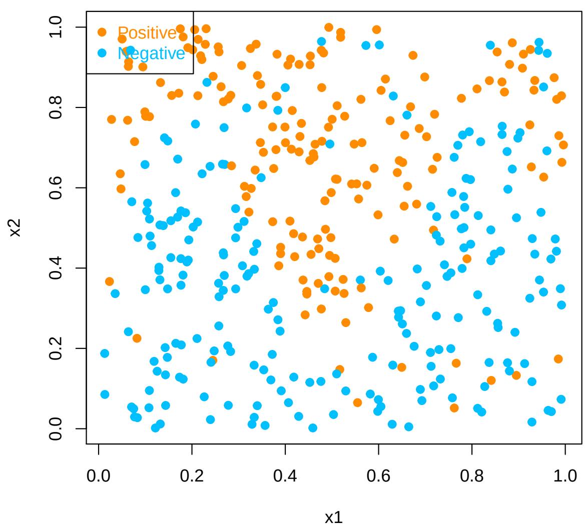
- Pre-calculate the $n \times n$ kernel matrix K of the observed data
- Write a function to define the objective function (this should not involve the original x, but uses K).
- Choose a reasonable λ value so that your optimization can run properly
- After solving the optimization problem, plot **fitted** labels (in-sample prediction) for all subjects
- If needed, modify your λ so that the model fits reasonably well (you do not have to optimize this tuning), and re-plot
- Summarize your in-sample classification error

```r
set.seed(1)
n = 400
p = 2 # dimension

# Generate the positive and negative examples
x <- matrix(runif(n * p), n, p)
side <- (x[, 2] > 0.5 + 0.3 * sin(3 * pi * x[, 1]))
y <-
  sample(c(1,-1), n, TRUE, c(0.9, 0.1)) * (side == 1) + sample(c(1,-1), n, TRUE, c(0.1, 0.9)) *
  (side == 0)

plot(
  x,
```

```
  col = ifelse(y > 0, "darkorange", "deepskyblue"),
  pch = 19,
  xlab = "x1",
  ylab = "x2"
)
legend(
  "topleft",
  c("Positive", "Negative"),
  col = c("darkorange", "deepskyblue"),
  pch = c(19, 19),
  text.col = c("darkorange", "deepskyblue")
)
```




```
#define a kernel function, assuming sigma = 1
kernel <- function(xi,xj){
  return(exp((-1/2)*sum((xi-xj)^2)))
}

#calculating n*n matrix of K
K <- matrix(0, nrow(x), nrow(x))
for (i in 1:nrow(x)){
  for (j in 1:nrow(x)){
    K[i,j] = kernel(x[i,],x[j,])
  }
}

#defining the loss function
kernel_loss <- function(k, y, beta, lambda)
{
  sum = 0
  for (i in 1:length(y)) {
    sum = sum + log(1 + exp(-y[i] * (t(k[,i])%*%beta))
```

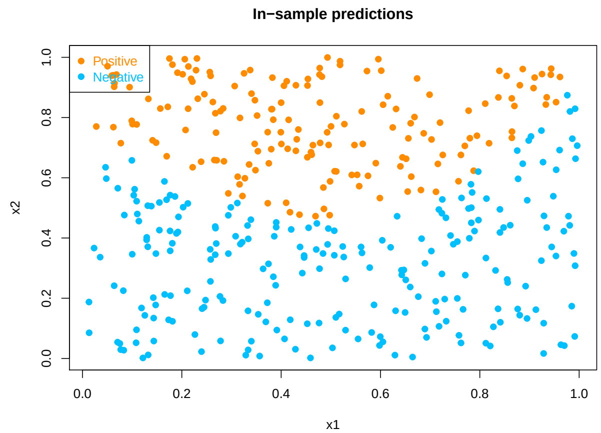
```r
  }
  beta_norm <- t(beta)%*%k%*%beta
  return(sum + lambda * beta_norm)
}

#optimising using
solution = optim(
  matrix(rep(0, nrow(x))),
  kernel_loss,
  k = K,
  y = y,
  lambda = 0.01,
  method = "BFGS"
)

#in sample prediction
pred <- ifelse( t(K)%*%solution$par >= 0 , 1, -1)
pred <- as.factor(pred)
y <- as.factor(y)

#plotting in-sample prediction
plot(
  x,
  col = ifelse(pred == 1, "darkorange", "deepskyblue"),
  pch = 19,
  xlab = "x1",
  ylab = "x2",
  main = "In-sample predictions"
)
legend(
  "topleft",
  c("Positive", "Negative"),
  col = c("darkorange", "deepskyblue"),
  pch = c(19, 19),
  text.col = c("darkorange", "deepskyblue")
)

#checking results
library(caret)
```




```r
confusionMatrix(pred, y)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  -1   1
##         -1 185  46
##         1   37 132
##
##                Accuracy : 0.7925
##                  95% CI : (0.7494, 0.8312)
##     No Information Rate : 0.555
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.5778
##
##  Mcnemar's Test P-Value : 0.3799
##
##             Sensitivity : 0.8333
##             Specificity : 0.7416
##          Pos Pred Value : 0.8009
##          Neg Pred Value : 0.7811
##              Prevalence : 0.5550
##          Detection Rate : 0.4625
##    Detection Prevalence : 0.5775
##       Balanced Accuracy : 0.7875
##
##        'Positive' Class : -1
##
```