Nonlinear Programming 1

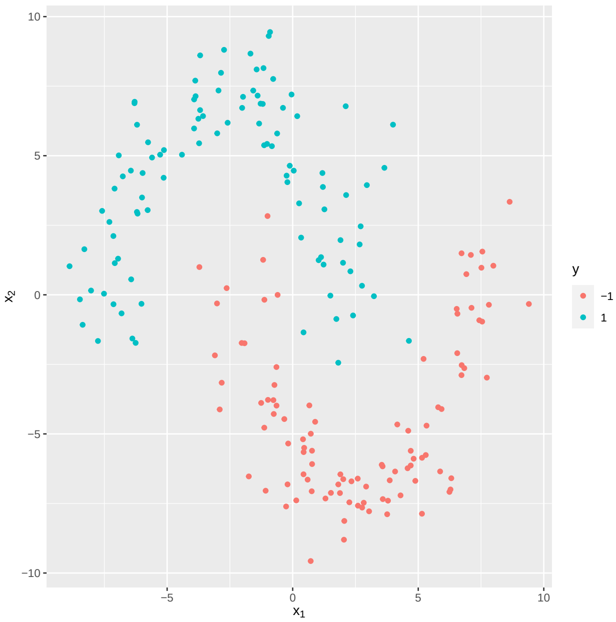
Exercise 1: Nonlinear SVM

(a)

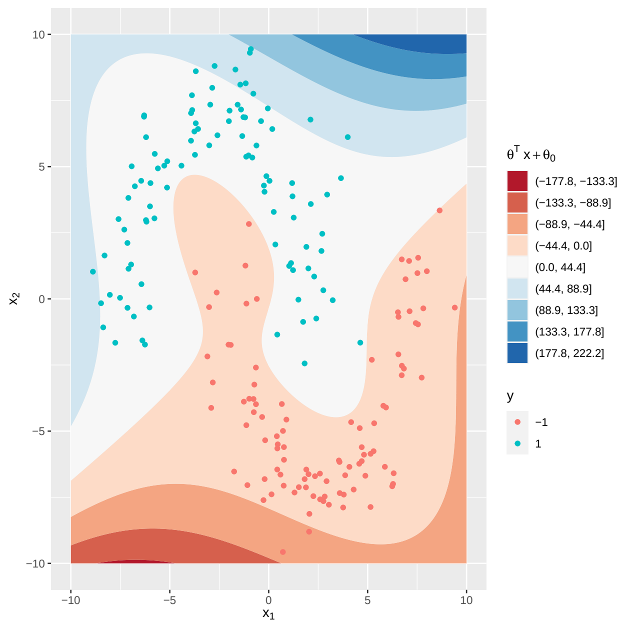
$$\mathcal{L} = 0.5\|\boldsymbol{\theta}\|^2 + C\sum_{i=1}^{n}\zeta^{(i)} - \sum_{i=1}^{n}\alpha^{(i)}(\mathbf{y}^{(i)}(\phi(\mathbf{x}^{(i)})^\top\boldsymbol{\theta} + \theta_0) - 1 + \zeta^{(i)}) - \sum_{i=1}^{n}\mu^{(i)}\zeta^{(i)}$$

(b)

```
library(ggplot2)
library(mlr3)
library(RColorBrewer)
library(CVXR)

##
## Attaching package:  'CVXR'

## The following object is masked from 'package:stats':
##
##     power

# generate 200 nonlinear separable binary observations
set.seed(123)
n = 200
moon_data = tgen("moons")$generate(n)$data()

moon_data$y = ifelse(moon_data$y == "A", 1, -1)
moon_data$y_dec = as.factor(moon_data$y)

ggplot(moon_data, aes(x=x1, y=x2)) +
 geom_point(aes(color=y_dec)) +
 xlab(expression(x[1])) +
 ylab(expression(x[2])) +
 labs(color=expression(y))
```



```r
X = as.matrix(moon_data[,c("x1", "x2")])
# define cubic polynomial transformation (without intercept)
cubic_trafo <- function(x) return(cbind(x[1], x[2], x[1]^2, x[2]^2, x[1]*x[2],
                                       x[1]^2*x[2], x[1]*x[2]^2, x[1]^3,
                                       x[2]^3))

Z = t(apply(t(X), 2, cubic_trafo))
C = 1.0

# define variables for cvxr
theta0 = Variable()
theta  = Variable(9)
slack = Variable(n)

objective = (1/2) * sum_squares(theta) + C * sum(slack)
constraints = list(moon_data$y * (Z %*% theta + theta0) >= 1 - slack, slack >= 0)
problem = Problem(Minimize(objective), constraints)
solution = solve(problem)

theta0_sol = solution$getValue(theta0)
theta_sol = solution$getValue(theta)

# create grid for plot
x = seq(-10, 10, by=0.05)
xx = expand.grid(X1 = x, X2 = x)
yxx = as.matrix(cubic_trafo(xx)) %*% theta_sol + theta0_sol

df = data.frame(xx = xx, yxx = yxx)
ggplot() +
 geom_contour_filled(data = df, aes(x = xx.X1, y = xx.X2, z = yxx), bins=10) +
 scale_fill_brewer(palette = "RdBu") +
 xlab(expression(x[1])) +
 ylab(expression(x[2])) +
 geom_point(data = moon_data, aes(x=x1, y=x2, color=y_dec)) +
 labs(color = expression(y), fill = expression(theta^T~x + theta[0]))
```



(c) Stationarity

$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = \boldsymbol{\theta} - \sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} \phi(\mathbf{x}^{(i)}) = 0$$

$$\nabla_{\theta_0} \mathcal{L} = - \sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} = 0$$

$$\nabla_{\boldsymbol{\zeta}} \mathcal{L} = C \cdot \mathbf{1}_n - \alpha - \mu = 0$$

Primal feasability

$$-(\mathbf{y}^{(i)}(\phi(\mathbf{x}^{(i)})^\top \boldsymbol{\theta} + \theta_0) - 1 + \zeta^{(i)}) \leq 0$$
$$-\zeta^{(i)} \leq 0$$

Dual feasability

$$\mu \geq 0$$

$$\alpha \geq 0$$

Complementary slackness

$$-\mu^{(i)}\zeta^{(i)} = 0 \quad i = 1, \ldots, n$$

$$-\alpha^{(i)}(\mathbf{y}^{(i)}(\phi(\mathbf{x}^{(i)})^\top \boldsymbol{\theta} + \theta_0) - 1 + \zeta^{(i)}) = 0 \quad i = 1, \ldots, n$$

(d) From the KKT conditions it follows that

$$\boldsymbol{\theta} = \sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} \phi(\mathbf{x}^{(i)}),$$

$$\sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} = 0,$$

$$C - \underbrace{\mu^{(i)}}_{\geq 0} = \alpha^{(i)} \Rightarrow C \geq \alpha^{(i)} \quad i = 1, \ldots, n.$$

Plugging these into the Lagrangian gives

$$0.5 \| \sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} \phi(\mathbf{x}^{(i)}) \|^2 + \sum_{i=1}^{n} \mu^{(i)} \zeta^{(i)} + \sum_{i=1}^{n} \alpha^{(i)} \zeta^{(i)} - \| \sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} \phi(\mathbf{x}^{(i)}) \|^2 + \sum_{i=1}^{n} \alpha^{(i)} - \sum_{i=1}^{n} \alpha^{(i)} \zeta^{(i)}) - \sum_{i=1}^{n} \mu^{(i)} \zeta^{(i)}$$

$$= -0.5 \| \sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} \phi(\mathbf{x}^{(i)}) \|^2 + \sum_{i=1}^{n} \alpha^{(i)} = -0.5 \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha^{(i)} \alpha^{(j)} \mathbf{y}^{(i)} \mathbf{y}^{(j)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle + \sum_{i=1}^{n} \alpha^{(i)}$$

Hence, the dual form of the nonlinear SVM is

$$\max_{\alpha} -0.5 \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha^{(i)} \alpha^{(j)} \mathbf{y}^{(i)} \mathbf{y}^{(j)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle + \sum_{i=1}^{n} \alpha^{(i)}$$

s.t.

$$\sum_{i=1}^{n} \alpha^{(i)} \mathbf{y}^{(i)} = 0,$$
$$0 \leq \alpha \leq C.$$

Here, we can use the kernel trick to evaluate $\langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle$ without explicitly computing the projections of each observation. (We only need to compute $\langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle$)

(e)
```r
gram = (X %*% t(X) + 1)^3 - 1

alpha = Variable(n)
P = diag(moon_data$y) %*% gram %*% diag(moon_data$y)
P = P + diag(n)*0.0000001


objective = sum(alpha) - (1/2) * quad_form(alpha, P)
constraints = list(t(alpha) %*% moon_data$y == 0,
                   alpha >= 0,
                   C >= alpha)
problem = Problem(Maximize(objective), constraints)
solution = solve(problem)

solution$status

## [1] "optimal"

D = diag(c(sqrt(3), sqrt(3), sqrt(3), sqrt(3), sqrt(6), sqrt(3), sqrt(3), 1, 1))
theta_sol = c(t(solution$getValue(alpha) * moon_data$y) %*% Z %*% D)
theta0_sol = -0.5 * (max((z_m = Z %*% D %*% theta_sol)[moon_data$y == -1]) +
                       min((z_m = Z %*% D %*% theta_sol)[moon_data$y == 1]))

x = seq(-10, 10, by=0.05)
xx = expand.grid(X1 = x, X2 = x)
yxx = as.matrix(cubic_trafo(xx)) %*% D %*% theta_sol + theta0_sol

df = data.frame(xx = xx, yxx = yxx)
ggplot() +
 geom_contour_filled(data = df, aes(x = xx.X1, y = xx.X2, z = yxx), bins=10) +
 scale_fill_brewer(palette = "RdBu") +
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 geom_point(data = moon_data, aes(x=x1, y=x2, color=y_dec)) +
 labs(color = expression(y), fill = expression(theta^T~x + theta[0]))
```