

# Comparing Full Methods

Amy Pitts

3/20/2022

## Data import + Cleaning

Cleaning involves

- removing the id variable
- re-factoring the outcome variable `diagnosis` to be 0 if B and if M. Then this variable is re-names `toy`.

## Test + Train

Next we will break the data into the test and train sets. The split will be 80-20.

```
partition <- function(p, data){
  set.seed(5)
  # generating a probability value
  part_p = runif(nrow(data), min = 0, max = 1)
  # assigning partition id based on probability value
  # parameter p sets proportion of train vs test
  part_id = ifelse(part_p <= p, "train", "test")
  # appending to data set
  data_new = cbind(data, part_id)

  return(data_new)
}
# here training proportion is set to 0.8
part_data <- partition(p = 0.8, data = dat)

trn_data <-
  part_data %>%
  filter(part_id == "train") %>%
  select(-part_id)

tst_data <- # this will come back into play for test error
  part_data %>%
  filter(part_id == "test") %>%
  select(-part_id)
```

I want to only check 3 variables

```
cor(trn_data$texture_mean, trn_data$radius_mean)
```

```
## [1] 0.3249025
```

```
cor(trn_data$radius_mean, trn_data$smoothness_mean)
```

```
## [1] 0.1527862
cor(trn_data$smoothness_mean, trn_data$texture_mean)

## [1] -0.02904833
# trn_data = trn_data %>%
#   select(y, texture_mean, radius_mean, smoothness_mean)
#   head(trn_data)

cor_dat <- data.frame(cor(dat)) %>%
  mutate(variable_left = names(data.frame(cor(dat)))) %>%
  relocate(variable_left) %>%
  pivot_longer(
    c(y:fractal_dimension_worst),
    names_to = "variables_top",
    values_to = "cor"
  ) %>%
  mutate(cor = abs(cor)) %>%
  arrange(desc(cor)) %>%
  filter(cor != 1) %>%
  filter(cor > 0.8)
head(cor_dat)

## # A tibble: 6 x 3
##   variable_left variables_top cor
##   <chr>         <chr>      <dbl>
## 1 radius_mean   perimeter_mean 0.998
## 2 perimeter_mean radius_mean    0.998
## 3 radius_worst  perimeter_worst 0.994
## 4 perimeter_worst radius_worst 0.994
## 5 radius_mean   area_mean     0.987
## 6 area_mean     radius_mean    0.987
```

## Comparing all Methods

We will be comparing:

- Waveley's Method
- Amy's Method
- base R glm
- glmnet ( $\lambda = 0$ )
- Jimmy's LASSO function with  $\lambda = 0$

### Waveley's Method

```
rep_col <- function(x, n){
  matrix(rep(x, each = n), ncol = n, byrow = TRUE)
}

logistic_stuff <- function(dat, beta){

  x <- dat[[1]] %>% unname() %>% as.matrix()
  y <- dat[[2]] %>% unname() %>% as.matrix()

  x_with_1 <- cbind(1, x)
```

```

u <- x_with_1 %*% beta
# return(u)

expu <- exp(u)

loglik <- sum(y*u - log(1 + expu))

p <- expu/(1 + expu)
# return(p)
# return(p)
grad <- t(x_with_1) %*% (y - p)

i_mat <- diag(nrow(p))
diag(i_mat) <- p*(1 - p)

hess <- -(t(x_with_1) %*% i_mat %*% x_with_1)

return(
  list(
    loglik = loglik,
    grad = grad,
    hess = hess
  ))
}

NewtonRaphson_w <- function(dat, func, start, tol = 1e-8, maxiter = 200) {
  i <- 0
  cur <- start
  stuff <- func(dat, cur)
  res <- c(0, stuff$loglik, cur)
  prevloglik <- -Inf

  while (i < maxiter && abs(stuff$loglik - prevloglik) > tol && !is.na(stuff$loglik)) {
    i <- i + 1
    prevloglik <- stuff$loglik
    prev <- cur
    # newhess <- ((stuff$hess + t(stuff$hess))/2)
    newhess <- stuff$hess

    # if (!is.negative.definite(newhess)) { # redirection
    #   while (!is.negative.definite(newhess)) {
    #     # subtracts identity matrix until a negative definite matrix is achieved
    #     newhess1 <- newhess - diag(nrow(newhess))
    #     # sanity check print("changing ascent direction")
    #     newhess <- ((newhess1 + t(newhess1))/2)
    #   }
    # }

    cur <- prev - solve(newhess) %*% stuff$grad
    stuff <- func(dat, cur)

    if (stuff$loglik < prevloglik) { # back tracking (half-step)
      j = 1

```

```

    while (stuff$loglik < prevloglik & (!is.na(stuff$loglik))) {
      halfstep = 1/(2^j)
      cur <- prev - halfstep*solve(newhess) %*% stuff$grad
      stuff <- func(dat, cur)
      # sanity check print("backtracking")
      j = j + 1
    }
  }
  res <- rbind(res, c(i, stuff$loglik, cur))
}
return(res)
}

rerun_NR <- function(beta_init){
  # calling the function
  ans_w <- NewtonRaphson_w(
    list(x = trn_data %>% select(-y) %>% as.matrix(),
         y = trn_data %>% select(y) %>% as.matrix()),
    logistic_stuff,
    beta_init)

  # organizing the results
  if (sum(is.na(ans_w[nrow(ans_w),])) > 0) {
    beta_est <- ans_w[nrow(ans_w) - 1, -c(1,2)]
  }

  if (sum(is.na(ans_w[nrow(ans_w),])) == 0) {
    beta_est <- ans_w[nrow(ans_w), -c(1,2)]
  }
  # results
  waveley_est <- tibble(beta_subscript = seq(0, (ncol(trn_data)-1)),
                        beta_estimates = beta_est) #>% knitr::kable()
  return(waveley_est)
}

beta_init <- rep(0.0001, ncol(trn_data)) %>% as.matrix()

beta_init <- rep(0.0001, ncol(trn_data)) %>% as.matrix()
w_0.0001 <- rerun_NR(beta_init)$beta_estimates

beta_init <- rep(0.001, ncol(trn_data)) %>% as.matrix()
w_0.001 <- rerun_NR(beta_init)$beta_estimates

```

## Amy's Method

```

loglike_func <- function(dat, betavec){
  # setting up an intercept
  dat_temp = dat %>%
    rename(intercept = y) %>%
    mutate(intercept = rep(1, nrow(dat) ))
  dat_x = unname(as.matrix(dat_temp)) # creating the x matrix

```

```

# finding the pi values
u = dat_x %>% betavec
pi <- exp(u) / (1+exp(u))

# loglikelihood
loglik <- sum(dat$y*u - log(1 + exp(u)))

#gradient
grad <- t(dat_x)%*(dat$y - pi)

# Hessian
W = matrix(0, nrow = dim(dat)[1], ncol = dim(dat)[1])
diag(W)= pi*(1-pi)
hess = -(t(dat_x)%% W %%(dat_x))

return(list(loglik = loglik, grad = grad, hess = hess))
}

#loglike_func(dat, betavec = c(rep(0.03, 31))) # test!

NewtonRaphson_a <- function(dat, start, tol = 1e-8, maxiter = 200){
  i = 0
  cur = start
  stuff = loglike_func(dat, cur)
  res <- c(i=0, "loglik" = stuff$loglik, "step" = 1, cur)
  prevloglik <- -Inf # To make sure it iterates
  while(i < maxiter && abs(stuff$loglik - prevloglik) > tol) {
    step = 1
    i <- i + 1
    prevloglik <- stuff$loglik

    # checking negative definite
    eigen_vals = eigen(stuff$hess)
    if(max(eigen_vals$values) <= 0 ){ # check neg def, if not change
      hess = stuff$hess
    } else{ # if it is pos def then need to adjust
      hess = stuff$hess - (max(eigen_vals$values) + 0.1)*diag(nrow(stuff$hess))
    }

    prev <- cur
    cur <- prev - rep(step, length(prev))*(solve(stuff$hess) %>% stuff$grad)
    stuff <- loglike_func(dat, cur) # log-lik, gradient, Hessian

    # doing half stepping
    while(stuff$loglik < prevloglik){
      stuff <- loglike_func(dat, prev)
      step <- step / 2 # this is where half steping happens
      cur <- prev - step*(solve(stuff$hess) %>% stuff$grad)
      stuff <- loglike_func(dat, cur)
    }
    # Add current values to results matrix

```

```

    res <- rbind(res, c(i, stuff$loglik, step, cur))
  }

  colnames(res) <- c("i", "loglik", "step", "intercept", names(dat[, -1]))
  return(res)
}
#Running the algorithm with random starting values

betavec = c(rep(0.0001, ncol(trn_data)))
ans0.0001 <- NewtonRaphson_a(trn_data, betavec)

# beta values
amy_est_0.0001 <- data.frame(ans0.0001) %>%
  select(-step, -loglik, -i) %>%
  filter(row_number() == n()) %>%
  pivot_longer(
    cols = everything(),
    names_to = "term",
    values_to = "a_0.0001"
  ) %>%
  mutate(`a_0.0001` = round(`a_0.0001`, 3))

```

It will also be interesting to look at the stability depending on initial values.

```

betavec = c(rep(0.001, ncol(trn_data)))
ans0.001 <- NewtonRaphson_a(trn_data, betavec)

# beta values
amy_est_0.001 <- data.frame(ans0.001) %>%
  select(-step, -loglik, -i) %>%
  filter(row_number() == n()) %>%
  pivot_longer(
    cols = everything(),
    names_to = "term",
    values_to = "a_0.001"
  ) %>%
  mutate(`a_0.001` = round(`a_0.001`, 3))

betavec = c(rep(0.01, ncol(trn_data)))
ans0.01 <- NewtonRaphson_a(trn_data, betavec)

# beta values
amy_est_0.01 <- data.frame(ans0.01) %>%
  select(-step, -loglik, -i) %>%
  filter(row_number() == n()) %>%
  pivot_longer(
    cols = everything(),
    names_to = "term",
    values_to = "a_0.01"
  ) %>%
  mutate(`a_0.01` = round(`a_0.01`, 3))

```

## Base R glm

```
# trn_data <- trn_data[c(1:455),]
glm_fit <- glm(y~., data=trn_data, family = "binomial")
result_glm <- summary(glm_fit)

glm_est <- glm_fit %>% broom::tidy() %>%
  select(term, estimate) %>%
  mutate(glm_est = round(estimate, 3)) %>%
  select(-estimate) %>%
  mutate(term = ifelse(term == "(Intercept)", "intercept", term))
```

## glmnet

```
library(glmnet)

## Loading required package: Matrix
##
## Attaching package: 'Matrix'
## The following objects are masked from 'package:tidyr':
##
##   expand, pack, unpack
## Loaded glmnet 4.1-2

xdat = as.matrix(trn_data %>% select(-y))
glmnet_fit <- glmnet(x = xdat, y = trn_data$y, family="binomial", lambda = 0)
glmnet_est <- as.vector(coef(glmnet_fit)) %>% round(3)
```

## Jimmy's Method (LASSO) but lambda = 0

```
# logistic function
logistic <- function(x) 1 / (1 + exp(-x))

# shrinkage function
S <- function(beta, gamma) {
  if(abs(beta) <= gamma) {
    0
  } else if(beta > 0) {
    beta - gamma
  } else {
    beta + gamma
  }
}

# probability adjustment function
p_adj <- function(p, epsilon) {
  if (p < epsilon) {
    0
  } else if(p > 1 - epsilon) {
    1
  } else {
    p
  }
}
```

```

}
}

# weight adjustment function
w_adj <- function(p, epsilon) {
  if ((p < epsilon) | (p > 1 - epsilon)) {
    epsilon
  } else {
    p * (1 - p)
  }
}

set.seed(1)
epsilon <- 10(-5)

n <- nrow(trn_data)
X <- trn_data[, -c(1)]
X <- as.matrix(cbind(rep(1, n), X))
y <- trn_data$y

lambda <- 0 # (max(t(X) %*% y) / n)

# initialize parameters
beta <- rep(0, ncol(X))
p <- map_dbl(logistic(- X %*% beta), p_adj, epsilon)
w <- map_dbl(p, w_adj, epsilon)
z <- X %*% beta + (y - p) / w

terminate <- 0
iter <- 1
while(terminate < 1) {

  beta_old <- beta
  # initially go through all parameters
  K <- 1:ncol(X)
  #if(iter > 1) {
  # K <- which(beta > 0)
  #}

  for(k in K) {
    x_k <- X[, k]
    x_notk <- X[, -k]
    b_notk <- beta[-k]

    # un-penalized coefficient update
    b_k_temp <- sum(w * (z - x_notk %*% b_notk) * x_k) / sum(w * x_k2)
    # shrinkage update
    b_k <- S(b_k_temp, lambda / mean(w * x_k2))

    # update beta vector along with other parameters
    beta[k] <- b_k
    #p <- map_dbl(logistic(- X %*% beta), p_adj, epsilon)
    #w <- map_dbl(p, w_adj, epsilon)
  }
}

```



```

    #z <- X %*% beta + (y - p) / w
  }

  iter <- iter + 1

  if(iter == 1000 | max(abs(beta - beta_old)) < 10^-10) {
    print(iter)
    terminate <- 1
  }
}

```

```
## [1] 1000
```

## Combining Results

```

combine_res <- amy_est_0.0001 %>%
  full_join(amy_est_0.001) %>%
  full_join(amy_est_0.01) %>%
  full_join(glm_est) %>%
  mutate(glmnet_est= glmnet_est)

## Joining, by = "term"
## Joining, by = "term"
## Joining, by = "term"

combine_res %>%
  mutate(
    glm_est = round(glm_est,3),
    w_0.0001 = round(w_0.0001,3),
    w_0.001 = round(w_0.001, 3),
    #j_est = round(beta,3)
  ) %>%
  #mutate(term = c(0:(ncol(trn_data)-1))) %>%
  knitr::kable()

```

term	a_0.0001	a_0.001	a_0.01	glm_est	glmnet_est	w_0.0001	w_0.001
intercept	-443.746	-208.587	-217.456	-1165.854	-394.803	-440.216	-176.105
radius_mean	-82.398	-25.090	-26.594	-226.537	-27.666	-81.695	-23.478
texture_mean	-1.083	-0.907	-1.182	-2.968	0.551	-1.074	-0.854
perimeter_mean	12.062	4.584	5.694	33.514	0.013	11.957	4.495
area_mean	0.197	0.018	-0.051	0.531	0.229	0.195	-0.009
smoothness_mean	689.557	248.111	258.230	1944.755	-25.726	683.657	233.946
compactness_mean	-1173.391	-551.774	-537.999	-3261.548	-1021.478	-1163.188	-458.713
concavity_mean	-564.588	-348.851	-400.338	-1344.234	-387.748	-560.612	-307.720
concave.points_mean	1858.833	1348.717	1411.895	4655.386	2238.209	1844.502	1112.090
symmetry_mean	-1161.107	-760.142	-781.333	-3092.685	-850.444	-1151.316	-609.451
fractal_dimension_mean	3515.343	2156.209	2004.182	9771.135	3071.874	3484.983	1695.822
radius_se	763.574	486.470	529.362	1960.594	438.904	757.534	421.324
texture_se	-11.605	-9.954	-10.952	-29.993	-6.644	-11.519	-8.909
perimeter_se	-21.247	-14.016	-16.195	-50.759	-9.283	-21.107	-13.984
area_se	-4.094	-2.450	-2.782	-10.755	-1.580	-4.060	-2.123
smoothness_se	-3947.158	-2961.395	-2961.740	-10030.701	-4492.049	-3916.295	-2466.660
compactness_se	719.542	311.800	392.120	2087.573	-1035.439	713.470	378.441
concavity_se	-631.281	-292.923	-294.554	-1798.657	265.090	-625.920	-275.294
concave.points_se	6698.376	4844.060	5137.757	16699.060	5971.022	6648.329	4172.128
symmetry_se	-1171.617	-816.787	-787.496	-2943.672	-1026.699	-1162.130	-613.508
fractal_dimension_se	-7303.521	-5367.256	-6069.727	-18435.908	-1387.765	-7249.560	-5089.317
radius_worst	-45.210	-49.079	-55.321	-109.899	-9.988	-44.875	-44.414
texture_worst	6.260	4.386	4.602	16.077	4.823	6.210	3.690
perimeter_worst	1.664	1.191	1.435	3.385	1.024	1.656	1.371
area_worst	0.421	0.488	0.547	1.046	0.215	0.417	0.424
smoothness_worst	396.284	325.164	330.644	964.315	672.007	393.308	266.992
compactness_worst	-415.650	-299.911	-328.047	-1045.701	-82.531	-412.484	-268.221
concavity_worst	522.362	323.819	339.607	1334.798	326.429	518.293	274.807
concave.points_worst	13.607	-53.989	-112.800	158.346	-76.691	12.834	-85.613
symmetry_worst	814.391	552.328	550.390	2115.083	707.835	807.668	435.517
fractal_dimension_worst	437.947	497.054	711.435	825.123	-597.772	435.993	570.389