Comparing Full Methods

Amy Pitts

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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(100)
  # 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)
```

Comparing all Methods

We will be comparing:

- Waveley’s Method

- Amy's Method
- base R glm
- glmnet (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)

    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)
}

beta_init <- rep(0.0001, 31) %>% as.matrix()

rerun_NR <- function(beta_init){
  # calling the function
  ans_w <- NewtonRaphson_w(
        list(x = tst_data %>% select(-y) %>% as.matrix(),
         y = tst_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, 30), beta_estimates = beta_est) #%>% knitr::kable()
  return(waveley_est)
}

beta_init <- rep(0.0001, 31) %>% as.matrix()
```

```
w_0.0001 <- rerun_NR(beta_init)$beta_estimates

beta_init <- rep(0.001, 31) %>% 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, 31))
ans0.0001 <- NewtonRaphson_a(tst_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, 31))
ans0.001 <- NewtonRaphson_a(tst_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, 31))
ans0.01 <- NewtonRaphson_a(tst_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

```
# tst_data <- tst_data[c(1:455),]
glm_fit <- glm(y~., data=tst_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 4.0-2
```

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

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)
  ) %>%
  knitr::kable()
```

term	a_0.0001	a_0.001	a_0.01	glm_est	glmnet_est	w_0.0001	w_0.001
intercept	-500.639	-317.865	-186.945	-531.955	-328.388	-117.773	-71.415
radius_mean	54.381	-2.384	-65.451	53.438	5.402	2.271	-0.432
texture_mean	0.899	-0.542	-1.403	0.707	-0.017	-0.828	-0.873
perimeter_mean	-5.612	1.559	6.998	-5.176	-0.005	0.063	0.153
area_mean	-0.025	-0.141	0.234	-0.042	0.005	-0.075	-0.088
smoothness_mean	-4371.611	-2344.025	-1055.376	-4367.474	-425.932	-652.243	-458.810
compactness_mean	-783.025	-131.699	-518.311	-800.934	-154.697	-168.444	-44.831
concavity_mean	-789.277	-715.764	-285.958	-808.732	48.627	-120.500	-122.239
concave.points_mean	2550.294	1219.064	729.534	2544.905	465.188	437.085	316.514
symmetry_mean	812.118	445.358	261.743	816.549	189.609	119.023	85.106
fractal_dimension_mean	6090.275	4085.480	1914.969	6258.990	1409.986	1074.682	868.945
radius_se	481.130	222.306	-23.340	487.902	98.597	77.819	45.078
texture_se	19.266	9.692	1.198	19.035	-7.211	0.325	-0.355
perimeter_se	-39.241	-32.990	-17.829	-39.871	-0.450	-5.075	-6.528
area_se	-1.527	0.832	2.132	-1.529	-0.468	0.011	0.476
smoothness_se	-12889.794	-4096.986	-2605.626	-12946.281	-3681.983	-2365.544	-954.608
compactness_se	633.706	59.812	374.751	798.625	269.835	102.873	9.519
concavity_se	-36.801	-305.758	-48.681	-51.676	138.117	33.722	-63.121
concave.points_se	2922.737	2955.799	2391.190	2975.569	908.110	658.999	684.712
symmetry_se	4172.068	2126.411	1538.266	4196.996	776.000	827.903	521.369
fractal_dimension_se	-21017.063	-9933.822	-13069.095	-21921.470	-10935.789	-4233.825	-2659.719
radius_worst	-24.930	-23.846	17.175	-25.764	4.594	-4.709	-6.083
texture_worst	-1.201	-0.099	0.841	-1.055	0.870	0.675	0.612
perimeter_worst	1.602	2.648	0.553	1.735	-0.024	0.509	0.607
area_worst	0.135	0.181	-0.193	0.137	-0.020	0.078	0.104
smoothness_worst	3081.347	1435.982	890.795	3100.188	854.070	554.271	326.673
compactness_worst	145.331	6.263	61.259	134.278	56.669	34.813	16.541
concavity_worst	143.531	178.861	69.313	147.728	-7.008	20.712	34.117
concave.points_worst	-166.634	-269.162	-219.285	-182.019	-130.643	-79.668	-83.688
symmetry_worst	-729.976	-380.210	-243.393	-731.735	-135.525	-128.321	-85.312
fractal_dimension_worst	565.925	387.287	585.239	626.682	270.973	124.092	75.301