Newton Raphson Full Model

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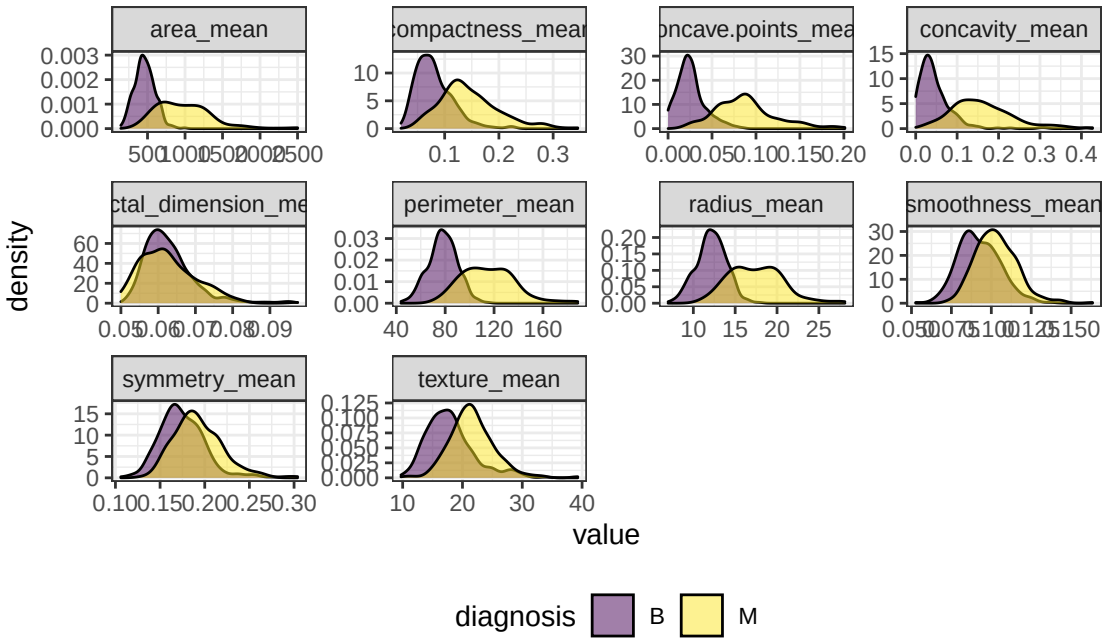
EDA

Let's import and take a look at the data.

Let's take a look at the distributions of other variables.




```
tbl_summary(bc, by = diagnosis)
```

```
## Table printed with `knitr::kable()`, not {gt}. Learn why at
## https://www.danieldsjoberg.com/gtsummary/articles/rmarkdown.html
## To suppress this message, include `message = FALSE` in code chunk header.
```

Characteristic	**B**, N = 357	**M**, N = 212
id	908,916 (874,662, 8,812,816)	895,366 (861,345, 8,911,290)
radius_mean	12.2 (11.1, 13.4)	17.3 (15.1, 19.6)
texture_mean	17.4 (15.2, 19.8)	21.5 (19.3, 23.8)
perimeter_mean	78 (71, 86)	114 (99, 130)
area_mean	458 (378, 551)	932 (705, 1,204)
smoothness_mean	0.091 (0.083, 0.101)	0.102 (0.094, 0.111)
compactness_mean	0.08 (0.06, 0.10)	0.13 (0.11, 0.17)
concavity_mean	0.04 (0.02, 0.06)	0.15 (0.11, 0.20)
concave.points_mean	0.02 (0.02, 0.03)	0.09 (0.06, 0.10)
symmetry_mean	0.171 (0.158, 0.189)	0.190 (0.174, 0.210)
fractal_dimension_mean	0.062 (0.059, 0.066)	0.062 (0.057, 0.067)
radius_se	0.26 (0.21, 0.34)	0.55 (0.39, 0.76)
texture_se	1.11 (0.80, 1.49)	1.10 (0.89, 1.43)
perimeter_se	1.85 (1.45, 2.39)	3.68 (2.72, 5.21)
area_se	20 (15, 25)	58 (36, 94)
smoothness_se	0.0065 (0.0052, 0.0085)	0.0062 (0.0051, 0.0080)
compactness_se	0.016 (0.011, 0.026)	0.029 (0.020, 0.039)
concavity_se	0.018 (0.011, 0.031)	0.037 (0.027, 0.050)
concave.points_se	0.009 (0.006, 0.012)	0.014 (0.011, 0.017)
symmetry_se	0.019 (0.016, 0.024)	0.018 (0.015, 0.022)
fractal_dimension_se	0.0028 (0.0021, 0.0042)	0.0037 (0.0027, 0.0049)
radius_worst	13.3 (12.1, 14.8)	20.6 (17.7, 23.8)
texture_worst	22.8 (19.6, 26.5)	28.9 (25.8, 32.7)
perimeter_worst	87 (78, 97)	138 (119, 160)
area_worst	547 (447, 670)	1,303 (970, 1,713)
smoothness_worst	0.125 (0.110, 0.138)	0.143 (0.130, 0.156)
compactness_worst	0.17 (0.11, 0.23)	0.36 (0.24, 0.45)
concavity_worst	0.14 (0.08, 0.22)	0.40 (0.33, 0.56)
concave.points_worst	0.07 (0.05, 0.10)	0.18 (0.15, 0.21)
symmetry_worst	0.27 (0.24, 0.30)	0.31 (0.28, 0.36)
fractal_dimension_worst	0.077 (0.070, 0.085)	0.088 (0.076, 0.103)

We want our outcome variable to be binary. Let's create a new outcome variable, `y`, which will be 1 if `diagnosis == 'M'` and 0 if 'diagnosis == 'B'.

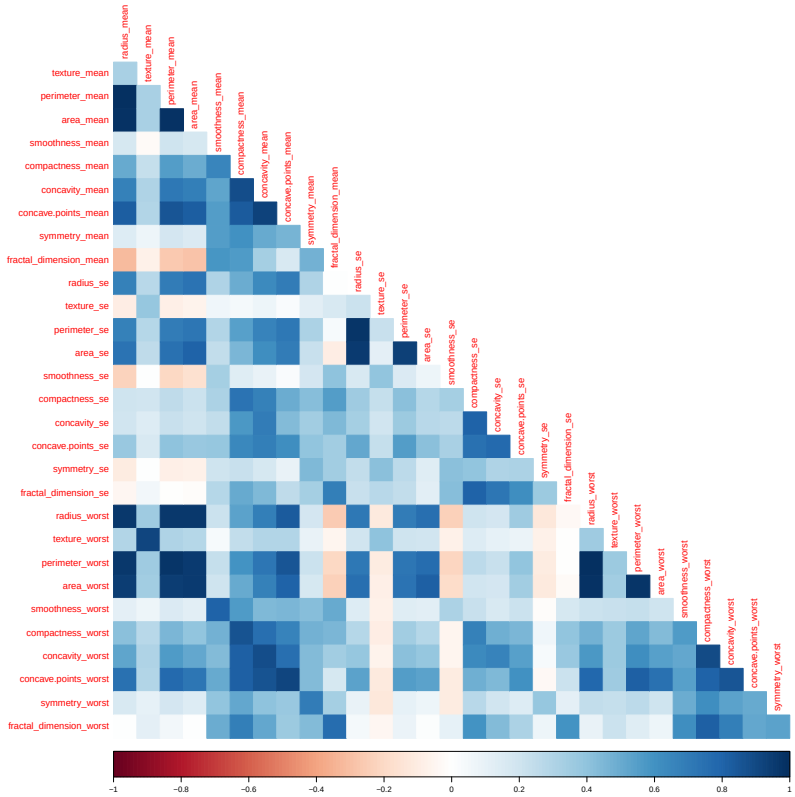
```
bc <- bc %>% mutate(y = ifelse(diagnosis == "M", 1, 0)) %>% relocate(y)
```

Multicollinearity Investigation

Let's look at the correlations for all predictors.

```
cor_cov_all <- cor(bc %>% select(-c(id, y, diagnosis)))

corrplot::corrplot(cor_cov_all,
                   method = "color",
                   type = "lower",
                   insig = "blank",
                   diag = FALSE)
```

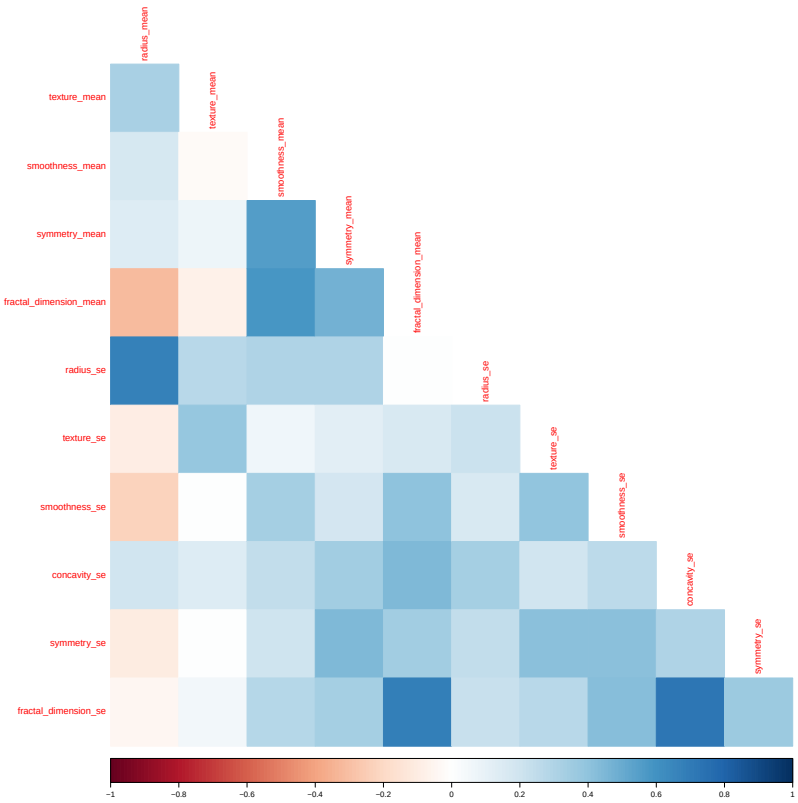


Yikes. Let's make some cuts ($r^2 > 0.9$) and reevaluate.

```
covariates <-
  bc %>%
  select(-c(id, y, diagnosis)) %>%
  dplyr::select(-contains("area")) %>%
  dplyr::select(-contains("perimeter")) %>%
  dplyr::select(-ends_with("_worst")) %>%
  dplyr::select(-c("concavity_mean",
                   "compactness_mean",
                   "concave.points_mean",
                   "compactness_se",
                   "concave.points_se"))

cor_cov <- cor(covariates)


corrplot::corrplot(cor_cov,
                   method = "color",
                   type = "lower",
                   insig = "blank",
                   diag = FALSE)
```



Better. We'll proceed with these predictors.

```
fin_names <- covariates %>% names()
```

Full Model

We want to establish logistic model using all variables in the dataset. We will do this by performing a Newton Raphson optimization in order to find the MLEs of the beta coefficients.

The likelihood function for a logistic model is defined as follows:

$$f(\beta_0, \beta_1, ..., \beta_{30}) = \sum_{i=1}^{n} \left(Y_i \left(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij} \right) - \log(1 + e^{\left(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}\right)}) \right)$$

Let $\pi_i = \frac{e^{\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}}}{1 + e^{\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}}}$. Then, the gradient of this function is defined as follows:

$$\nabla f(\beta_0, \beta_1, ..., \beta_p) = \begin{pmatrix} \sum_{i=1}^{n} Y_i - \pi_i \\ \sum_{i=1}^{n} x_{i1}(Y_i - \pi_i) \\ \sum_{i=1}^{n} x_{i2}(Y_i - \pi_i) \\ \vdots \\ \sum_{i=1}^{n} x_{ip}(Y_i - \pi_i) \end{pmatrix}$$

Finally, we define the Hessian of this function as follows:

$$\nabla^2 f(\beta_0, \beta_1, ..., \beta_p) = -\sum_{i=1}^{n} \begin{pmatrix} 1 \\ x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix} (1 \; x_{i1} \; x_{i2} \; \dots \; x_{ip}) \, \pi_i(1-\pi_i)$$

$$= -\begin{pmatrix} \sum_{i=1}^n \pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{ip}\pi_i(1-\pi_i) \\ \sum_{i=1}^n x_{i1}\pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}^2\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{ip}x_{i1}\pi_i(1-\pi_i) \\ \sum_{i=1}^n x_{i2}\pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}x_{i2}\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{ip}x_{i2}\pi_i(1-\pi_i) \\ \vdots & \ddots & \ddots & \vdots \\ \sum_{i=1}^n x_{ip}\pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}x_{ip}\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{ip}^2\pi_i(1-\pi_i) \end{pmatrix}$$

$$= (1 \; x_{i1} \; x_{i2} \; \dots \; x_{ip}) \, I(\pi_i(1-\pi_i)) \begin{pmatrix} 1 \\ x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix}$$

Let's create a function that produces the log-likelihood, gradient vector, and hessian matrix, given a dataset and beta vector:

```
loglike_func <- function(dat, betavec){

  dat = bc_train

  # x matrix
  dat_temp <-
    dat %>%
    mutate(intercept = 1) %>%
    select(-y) %>%
    relocate(intercept)

  dat_x <-
    dat_temp %>%
    as.matrix() %>%
    unname()

  # pi vector
  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 <- diag(nrow(pi))
  diag(W) <- pi*(1 - pi)
  hess <- -(t(dat_x) %*% W %*% (dat_x))

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

```
}
```

Now, let's construct a Newton Raphson algorithm to determine β_i coefficients that maximize the likelihood of the function.

```
NewtonRaphson <- 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

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

    # step halving
    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)
}
```

Splitting Testing and Training Data

Using a function from `partition.R`, we will split our data into testing and training. We will include only the variables we have identified as being sufficiently uncorrelated.

```
col.num <- which(colnames(bc) %in% fin_names) # get those variables
bc_trunc <- bc[, c(1, col.num)]
```

```
bc_test_train <- partition(0.8, bc_trunc)

bc_test <- bc_test_train %>% filter(part_id == "test") %>% select(-part_id)
bc_train <- bc_test_train %>% filter(part_id == "train") %>% select(-part_id)
```

Running Newton-Raphson Algorithm

Let's establish a beta vector and run the Newton-Raphson algorithm we've established on the training data.

```
betavec <- c(rep(0.01, ncol(bc_train))) %>% as.matrix()
nr1 <- NewtonRaphson(bc_train, betavec)
beta_est <- nr1[nrow(nr1), -c(1:3)] %>% as.vector()
```

Compare with GLM and GLMNET

Let's run GLM.

```
glm_fit <- glm(y~., data = bc_train, family = "binomial")
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

```
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)) %>% pull(glm_est)
```

Now, let's run GLMNET.

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

```
tibble(
  beta_sub = 0:(length(beta_est) - 1),
  nr_est = beta_est,
  glm_est = glm_est,
  glmnet_est = glmnet_est
)
```

```
## # A tibble: 12 x 4
##    beta_sub   nr_est  glm_est glmnet_est
##       <int>    <dbl>    <dbl>      <dbl>
##  1        0  -54.6    -54.6      -54.6
##  2        1    1.39     1.39       1.39
##  3        2    0.549    0.549      0.549
##  4        3   80.8     80.8       81.1
##  5        4   34.6     34.6       34.6
##  6        5  179.     179.       178.
##  7        6    8.71     8.71       8.70
##  8        7   -0.908   -0.908     -0.908
##  9        8  -43.8    -43.8      -44.3
## 10        9   39.6     39.6       39.6
```

```
## 11       10 -134.    -134.      -134.
## 12       11 -685.    -685.      -683.
```

AUC

```
auc_calc_full <- function(beta_est, test_data){
  # pulling out the terms used in the full model (should be all)

  # we have this flexible in case we want to test fewer variables
  # terms <- beta_est %>% pull(term)
  # col.num <- which(colnames(test_data) %in% terms)
  # select the desired x values

  xvals <- test_data[,-1] %>%
     mutate(
       intercept = 1 # create a intercept variable
    ) %>%
    relocate(intercept) # move it to the front

  pred <- as.matrix(xvals) %*% beta_est # get the cross product of the linear model
  logit_pred <- exp(pred) / (1 + exp(pred)) # link function to get probabilities

  auc_val <- auc(test_data$y, as.vector(logit_pred)) # calculating the AUC

  # roc(tst_data$y, as.vector(logit_pred)) %>% plot( legacy.axes=TRUE) # graphs AUC
  return(auc_val)

}

auc <- auc_calc_full(beta_est, bc_test)
```

```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls < cases
```

The AUC of the Newton-Raphson Model is 0.973454.