# Tinkering

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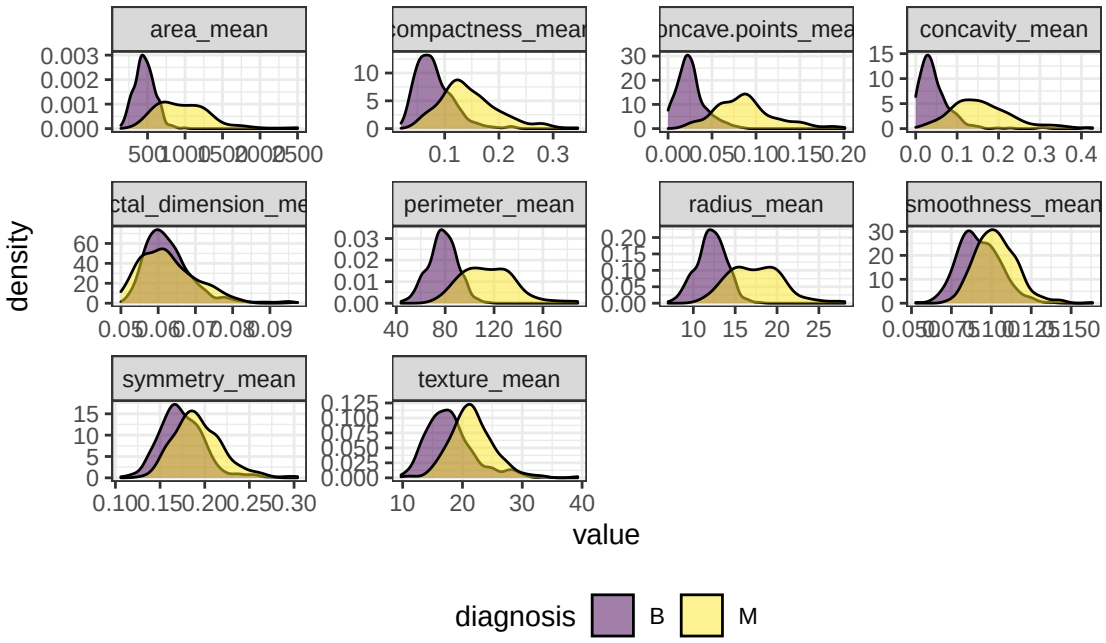
## EDA

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) |

| **Characteristic** | **B**, N = 357 | **M**, N = 212 |
|---|---|---|
| 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) |

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

## Logistic Function

The likelihood function is defined as follows:

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

Let $\pi_i = \frac{e^{\beta_0 + \sum_{j=1}^{30} \beta_j x_{ij}}}{1 + e^{\beta_0 + \sum_{j=1}^{30} \beta_j x_{ij}}}$. Then, the gradient of this function is defined as follows:

$$\nabla f(\beta_0, \beta_1, ..., \beta_{30}) = \begin{pmatrix} \sum_{i=1}^{n} Y_i - \pi_i \\ \sum_{i=1}^{n} x_{i1}(Y_i - \pi_i) \\ \sum_{i=1}^{n} x_{i2}(Y_i - \pi_i) \\ \vdots \\ \sum_{i=1}^{n} x_{i30}(Y_i - \pi_i) \end{pmatrix}$$

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

$$\nabla^2 f(\beta_0, \beta_1, ..., \beta_{30}) = -\sum_{i=1}^{n} \begin{pmatrix} 1 \\ x_{i1} \\ x_{i2} \\ \vdots \\ x_{i30} \end{pmatrix} (1 \; x_{i1} \; x_{i2} \; \dots \; x_{i30}) \, \pi_i(1-\pi_i)$$

$$= -\begin{pmatrix} \sum_{i=1}^n \pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{i30}\pi_i(1-\pi_i) \\ \sum_{i=1}^n x_{i1}\pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}^2\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{i30}x_{i1}\pi_i(1-\pi_i) \\ \sum_{i=1}^n x_{i2}\pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}x_{i2}\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{i30}x_{i2}\pi_i(1-\pi_i) \\ \vdots & \ddots & \ddots & \vdots \\ \sum_{i=1}^n x_{i30}\pi_i(1-\pi_i) & \sum_{i=1}^n x_{i1}x_{i30}\pi_i(1-\pi_i) & \dots & \sum_{i=1}^n x_{i30}^2\pi_i(1-\pi_i) \end{pmatrix}$$

$$= (1 \; x_{i1} \; x_{i2} \; \dots \; x_{i30}) \, I(\pi_i(1-\pi_i)) \begin{pmatrix} 1 \\ x_{i1} \\ x_{i2} \\ \vdots \\ x_{i30} \end{pmatrix}$$

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

```
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
```

```
  ))
}
```

## Newton-Raphson Algorithm

Now, let's write a Newton-Raphson algorithm to find the beta coefficients that maximize likelihood.

The unmodified estimate of $\theta_i = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_3 0 \end{bmatrix}$ at each step $i$ of the Newton Raphson algorithm is:

$$\theta_i = \theta_{i-1} - [\nabla^2 f(\theta_{i-1})]^{-1} \nabla f(\theta_{i-1})$$

In this modified Newton Raphson algorithm, we want to first ensure that the $\nabla^2 f(\theta_{i-1})$ is either negative definite or replaced with a similar matrix that is negative definite. To do this, we will update the algorithm to be as follows:

$$\theta_i = \theta_{i-1} - [\nabla^2 f(\theta_{i-1}) - kI]^{-1} \nabla f(\theta_{i-1}),$$

where $I$ is the identity matrix and $k$ is a constant that allows $\nabla^2 f(\theta_{i-1}) - kI$ to be negative definite. If $\nabla^2 f(\theta_{i-1})$ is already negative definite, $k$ will be 0.

Next, we want to add step-halving into our algorithm. We will proceed as follows:

$$\theta_i = \theta_{i-1} - \frac{1}{2^j} [\nabla^2 f(\theta_{i-1}) - kI]^{-1} \nabla f(\theta_{i-1}),$$

where $j$ is chosen in a stepwise fashion, until $f(\theta_i) > f(\theta_{i-1})$.

```
NewtonRaphson <- 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 - 0.0001*diag(31)
       # 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)
}
```

Let's start with all beta coefficients being 0.001.

```
beta_init <- rep(0.001, 31) %>% as.matrix()

test1 <- logistic_stuff(
  list(x = bc[,-c(1,2, 3)] %>% as.matrix(),
       y = bc$bin_out %>% as.matrix()),
  beta = beta_init)

ans <- NewtonRaphson(
      list(x = bc[,-c(1,2, 3)] %>% as.matrix(),
       y = bc$bin_out %>% as.matrix()),
       logistic_stuff,
       beta_init)
```

The beta estimates are as follows:

```
if (sum(is.na(ans[nrow(ans),])) > 0) {
  beta_est <- ans[nrow(ans) - 1, -c(1,2)]
}

if (sum(is.na(ans[nrow(ans),])) == 0) {
  beta_est <- ans[nrow(ans), -c(1,2)]
}

tibble(beta_subscript = seq(0, 30), beta_estimates = beta_est) %>% knitr::kable()
```

| beta_subscript | beta_estimates |
|---|---|
| 0 | -35.6788855 |
| 1 | -25.8450679 |
| 2 | 0.2364029 |
| 3 | 0.5233921 |
| 4 | 0.1930977 |
| 5 | 374.2231831 |
| 6 | -274.0661692 |
| 7 | 112.3745441 |
| 8 | 197.4735980 |
| 9 | -81.7535878 |
| 10 | 159.0248149 |

| beta_subscript | beta_estimates |
|---|---|
| 11 | -8.7382958 |
| 12 | -3.6859107 |
| 13 | -3.5505959 |
| 14 | 0.6320060 |
| 15 | 229.4048089 |
| 16 | 491.9823911 |
| 17 | -394.7461298 |
| 18 | 1835.8287537 |
| 19 | -331.3771487 |
| 20 | -5753.5678242 |
| 21 | 9.2644874 |
| 22 | 0.8250521 |
| 23 | 0.1906329 |
| 24 | -0.0454310 |
| 25 | -131.4051756 |
| 26 | -43.7531684 |
| 27 | 47.8195818 |
| 28 | -22.8843059 |
| 29 | 80.0735290 |
| 30 | 555.5843554 |

## Lasso

Now, let's try lasso.

$$f(\beta_0, \beta_1, \ldots, \beta_{30}) \approx -\frac{1}{2n}\sum_{i=1}^{n} w_i \left( z_i - (\mathbf{1} \quad \mathbf{x_i}) \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{30} \end{pmatrix} \right)^2 + C(\tilde{\beta_0}, \tilde{\beta_1}, \ldots, \tilde{\beta_{30}})$$

$$z_i = (\mathbf{1} \quad \mathbf{x_i}) \begin{pmatrix} \tilde{\beta_1} \\ \tilde{\beta_2} \\ \vdots \\ \tilde{\beta_{30}} \end{pmatrix} + \frac{\mathbf{y_i} - \tilde{\mathbf{p}}_\mathbf{i}(\mathbf{x_i})}{\tilde{\mathbf{p}}_\mathbf{i}(\mathbf{x_i})(\mathbf{1} - \tilde{\mathbf{p}}_\mathbf{i}(\mathbf{x_i}))}$$

$$w_i = \tilde{p_i}(x_i)(1 - \tilde{p_i}(x_i))$$

$$\tilde{p_i} = \frac{\exp\left( (\mathbf{1} \quad \mathbf{x_i}) \begin{pmatrix} \tilde{\beta_1} \\ \tilde{\beta_2} \\ \vdots \\ \tilde{\beta_{30}} \end{pmatrix} \right)}{1 + \exp\left( (\mathbf{1} \quad \mathbf{x_i}) \begin{pmatrix} \tilde{\beta_1} \\ \tilde{\beta_2} \\ \vdots \\ \tilde{\beta_{30}} \end{pmatrix} \right)}$$

$$\min_{(\beta_0, \beta_1, \ldots, \beta_{30})} L(\beta_0, \beta_1, \ldots, \beta_{30}) = \left\{ -l(\beta_0, \beta_1, \ldots, \beta_{30}) + \lambda \sum_{j=0}^{30} |\beta_j| \right\}$$

**Quadratic Approximation**

```
quad_log_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
  ))

}
```