

# Research Log Project Machine Learning

Diagnosing malignancy of breast masses using Machine Learning

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# 1 Preparing R environment

For the data analysis and further processes multiple libraries are needed, they are loaded in here. A few other options/settings are also configured here.

```
# Create vector with all packages that are required
packages <- c("tidyverse", "pander", "ggplot2", "data.table", "ggpubr")
# Load each package in the vector with lapply
invisible(lapply(packages, library, character.only = TRUE))
# Drop the packages variable from memory since it will not be used again
remove(packages)

# Disable printing 'table continues' lines between split sections
panderOptions("table.continues", "")
# Change affix after table caption if it's a split table
panderOptions("table.continues.affix", "(table continues below)")
```

## 2 Exploratory Data Analysis

### 2.1 About the chosen data set

#### Origin of the data

The data set that is used is the *Wisconsin Breast Cancer (Diagnostic) Data Set*, which is publicly available from the UCI Machine Learning Repository. There are two published research articles, from the same team of researchers, where the data set was first used, namely [1] and [2]. The samples for the data were collected from 569 patients at the University of Wisconsin Hospital with the goal of creating a machine learning model that was faster, improved the correctness and increased the objectivity of the diagnosis process of breast cancer.

#### Collection of the data

The data was gathered by first collecting the fine needle aspirates (FNA), which are expressed on a glass slide and stained. A color video camera mounted on top of a microscope, where the images were projected into the camera with a 63x objective and 2.5x ocular. The image was then captured by a color frame grabber board as a 512x480, 8-bit-per-pixel Targa file.

The digitized image is then analyzed in the program Xcyt (custom made by Nick Street). First the user marks approximate initial boundaries of the nuclei and then the actual boundaries are further defined with an active contour model known as “Snake”. In the end the snake reaches a point where it’s curve accurately corresponds to the boundary of a cell nucleus. From the snake-generated cell nuclei boundaries 10 features are extracted, these are numerically modeled such that larger values will typically indicate a higher likelihood of malignancy.

The ten features that are extracted for each cell nucleus are the following:

1. Radius (mean of distances from center to points on the perimeter)
2. Texture (standard deviation of gray-scale values)
3. Perimeter (the total distance between all the points of the snake-generated boundary)
4. Area (the nuclear area is the sum of pixels on the interior, with half of the pixels of the perimeter)
5. Smoothness (local variation in radius lengths)
6. Compactness ( $\text{perimeter}^2 / \text{area} - 1.0$ )
7. Concavity (severity of concave portions of the contour)
8. Concave points (number of concave portions of the contour)
9. Symmetry (difference in length of perpendicular lines to the longest chord through the center, in both directions)
10. Fractal dimension (approximated using Mandelbrot’s “coastline approximation” - 1)

For each feature and for every image, three final values were computed and saved to the data set, namely the mean, standard error and the extreme (largest) value.

#### Data structure and codebook

The data set has 569 instances/rows with 32 columns, an ID column, a classification column with the diagnosis (benign or malignant) and 30 columns describing the nuclei boundaries (10x mean/extreme/se). Because the data set itself does not come with an annotated header with column names, a codebook has been manually made. This codebook has the abbreviated column name, the full column name, the data type and a description for each feature/column.

Below is an overview of the columns in the data set, shown using the contents of the codebook after it has been loaded in:

```
codebook <- readr::read_delim("data/codebook.txt", delim = "|", show_col_types = FALSE)

# Pretty print the codebook (without descriptions) using pander
pander::pander(codebook[,1:3], style = "rmarkdown", caption = "Overview of created codebook excluding d
```

Table 1: Overview of created codebook excluding descriptions

| Column Name       | Full Name                        | Type |
|-------------------|----------------------------------|------|
| id                | ID                               | dbl  |
| diagnosis         | Diagnosis                        | fct  |
| radius_mean       | Mean Radius                      | dbl  |
| texture_mean      | Mean Texture                     | dbl  |
| perimeter_mean    | Mean Perimeter                   | dbl  |
| area_mean         | Mean Area                        | dbl  |
| smoothness_mean   | Mean Smoothness                  | dbl  |
| compactness_mean  | Mean Compactness                 | dbl  |
| concavity_mean    | Mean Concavity                   | dbl  |
| concave_pts_mean  | Mean Concave Points              | dbl  |
| symmetry_mean     | Mean Symmetry                    | dbl  |
| fractal_dim_mean  | Mean Fractal Dimension           | dbl  |
| radius_se         | Radius Standard Error            | dbl  |
| texture_se        | Texture Standard Error           | dbl  |
| perimeter_se      | Perimeter Standard Error         | dbl  |
| area_se           | Area Standard Error              | dbl  |
| smoothness_se     | Smoothness Standard Error        | dbl  |
| compactness_se    | Compactness Standard Error       | dbl  |
| concavity_se      | Concavity Standard Error         | dbl  |
| concave_pts_se    | Concave Points Standard Error    | dbl  |
| symmetry_se       | Symmetry Standard Error          | dbl  |
| fractal_dim_se    | Fractal Dimension Standard Error | dbl  |
| radius_worst      | Worst Radius                     | dbl  |
| texture_worst     | Worst Texture                    | dbl  |
| perimeter_worst   | Worst Perimeter                  | dbl  |
| area_worst        | Worst Area                       | dbl  |
| smoothness_worst  | Worst Smoothness                 | dbl  |
| compactness_worst | Worst Compactness                | dbl  |
| concavity_worst   | Worst Concavity                  | dbl  |
| concave_pts_worst | Worst Concave Points             | dbl  |
| symmetry_worst    | Worst Symmetry                   | dbl  |
| fractal_dim_worst | Worst Fractal Dimension          | dbl  |

As can be seen, all the features are of the type double except the main diagnosis classification factor.

## 2.2 Loading in the data set

The data will be loaded in with the `read_csv` function from the `readr` package, this function returns the data as a tibble data frame. This function allows a vector with column names to be given with an argument, the names from the column `Column Name` of the codebook will be used.

```
data <- readr::read_csv("data/wdbc.data", col_names = codebook[[1]], show_col_types = FALSE)

# Print the amount of samples and columns
cat("Amount of samples:", dim(data)[1], "\tColumns in dataframe:", dim(data)[2], "\n")
```

```
## Amount of samples: 569    Columns in dataframe: 32
```

The amount of samples and columns are as expected, so in this aspect the data set has been read correctly. However, what is more important is if the values are read correctly, since the values are that what is actually going to be used.

```
str(data)

## spec_tbl_df [569 x 32] (S3: spec_tbl_df/tbl_df/tbl/data.frame)
##  $ id                : num [1:569] 842302 842517 84300903 84348301 84358402 ...
##  $ diagnosis          : chr [1:569] "M" "M" "M" "M" ...
##  $ radius_mean        : num [1:569] 18 20.6 19.7 11.4 20.3 ...
##  $ texture_mean       : num [1:569] 10.4 17.8 21.2 20.4 14.3 ...
##  $ perimeter_mean     : num [1:569] 122.8 132.9 130 77.6 135.1 ...
##  $ area_mean          : num [1:569] 1001 1326 1203 386 1297 ...
##  $ smoothness_mean    : num [1:569] 0.1184 0.0847 0.1096 0.1425 0.1003 ...
##  $ compactness_mean   : num [1:569] 0.2776 0.0786 0.1599 0.2839 0.1328 ...
##  $ concavity_mean     : num [1:569] 0.3001 0.0869 0.1974 0.2414 0.198 ...
##  $ concave_pts_mean   : num [1:569] 0.1471 0.0702 0.1279 0.1052 0.1043 ...
##  $ symmetry_mean      : num [1:569] 0.242 0.181 0.207 0.26 0.181 ...
##  $ fractal_dim_mean   : num [1:569] 0.0787 0.0567 0.06 0.0974 0.0588 ...
##  $ radius_se          : num [1:569] 1.095 0.543 0.746 0.496 0.757 ...
##  $ texture_se         : num [1:569] 0.905 0.734 0.787 1.156 0.781 ...
##  $ perimeter_se       : num [1:569] 8.59 3.4 4.58 3.44 5.44 ...
##  $ area_se           : num [1:569] 153.4 74.1 94 27.2 94.4 ...
##  $ smoothness_se      : num [1:569] 0.0064 0.00522 0.00615 0.00911 0.01149 ...
##  $ compactness_se     : num [1:569] 0.049 0.0131 0.0401 0.0746 0.0246 ...
##  $ concavity_se       : num [1:569] 0.0537 0.0186 0.0383 0.0566 0.0569 ...
##  $ concave_pts_se     : num [1:569] 0.0159 0.0134 0.0206 0.0187 0.0188 ...
##  $ symmetry_se        : num [1:569] 0.03 0.0139 0.0225 0.0596 0.0176 ...
##  $ fractal_dim_se     : num [1:569] 0.00619 0.00353 0.00457 0.00921 0.00511 ...
##  $ radius_worst       : num [1:569] 25.4 25 23.6 14.9 22.5 ...
##  $ texture_worst      : num [1:569] 17.3 23.4 25.5 26.5 16.7 ...
##  $ perimeter_worst    : num [1:569] 184.6 158.8 152.5 98.9 152.2 ...
##  $ area_worst         : num [1:569] 2019 1956 1709 568 1575 ...
##  $ smoothness_worst   : num [1:569] 0.162 0.124 0.144 0.21 0.137 ...
##  $ compactness_worst  : num [1:569] 0.666 0.187 0.424 0.866 0.205 ...
##  $ concavity_worst    : num [1:569] 0.712 0.242 0.45 0.687 0.4 ...
##  $ concave_pts_worst  : num [1:569] 0.265 0.186 0.243 0.258 0.163 ...
##  $ symmetry_worst     : num [1:569] 0.46 0.275 0.361 0.664 0.236 ...
##  $ fractal_dim_worst  : num [1:569] 0.1189 0.089 0.0876 0.173 0.0768 ...
```

Luckily it looks like the values for every column have correctly been read, but there is one thing that could still be changed; the diagnosis column. It would be more helpful if diagnosis was a factor and not just a character column.

```
data$diagnosis <- factor(data$diagnosis, labels = c("Benign", "Malignant"))

ggplot(data, aes(x = diagnosis, fill = diagnosis)) + geom_bar() +
  geom_text(stat='count', aes(label = after_stat(count)), nudge_y = -15) +
  scale_fill_hue(direction = 1, h.start=180)
```

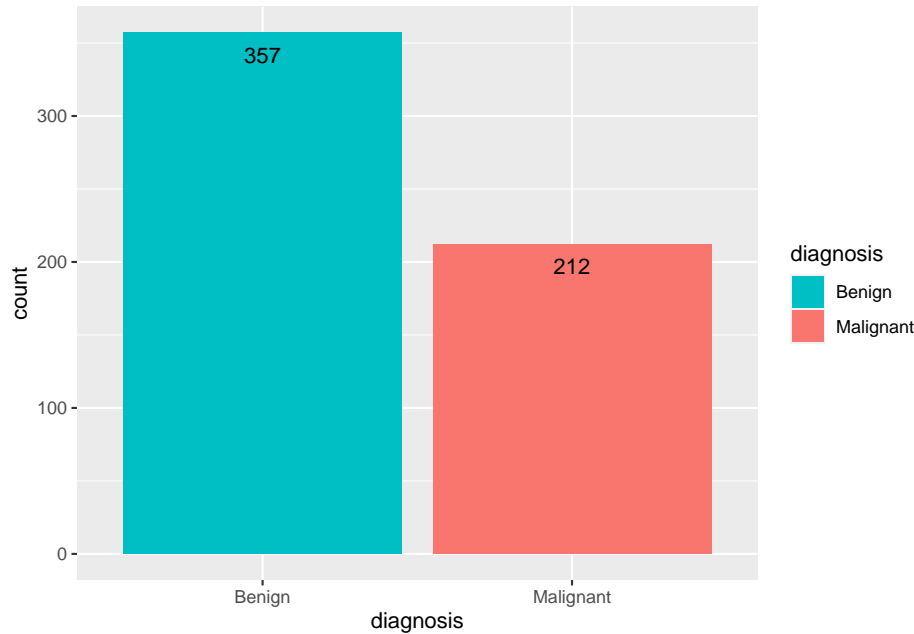


Figure 1: Distribution of diagnosis classification

There are more benign cases than malignant, this means the data set is not entirely balanced and could cause bias if not handled correctly.

For the analysis and the creation of the machine learning model the ID column is not needed, it can therefore be dropped from the data frame.

```
data <- dplyr::select(data, -id)
colnames(data)
```

```
## [1] "diagnosis"      "radius_mean"    "texture_mean"
## [4] "perimeter_mean" "area_mean"      "smoothness_mean"
## [7] "compactness_mean" "concavity_mean" "concave_pts_mean"
## [10] "symmetry_mean"   "fractal_dim_mean" "radius_se"
## [13] "texture_se"      "perimeter_se"    "area_se"
## [16] "smoothness_se"   "compactness_se"  "concavity_se"
## [19] "concave_pts_se"  "symmetry_se"     "fractal_dim_se"
## [22] "radius_worst"    "texture_worst"   "perimeter_worst"
## [25] "area_worst"      "smoothness_worst" "compactness_worst"
## [28] "concavity_worst" "concave_pts_worst" "symmetry_worst"
## [31] "fractal_dim_worst"
```

## 2.3 Data inspection

### Checking for missing values

A good understanding of what the data is like is important, namely how the data is distributed and if there is data corruption. Thing to check are if there are outliers and if there is any skewed or missing data.

```
cat("Missing values:", any(is.na(data)))
```

```
## Missing values: FALSE
```

Luckily there are no missing values in the data set. But now it is good to get an idea of what the values of the columns look like, what ranges do they fall in? This is done by the function `summary()`, it will show basic statistics about the columns to create an overview.

### Overall data summary

```
pander::pander(summary(data), caption = "Summary with basic statistics about the data columns")
```

Table 2: Summary with basic statistics about the data columns  
(table continues below)

| diagnosis     | radius_mean    | texture_mean  | perimeter_mean |
|---------------|----------------|---------------|----------------|
| Benign :357   | Min. : 6.981   | Min. : 9.71   | Min. : 43.79   |
| Malignant:212 | 1st Qu.:11.700 | 1st Qu.:16.17 | 1st Qu.: 75.17 |
| NA            | Median :13.370 | Median :18.84 | Median : 86.24 |
| NA            | Mean :14.127   | Mean :19.29   | Mean : 91.97   |
| NA            | 3rd Qu.:15.780 | 3rd Qu.:21.80 | 3rd Qu.:104.10 |
| NA            | Max. :28.110   | Max. :39.28   | Max. :188.50   |

| area_mean      | smoothness_mean | compactness_mean | concavity_mean  |
|----------------|-----------------|------------------|-----------------|
| Min. : 143.5   | Min. :0.05263   | Min. :0.01938    | Min. :0.00000   |
| 1st Qu.: 420.3 | 1st Qu.:0.08637 | 1st Qu.:0.06492  | 1st Qu.:0.02956 |
| Median : 551.1 | Median :0.09587 | Median :0.09263  | Median :0.06154 |
| Mean : 654.9   | Mean :0.09636   | Mean :0.10434    | Mean :0.08880   |
| 3rd Qu.: 782.7 | 3rd Qu.:0.10530 | 3rd Qu.:0.13040  | 3rd Qu.:0.13070 |
| Max. :2501.0   | Max. :0.16340   | Max. :0.34540    | Max. :0.42680   |

| concave_pts_mean | symmetry_mean  | fractal_dim_mean | radius_se      |
|------------------|----------------|------------------|----------------|
| Min. :0.00000    | Min. :0.1060   | Min. :0.04996    | Min. :0.1115   |
| 1st Qu.:0.02031  | 1st Qu.:0.1619 | 1st Qu.:0.05770  | 1st Qu.:0.2324 |
| Median :0.03350  | Median :0.1792 | Median :0.06154  | Median :0.3242 |
| Mean :0.04892    | Mean :0.1812   | Mean :0.06280    | Mean :0.4052   |
| 3rd Qu.:0.07400  | 3rd Qu.:0.1957 | 3rd Qu.:0.06612  | 3rd Qu.:0.4789 |
| Max. :0.20120    | Max. :0.3040   | Max. :0.09744    | Max. :2.8730   |



| texture_se     | perimeter_se   | area_se         | smoothness_se    |
|----------------|----------------|-----------------|------------------|
| Min. :0.3602   | Min. : 0.757   | Min. : 6.802    | Min. :0.001713   |
| 1st Qu.:0.8339 | 1st Qu.: 1.606 | 1st Qu.: 17.850 | 1st Qu.:0.005169 |
| Median :1.1080 | Median : 2.287 | Median : 24.530 | Median :0.006380 |
| Mean :1.2169   | Mean : 2.866   | Mean : 40.337   | Mean :0.007041   |
| 3rd Qu.:1.4740 | 3rd Qu.: 3.357 | 3rd Qu.: 45.190 | 3rd Qu.:0.008146 |
| Max. :4.8850   | Max. :21.980   | Max. :542.200   | Max. :0.031130   |

| compactness_se   | concavity_se    | concave_pts_se   | symmetry_se      |
|------------------|-----------------|------------------|------------------|
| Min. :0.002252   | Min. :0.00000   | Min. :0.000000   | Min. :0.007882   |
| 1st Qu.:0.013080 | 1st Qu.:0.01509 | 1st Qu.:0.007638 | 1st Qu.:0.015160 |
| Median :0.020450 | Median :0.02589 | Median :0.010930 | Median :0.018730 |
| Mean :0.025478   | Mean :0.03189   | Mean :0.011796   | Mean :0.020542   |
| 3rd Qu.:0.032450 | 3rd Qu.:0.04205 | 3rd Qu.:0.014710 | 3rd Qu.:0.023480 |
| Max. :0.135400   | Max. :0.39600   | Max. :0.052790   | Max. :0.078950   |

| fractal_dim_se    | radius_worst  | texture_worst | perimeter_worst |
|-------------------|---------------|---------------|-----------------|
| Min. :0.0008948   | Min. : 7.93   | Min. :12.02   | Min. : 50.41    |
| 1st Qu.:0.0022480 | 1st Qu.:13.01 | 1st Qu.:21.08 | 1st Qu.: 84.11  |
| Median :0.0031870 | Median :14.97 | Median :25.41 | Median : 97.66  |
| Mean :0.0037949   | Mean :16.27   | Mean :25.68   | Mean :107.26    |
| 3rd Qu.:0.0045580 | 3rd Qu.:18.79 | 3rd Qu.:29.72 | 3rd Qu.:125.40  |
| Max. :0.0298400   | Max. :36.04   | Max. :49.54   | Max. :251.20    |

| area_worst     | smoothness_worst | compactness_worst | concavity_worst |
|----------------|------------------|-------------------|-----------------|
| Min. : 185.2   | Min. :0.07117    | Min. :0.02729     | Min. :0.0000    |
| 1st Qu.: 515.3 | 1st Qu.:0.11660  | 1st Qu.:0.14720   | 1st Qu.:0.1145  |
| Median : 686.5 | Median :0.13130  | Median :0.21190   | Median :0.2267  |
| Mean : 880.6   | Mean :0.13237    | Mean :0.25427     | Mean :0.2722    |
| 3rd Qu.:1084.0 | 3rd Qu.:0.14600  | 3rd Qu.:0.33910   | 3rd Qu.:0.3829  |
| Max. :4254.0   | Max. :0.22260    | Max. :1.05800     | Max. :1.2520    |

| concave_pts_worst | symmetry_worst | fractal_dim_worst |
|-------------------|----------------|-------------------|
| Min. :0.00000     | Min. :0.1565   | Min. :0.05504     |
| 1st Qu.:0.06493   | 1st Qu.:0.2504 | 1st Qu.:0.07146   |
| Median :0.09993   | Median :0.2822 | Median :0.08004   |
| Mean :0.11461     | Mean :0.2901   | Mean :0.08395     |
| 3rd Qu.:0.16140   | 3rd Qu.:0.3179 | 3rd Qu.:0.09208   |
| Max. :0.29100     | Max. :0.6638   | Max. :0.20750     |

By glancing over the summary created above a few things can be noticed and questions can arise, for example the `area_mean`, `concave_pts_mean`, `radius_se`, `perimeter_se` and `area_worst` columns. These, among other columns, have a wide range of values with their minimum or maximum values far from the quantiles or median.

This could mean that there are outliers in the data, the questions that arise because of this is if these points are actually outliers and if they should be excluded from the data. It can however not be determined with just the summary above if these are actually outliers and if they need to be removed.

## Univariate analysis

To check if points are outliers the data needs to be visualized, this can be done by creating a box plot and/or density plot for each of the columns. Creating them separately for all 30 feature columns would result in 60 plots, which is a lot and perhaps too many. To reduce the amount of total plots, the density plots will instead be visualized using violin plots with the box plots inside of them. Because printing all the data of a feature column in a single box or violin does not show what is desired, the plots will be split on the diagnosis classification factor.

There is not a function in `ggplot` to create these split violin plots, the source code file `split_violin_plot.R` contains a function that uses `ggplot` as a basis to create split violin plots. Then, using this function from the source file, another function is created that assembles the full plot including the box plot, plot title and themes. After this a list of column names can be given and a plot will be generated for each of them and they will be arranged with a common legend to the output file. So there is a clearer overview where the data can be compared the plots for the feature columns will be split on their specification, resulting in three arranged layouts with the mean-, standard error- and worst plots.

```
source("split_violin_plot.R")

createSplitViolinPlot <- function(col_name) {
  ggplot(data, aes(x = "", y = !!sym(col_name), fill = diagnosis)) +
    geom_split_violin(alpha = 0.6, trim = FALSE) +
    geom_boxplot(width = 0.2, alpha = 0.6, fatten = NULL, show.legend = F) +
    stat_summary(fun.data = "mean_se", geom = "pointrange", show.legend = F,
                 position = position_dodge(0.2), size = 0.3) +
    scale_fill_brewer(palette = "Dark2", name = "Diagnosis:") +
    ggtitle(filter(codebook, `Column Name` == col_name)$`Full Name`) +
    theme_minimal() + labs(y = NULL, x = NULL) +
    theme(plot.title = element_text(size = 9, hjust = 0.5))
}

createAndArrangePlots <- function(extension) {
  # Create plots and put them in a list
  plot_list <- lapply(colnames(data)[colnames(data) %like% extension], createSplitViolinPlot)
  # Print the plots in an arranged grid with the legend at the bottom
  ggpubr::ggarrange(plotlist = plot_list, ncol = 4, nrow = 3,
                    common.legend = TRUE, legend = "bottom")
}

# Create split violin plots for all mean feature columns
createAndArrangePlots("_mean")

# Create split violin plots for all standard error feature columns
createAndArrangePlots("_se")

# Create split violin plots for all worst/extreme feature columns
createAndArrangePlots("_worst")
```

Looking at the resulting plots it can easily be seen if there is a distinctive correlation between the classification factor and the values of feature columns. The couple of columns that stand out the most are the `Radius`, `Perimeter`, `Area`, `Concave Points` and `Radius` feature columns, these all seem to have a clear distinction between the diagnosis classification.

Another thing that should be noted is that in most of the standard error columns a lot of outliers can be seen, for now nothing will be done with these but it is a good thing to know might problems arise later on.

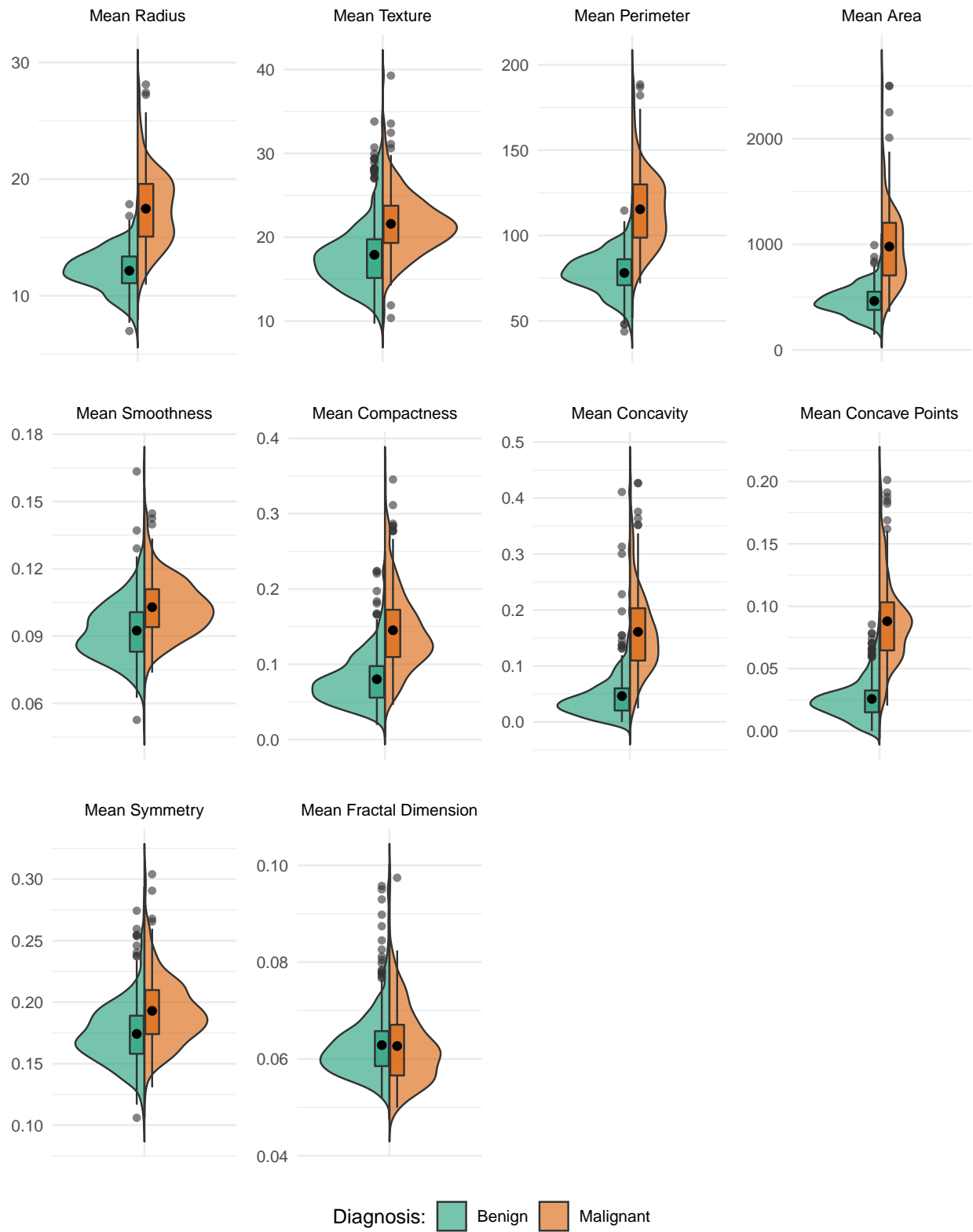


Figure 2: Split violin plots joined with box plots of 'mean' feature columns

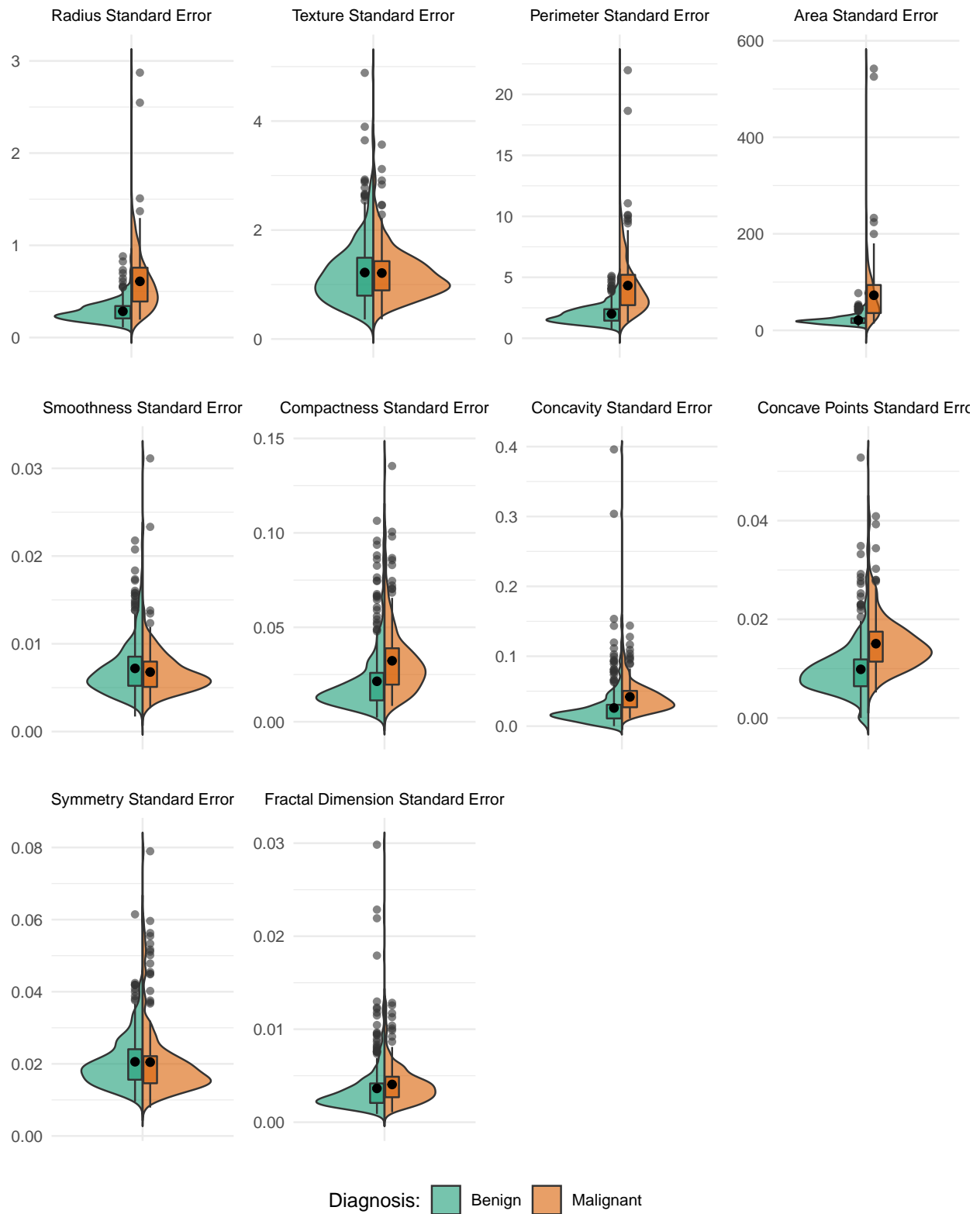


Figure 3: Split violin plots joined with box plots of 'standard error' feature columns

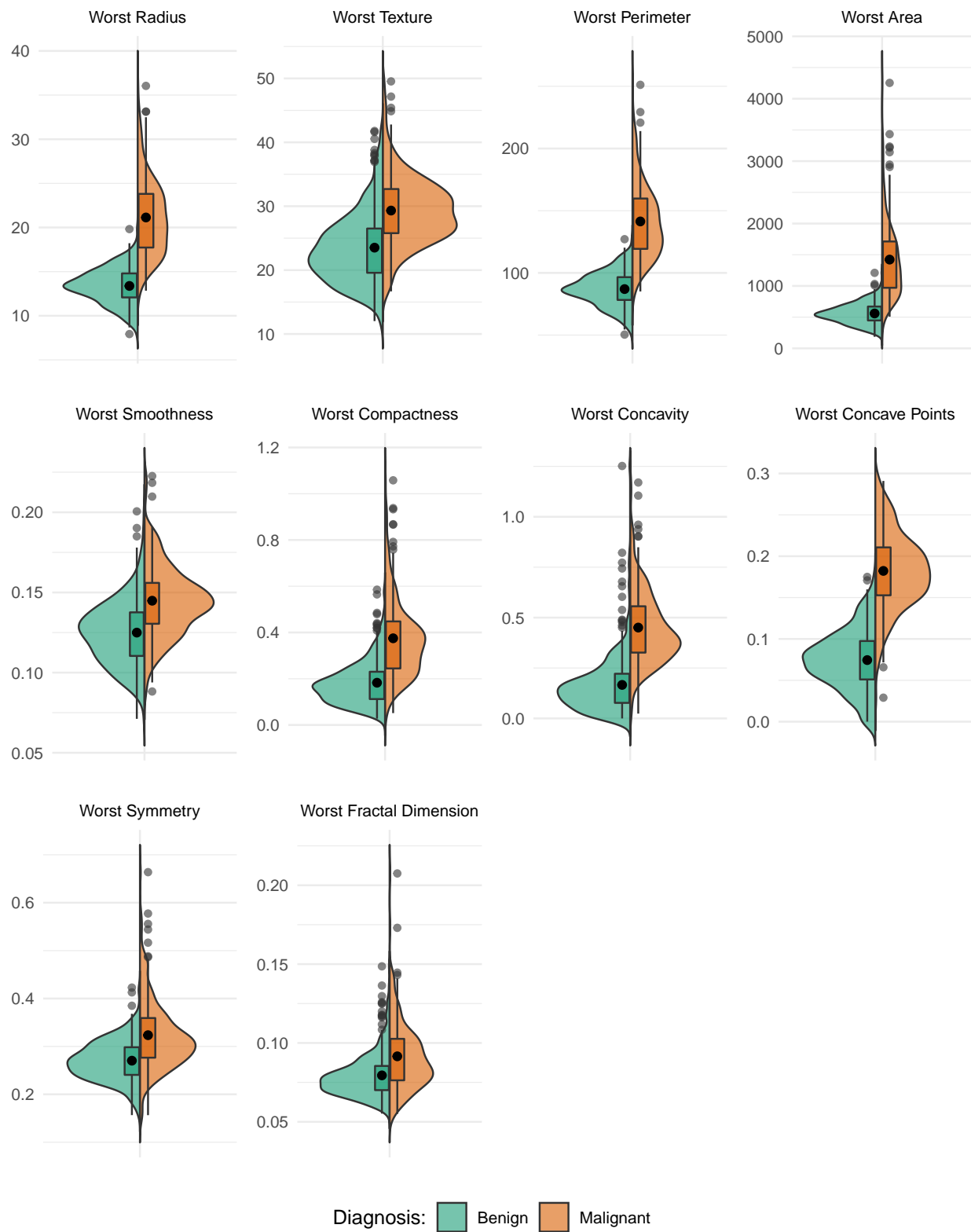


Figure 4: Split violin plots joined with box plots of 'worst/extreme' feature columns

## Bivariate analysis

To identify the correlations between features and visualize them, the perfect way is to create a heatmap. It visualizes the strength of the correlation between all columns, so all possible combinations can be seen. The heatmap takes a correlation matrix and displays its values with colors so correlations can easily be visually seen.

```
# Create correlation matrix with only the numerical feature columns
cor_matrix <- stats::cor(select(data, -diagnosis))
cor_matrix <- as_tibble(cor_matrix)
column_names <- colnames(cor_matrix)

# Insert column with feature column names and set it as the left most column
cor_matrix <- cor_matrix %>%
  mutate(col_names = all_of(column_names)) %>%
  select(31, 1:30)

# Convert data to long format
cor_matrix_long <- pivot_longer(data = cor_matrix, cols = all_of(column_names),
                                names_to = "variable", values_to = "cor")

ggplot(data = cor_matrix_long, aes(x = col_names, y = variable, fill = cor)) +
  geom_tile() + labs(x = NULL, y = NULL) +
  scale_fill_gradient(high = "purple", low = "white" ) +
  theme(axis.text.x = element_text(angle = 45, hjust=1))
```

When looking at the heatmap it can be seen very clearly that multiple features are heavily correlated together. Next, it could be a good idea to create scatterplots with trend lines of these heavily correlated feature pairs.

## Data clustering

```
# Tree, Scatter plot, PCA plot
```

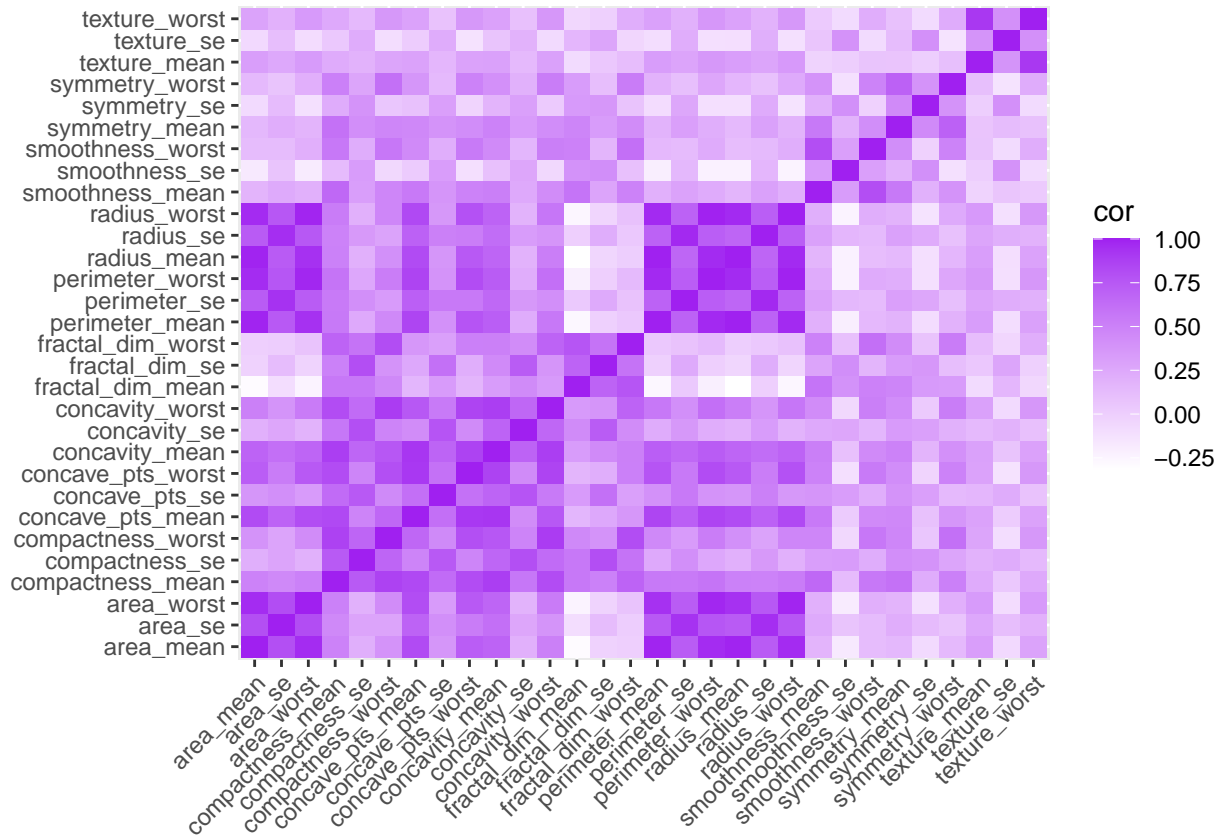


Figure 5: Heatmap showing pairwise correlation between feature columns

## References

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