

DATA 624: PREDICTIVE ANALYTICS HW4

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```
library(mlbench)
library(dplyr)
library(ggplot2)
library(tsibble)
library(tidyr)
library(corrplot)
library(cowplot)
library(psych)
library(MASS)
library(gridExtra)
library(tidyr)
```

Instructions

Do problems 3.1 and 3.2 in the Kuhn and Johnson book Applied Predictive Modeling. Please submit your Rpubs link along with your .pdf for your run code.

3.1

The UC Irvine Machine Learning Repository⁶ contains a data set related to glass identification. The data consist of 214 glass samples labeled as one of seven class categories. There are nine predictors, including the refractive index and percentages of eight elements: Na, Mg, Al, Si, K, Ca, Ba, and Fe. The data can be accessed via:

```
data(Glass)
str(Glass)
```

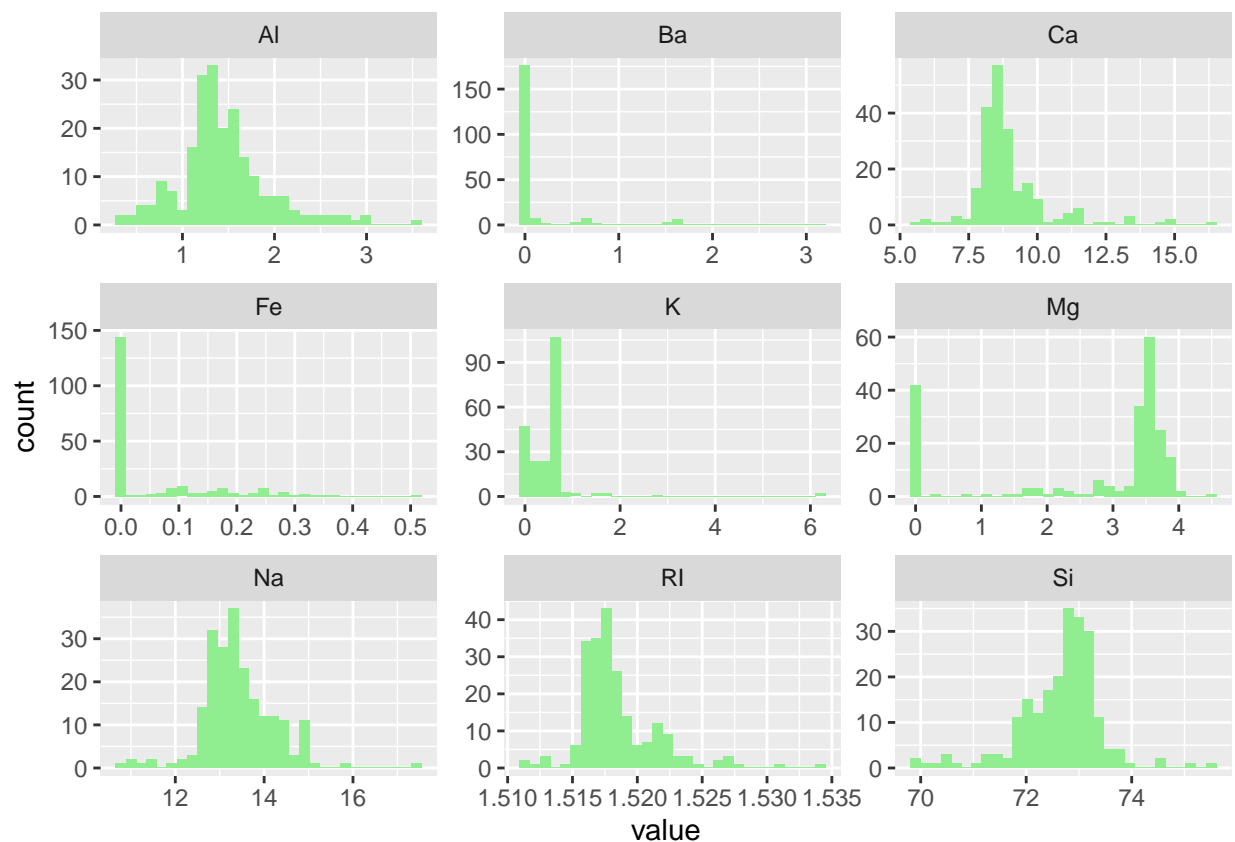
```
## 'data.frame':   214 obs. of  10 variables:
## $ RI : num  1.52 1.52 1.52 1.52 1.52 ...
## $ Na : num  13.6 13.9 13.5 13.2 13.3 ...
## $ Mg : num  4.49 3.6 3.55 3.69 3.62 3.61 3.6 3.61 3.58 3.6 ...
## $ Al : num  1.1 1.36 1.54 1.29 1.24 1.62 1.14 1.05 1.37 1.36 ...
## $ Si : num  71.8 72.7 73 72.6 73.1 ...
## $ K : num  0.06 0.48 0.39 0.57 0.55 0.64 0.58 0.57 0.56 0.57 ...
## $ Ca : num  8.75 7.83 7.78 8.22 8.07 8.07 8.17 8.24 8.3 8.4 ...
## $ Ba : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Fe : num  0 0 0 0 0 0.26 0 0 0 0.11 ...
## $ Type: Factor w/ 6 levels "1","2","3","5",...: 1 1 1 1 1 1 1 1 1 1 ...
```

(a)

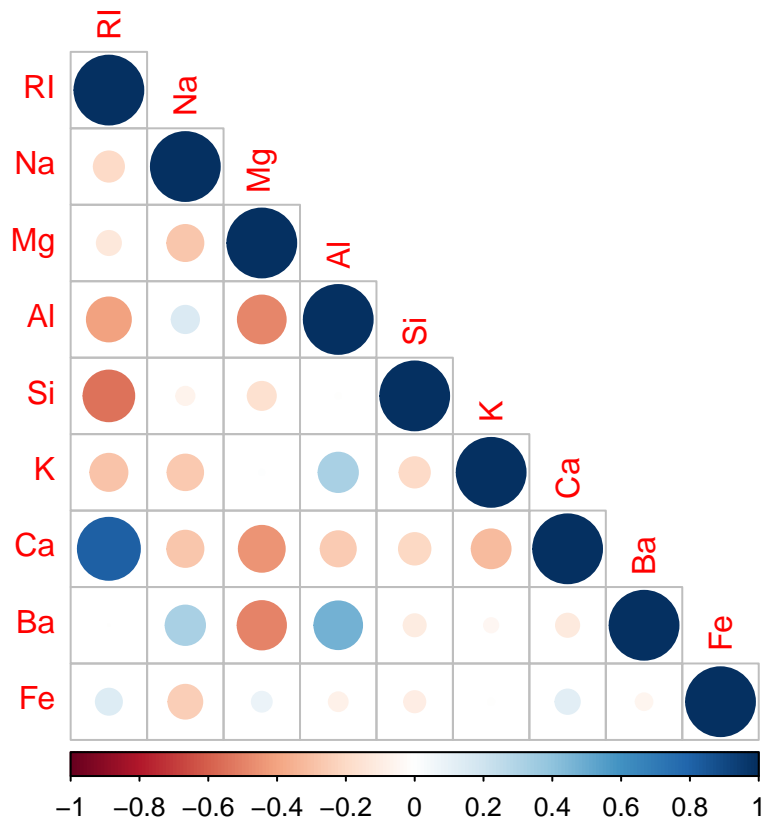
Using visualizations, explore the predictor variables to understand their distributions as well as the relationships between predictors.

```
Glass %>%  
  dplyr::select(-10)%>%  
  gather() %>%  
  ggplot(aes(x=value))+  
  geom_histogram(fill="lightgreen")+  
  facet_wrap(~key,scales = "free")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



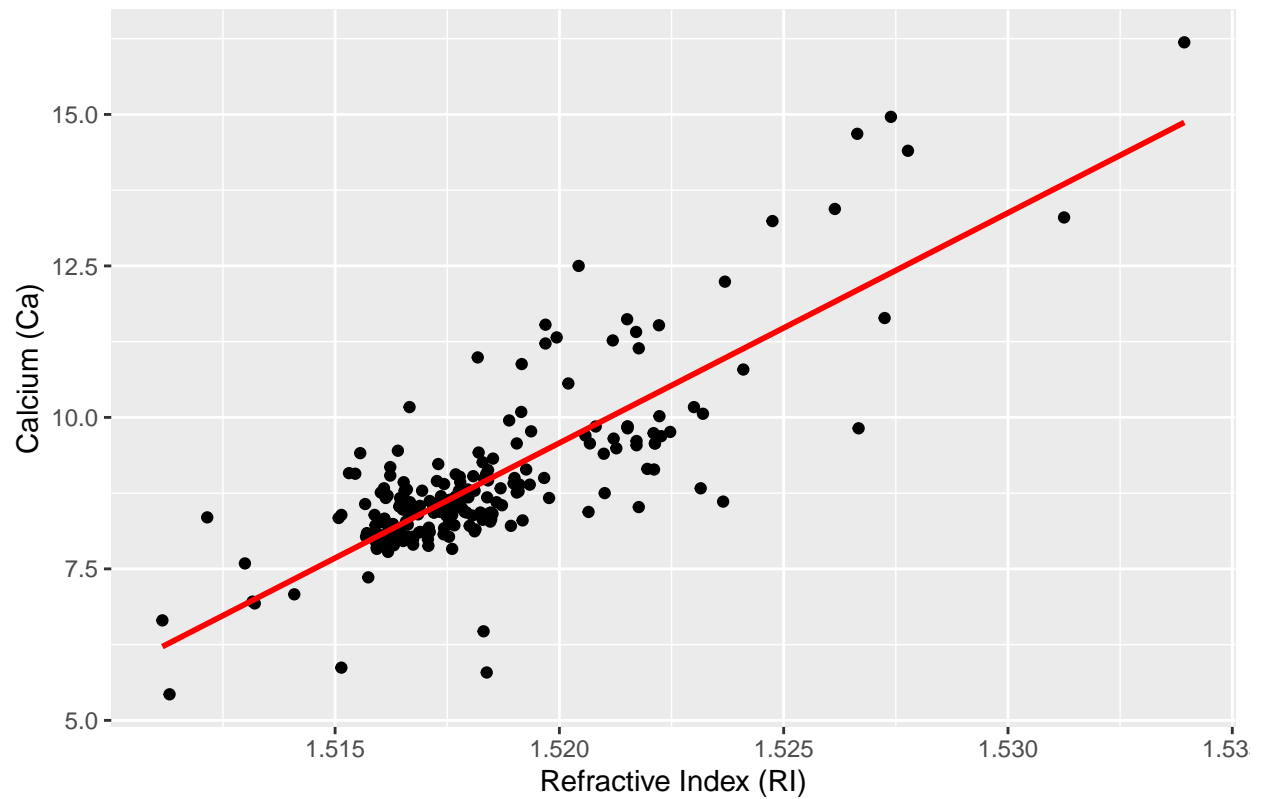
```
corrplot(cor(Glass%>%dplyr::select(-10)),type="lower")
```



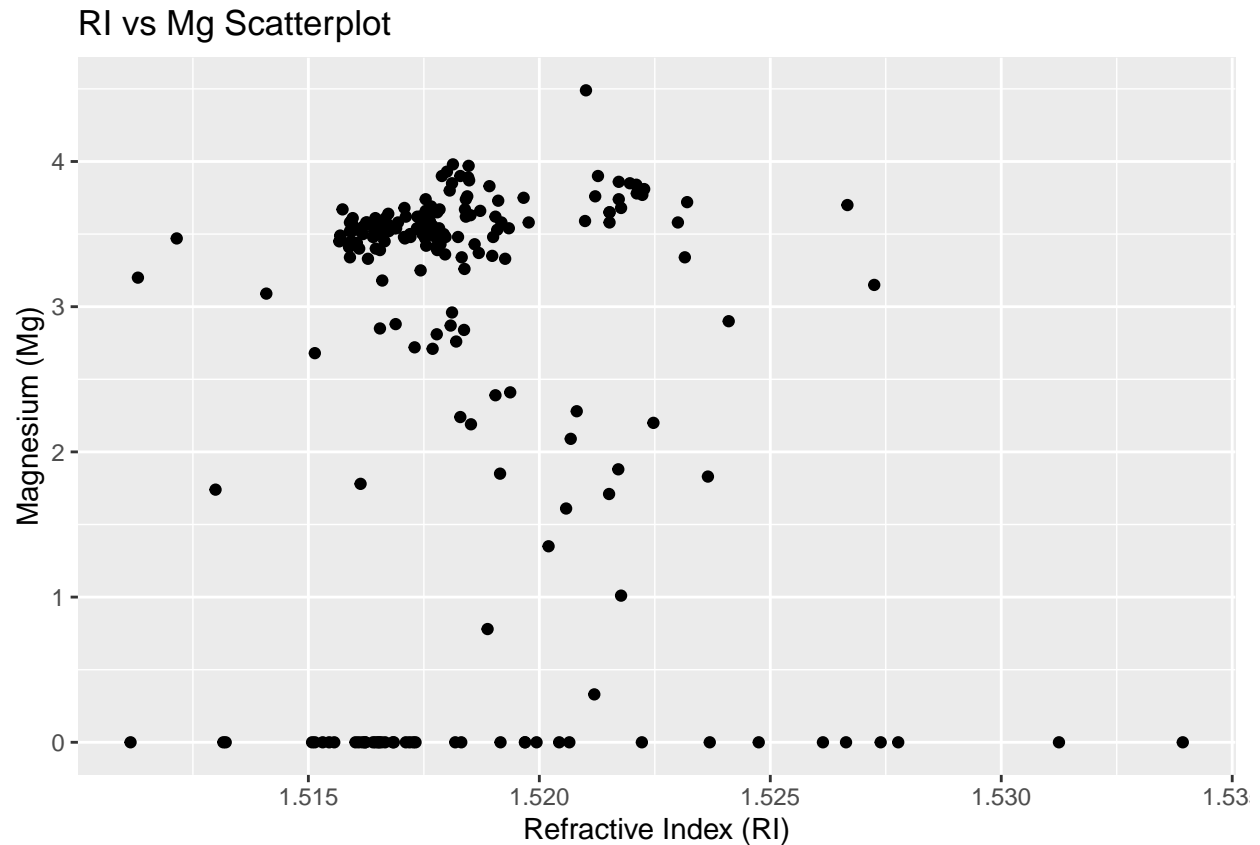
```
Glass%>%
  dplyr::select("RI", "Ca")%>%
  ggplot(aes(x=RI, y=Ca))+
  geom_point()+
  geom_smooth(method="lm", se = FALSE, color="red")+
  labs(x = "Refractive Index (RI)", y = "Calcium (Ca)",
       title = "RI vs Ca Scatterplot" )
```

```
## `geom_smooth()` using formula = 'y ~ x'
```

RI vs Ca Scatterplot



```
Glass%>%  
  dplyr::select("RI", "Mg")%>%  
  ggplot(aes(x=RI, y=Mg))+  
  geom_point()+  
  labs(x = "Refractive Index (RI)", y = "Magnesium (Mg)",  
       title = "RI vs Mg Scatterplot" )
```



In order to make the plots `Type` was excluded, as the values were not numeric and did not provide any real insight if it were to be plotted.

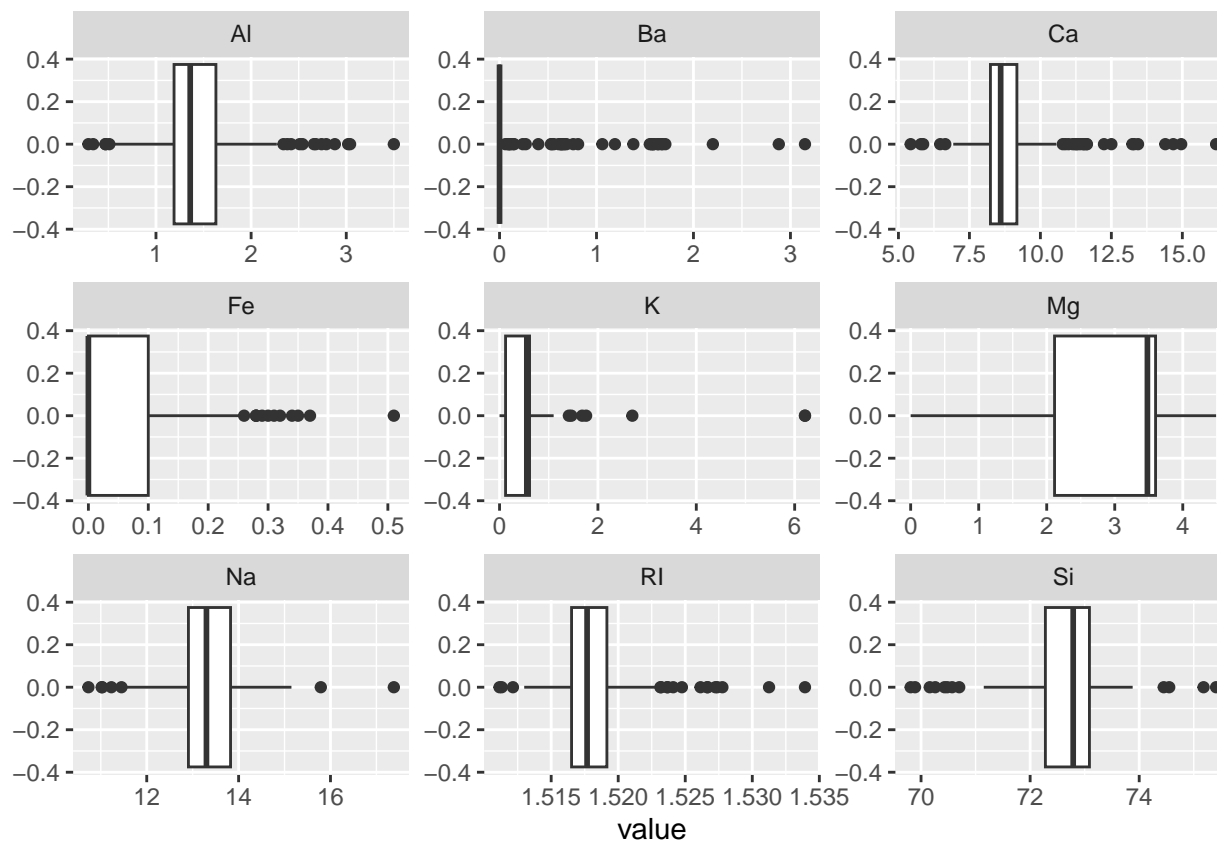
Noting the plots I can assess the following:

- All plots with exception of `Mg` and `Si` appear to be right skewed to some degree
- Of the right skewed properties `Ba` and `Fe` is centered around 0
- `Ai` and `Ba` is the most centered
- `RI` and `Ca` is shown to have the highest positive correlation while `RI` and `Mg` has the lowest.
- none of the degrees of relationship seems prominent

(b)

Do there appear to be any outliers in the data? Are any predictors skewed?

```
Glass %>%
  dplyr::select(-10)%>%
  gather() %>%
  ggplot(aes(value))+
  geom_boxplot()+
  facet_wrap(~key,scales = "free")
```



All of the attribute except for Mg have outliers in the data. Skewness is shown below. As noted all have a degree of skewness, right and left skewness is described in (a) with Ba having the most notable degree.

```
data.frame(describe(Glass))%>%
  dplyr::select(skew)
```

```
##           skew
## RI      1.6027151
## Na      0.4478343
## Mg     -1.1364523
## Al      0.8946104
## Si     -0.7202392
## K       6.4600889
## Ca      2.0184463
## Ba      3.3686800
## Fe      1.7298107
## Type*   1.0377535
```

(c)

Are there any relevant transformations of one or more predictors that might improve the classification model?

```
df_glass<-Glass
df_glass$log_Ba<-log(Glass$Ba)
df_glass$log_Fe<-log(Glass$Fe)
```

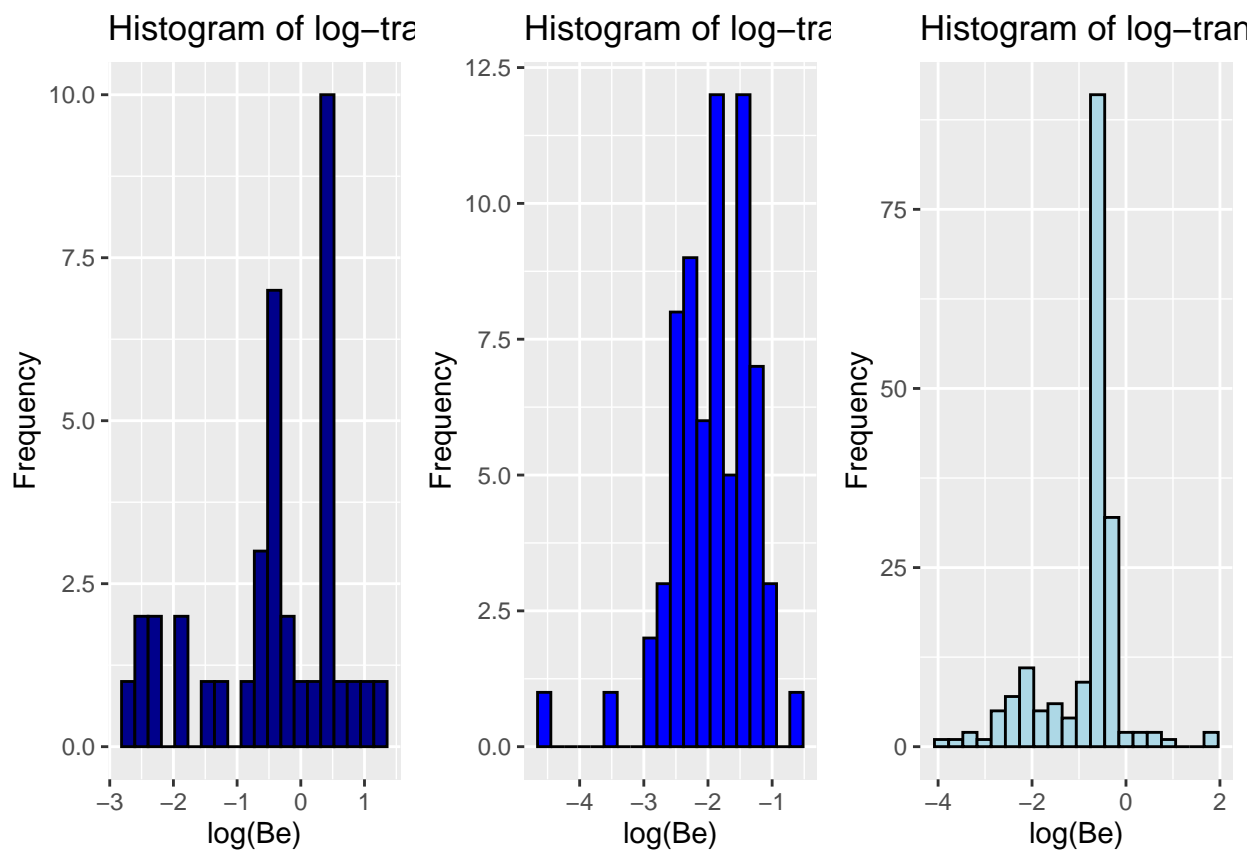
```
df_glass$log_K<-log(Glass$K)

plot_Ba <- ggplot(df_glass, aes(x = log_Ba)) +
  geom_histogram(bins = 20, fill = "darkblue",
    color = "black") +
  labs(title = "Histogram of log-transformed Ba",
    x = "log(Be)", y = "Frequency")

plot_Fe<-ggplot(df_glass, aes(x = log_Fe)) +
  geom_histogram(bins = 20, fill = "blue",
    color = "black") +
  labs(title = "Histogram of log-transformed Fe",
    x = "log(Be)", y = "Frequency")

plot_K<-ggplot(df_glass, aes(x = log_K)) +
  geom_histogram(bins = 20, fill = "lightblue",
    color = "black") +
  labs(title = "Histogram of log-transformed K",
    x = "log(Be)", y = "Frequency")

plot_grid(plot_Ba,plot_Fe,plot_K, ncol = 3)
```



```
# Box-Cox transformation for specified columns
df_glass_transformed <- df_glass
```

```

# Columns for Box-Cox transformation
columns <- c("RI", "Na", "Al", "Si", "Ca")

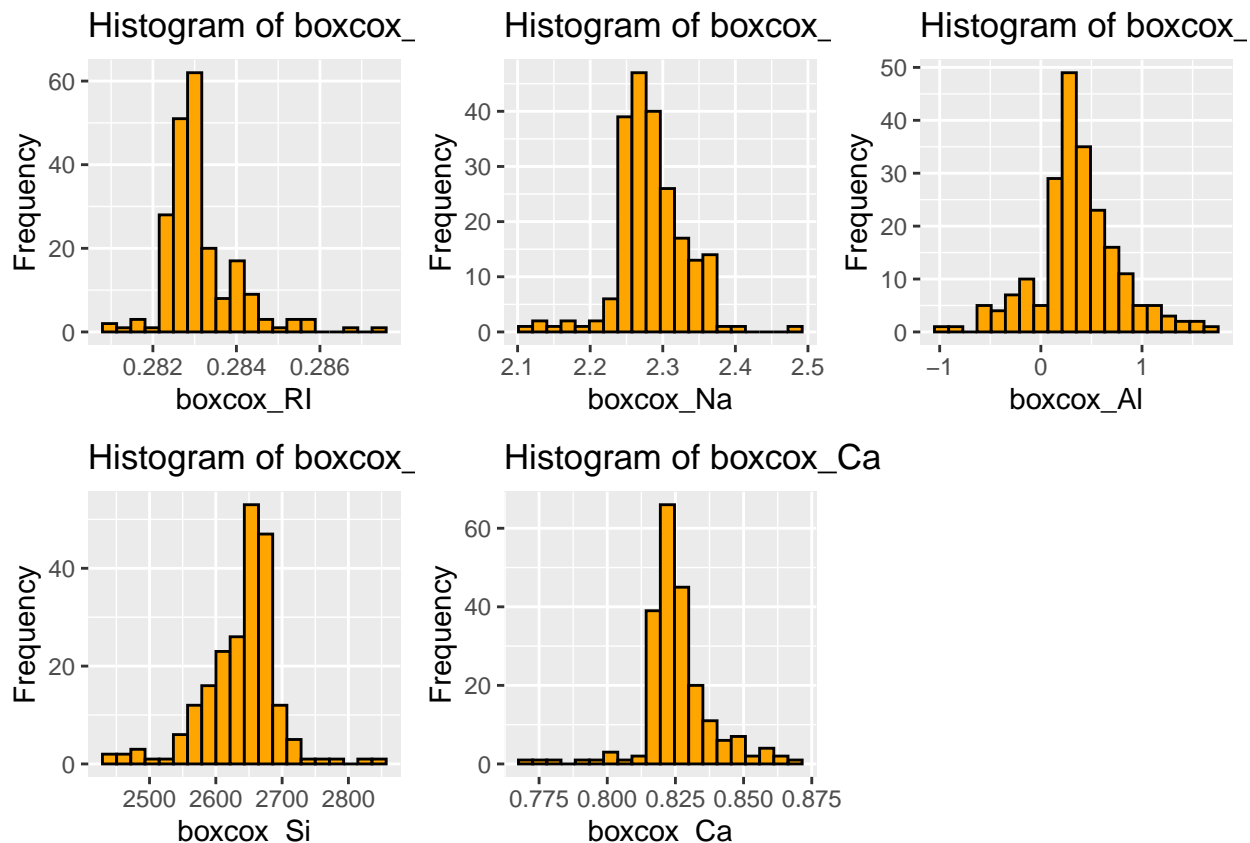
for (col in columns) {
  transformed_col <- boxcox(df_glass[[col]] ~ 1, plotit=FALSE)
  lambda <- transformed_col$x[which.max(transformed_col$y)]
  if (lambda == 0) {
    df_glass_transformed[[paste0("boxcox_", col)]] <- log(df_glass[[col]])
  } else {
    df_glass_transformed[[paste0("boxcox_", col)]] <- (df_glass[[col]]^lambda - 1) / lambda
  }
}

# Replace null values with 0
df_glass_transformed[is.na(df_glass_transformed)] <- 0

# Create ggplot visualizations for each transformed column
plots <- list()
for (col in paste0("boxcox_", columns)) {
  plots[[col]] <- ggplot(df_glass_transformed, aes(x = !!sym(col))) +
    geom_histogram(bins = 20, fill = "orange", color = "black") +
    labs(title = paste("Histogram of", col), x = col, y = "Frequency")
}

# Arrange plots in columns of 3
grid.arrange(grobs = plots, ncol = 3)

```

```
rm(list = ls(pattern = "(lambda|plot|glass|^col|col$)"))
```

3.2

The soybean data can also be found at the UC Irvine Machine Learning Repository. Data were collected to predict disease in 683 soybeans. The 35 predictors are mostly categorical and include information on the environmental conditions (e.g., temperature, precipitation) and plant conditions (e.g., left spots, mold growth). The outcome labels consist of 19 distinct classes.

The data can be loaded via:

```
data(Soybean)
## See ?Soybean for details
```

(a)

Investigate the frequency distributions for the categorical predictors. Are any of the distributions degenerate in the ways discussed earlier in this chapter?

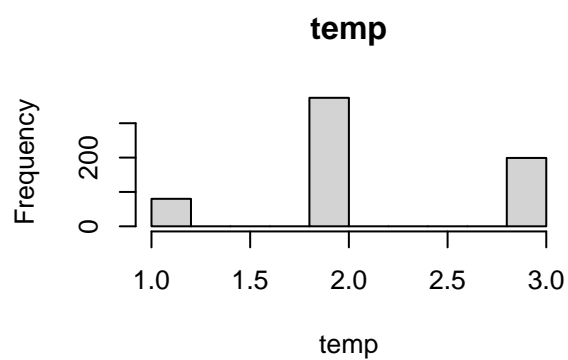
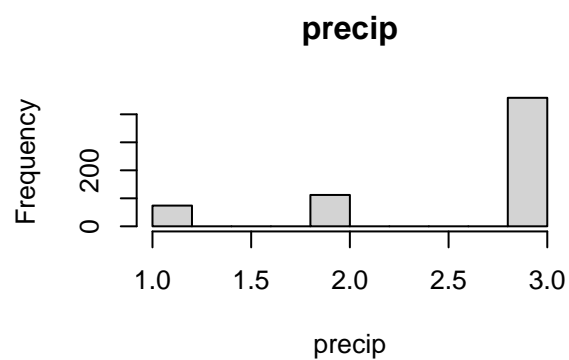
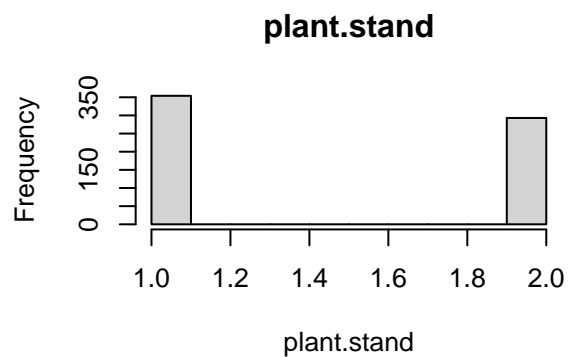
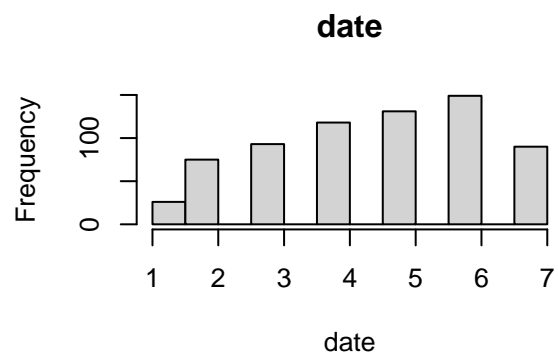
```
str(Soybean)
```

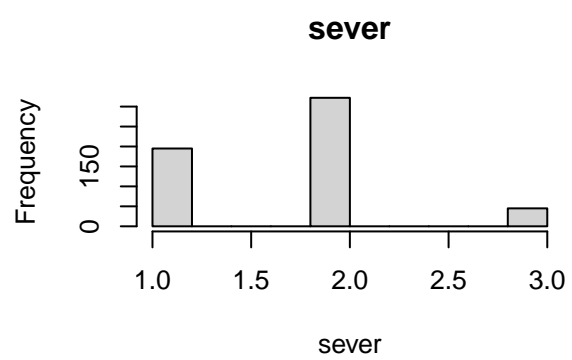
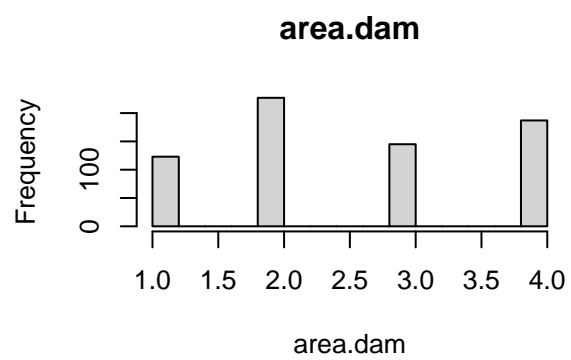
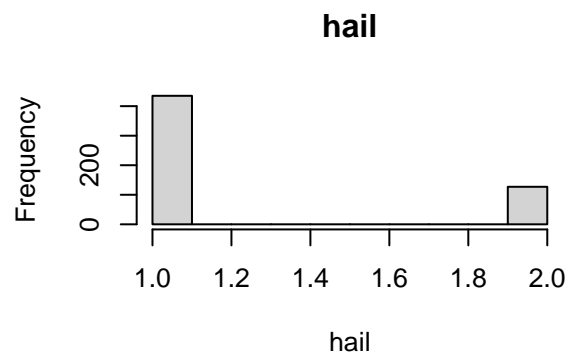
```
## 'data.frame':   683 obs. of  36 variables:
## $ Class       : Factor w/ 19 levels "2-4-d-injury",...: 11 11 11 11 11 11 11 11 11 11 ...
```

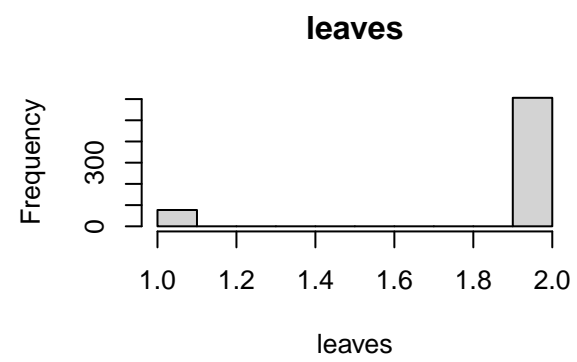
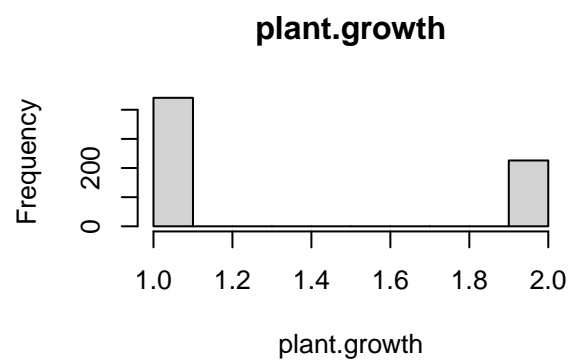
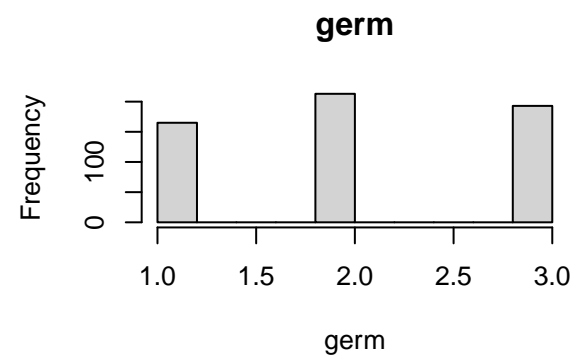
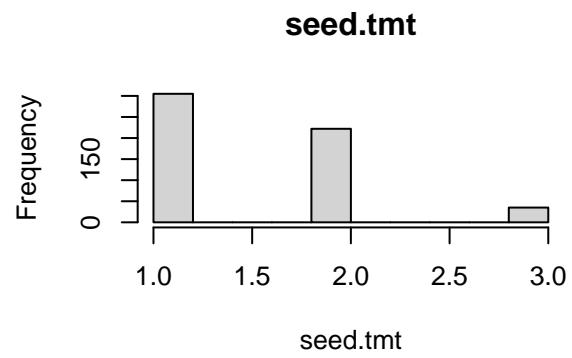
```
## $ date          : Factor w/ 7 levels "0","1","2","3",...: 7 5 4 4 7 6 6 5 7 5 ...
## $ plant.stand   : Ord.factor w/ 2 levels "0"<"1": 1 1 1 1 1 1 1 1 1 1 ...
## $ precip        : Ord.factor w/ 3 levels "0"<"1"<"2": 3 3 3 3 3 3 3 3 3 3 ...
## $ temp          : Ord.factor w/ 3 levels "0"<"1"<"2": 2 2 2 2 2 2 2 2 2 2 ...
## $ hail          : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 2 1 1 ...
## $ crop.hist     : Factor w/ 4 levels "0","1","2","3": 2 3 2 2 3 4 3 2 4 3 ...
## $ area.dam      : Factor w/ 4 levels "0","1","2","3": 2 1 1 1 1 1 1 1 1 1 ...
## $ sever         : Factor w/ 3 levels "0","1","2": 2 3 3 3 2 2 2 2 2 3 ...
## $ seed.tmt      : Factor w/ 3 levels "0","1","2": 1 2 2 1 1 1 2 1 2 1 ...
## $ germ          : Ord.factor w/ 3 levels "0"<"1"<"2": 1 2 3 2 3 2 1 3 2 3 ...
## $ plant.growth  : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...
## $ leaves        : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...
## $ leaf.halo     : Factor w/ 3 levels "0","1","2": 1 1 1 1 1 1 1 1 1 1 ...
## $ leaf.marg     : Factor w/ 3 levels "0","1","2": 3 3 3 3 3 3 3 3 3 3 ...
## $ leaf.size     : Ord.factor w/ 3 levels "0"<"1"<"2": 3 3 3 3 3 3 3 3 3 3 ...
## $ leaf.shread   : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ leaf.malf     : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ leaf.mild     : Factor w/ 3 levels "0","1","2": 1 1 1 1 1 1 1 1 1 1 ...
## $ stem          : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...
## $ lodging       : Factor w/ 2 levels "0","1": 2 1 1 1 1 1 2 1 1 1 ...
## $ stem.cankers  : Factor w/ 4 levels "0","1","2","3": 4 4 4 4 4 4 4 4 4 4 ...
## $ canker.lesion : Factor w/ 4 levels "0","1","2","3": 2 2 1 1 2 1 2 2 2 2 ...
## $ fruiting.bodies: Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...
## $ ext.decay     : Factor w/ 3 levels "0","1","2": 2 2 2 2 2 2 2 2 2 2 ...
## $ mycelium      : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ int.discolor  : Factor w/ 3 levels "0","1","2": 1 1 1 1 1 1 1 1 1 1 ...
## $ sclerotia     : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ fruit.pods    : Factor w/ 4 levels "0","1","2","3": 1 1 1 1 1 1 1 1 1 1 ...
## $ fruit.spots   : Factor w/ 4 levels "0","1","2","4": 4 4 4 4 4 4 4 4 4 4 ...
## $ seed          : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ mold.growth   : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ seed.discolor : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ seed.size     : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ shriveling    : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ roots         : Factor w/ 3 levels "0","1","2": 1 1 1 1 1 1 1 1 1 1 ...
```

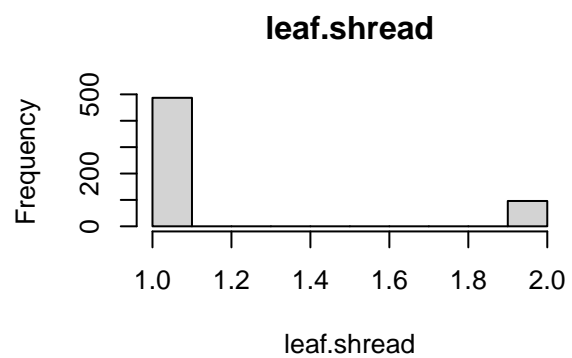
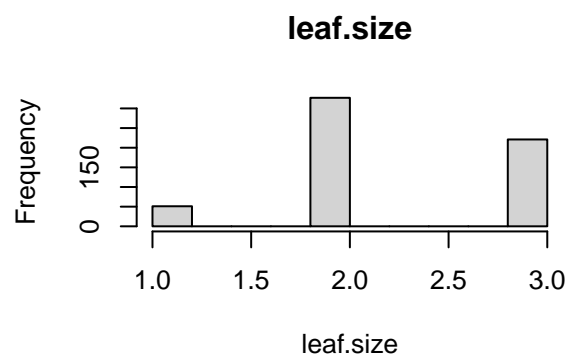
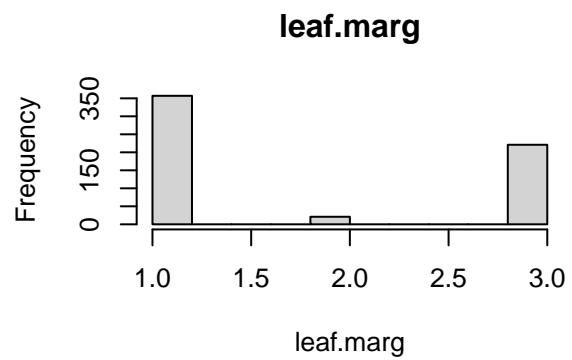
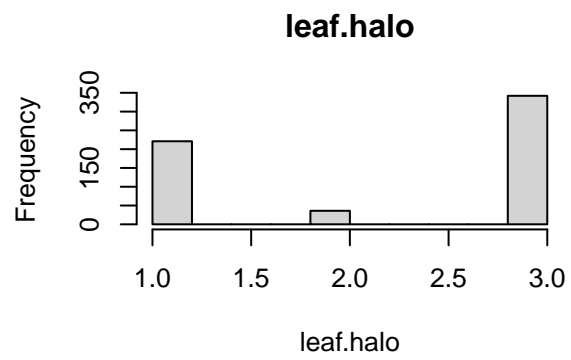
```
df_soybean <- Soybean#%>%dplyr::select(-1)

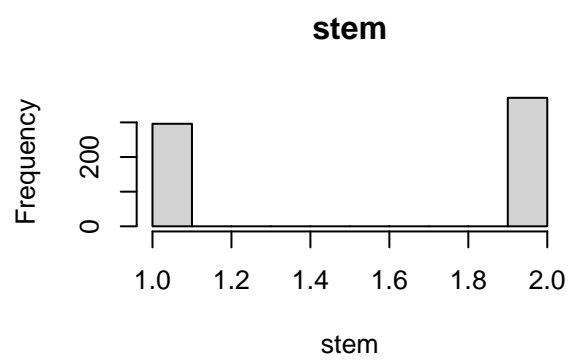
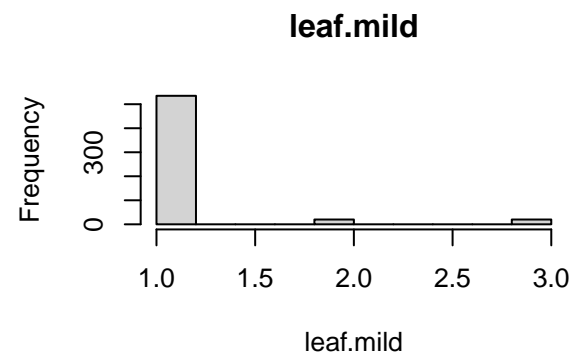
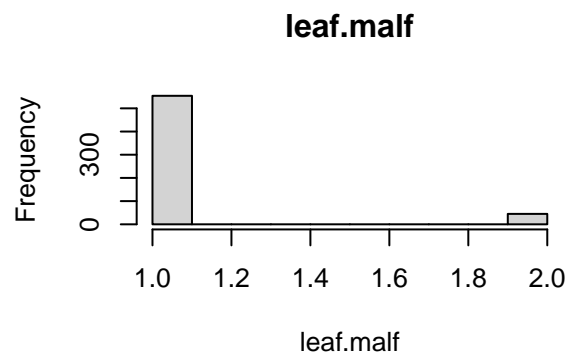
par(mfrow=c(2,2))
for (col in 2:ncol(Soybean)) {
  hist( as.numeric(Soybean[,col]),main = colnames(Soybean)[col], xlab = colnames(Soybean)[col])
}
```

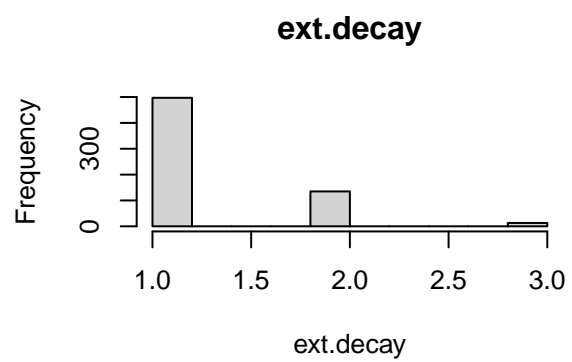
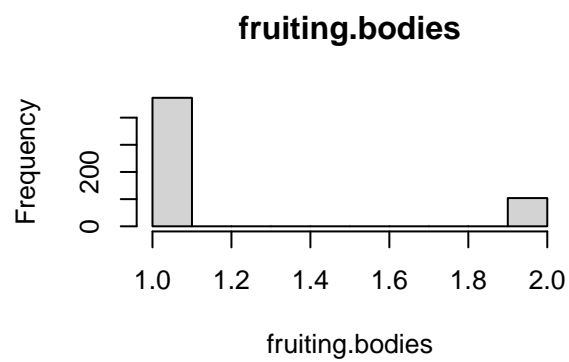
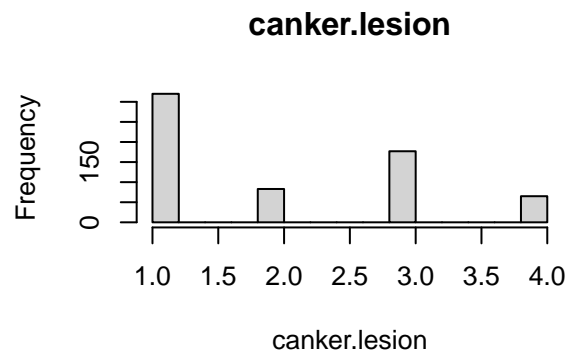
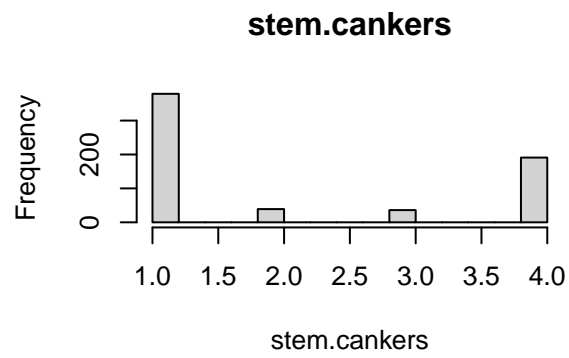


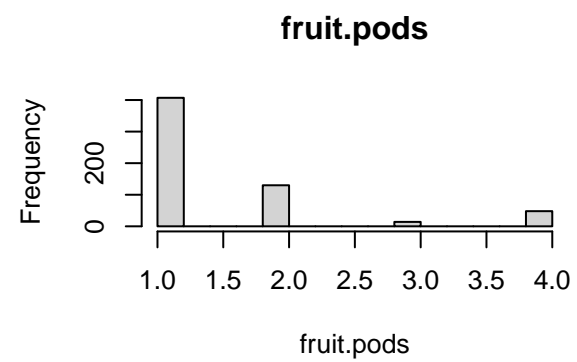
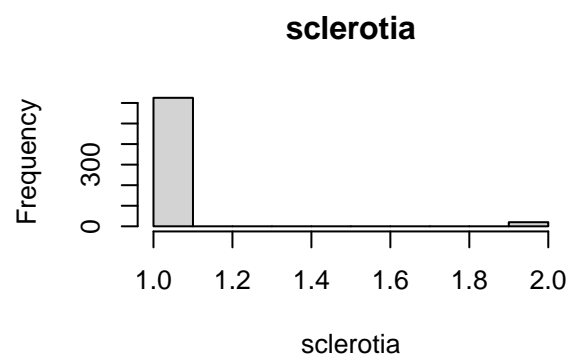
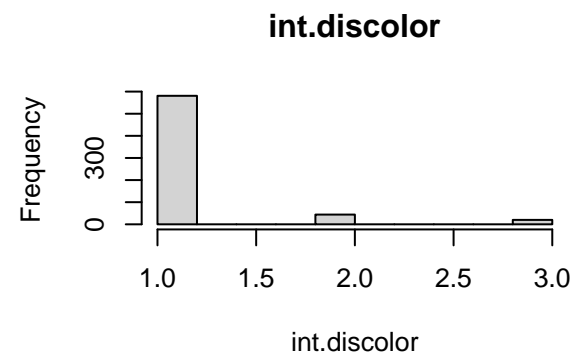
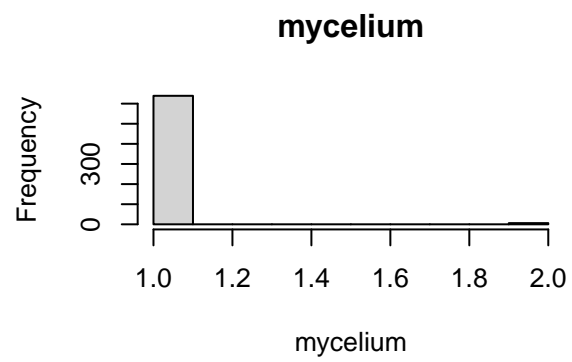


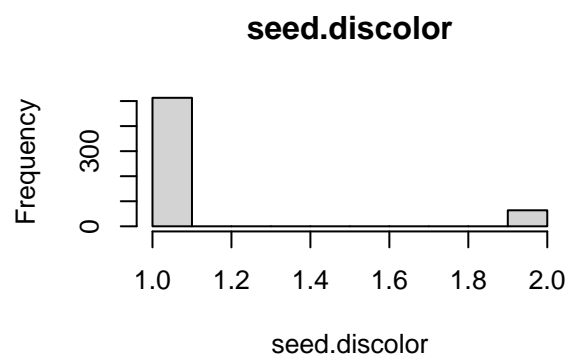
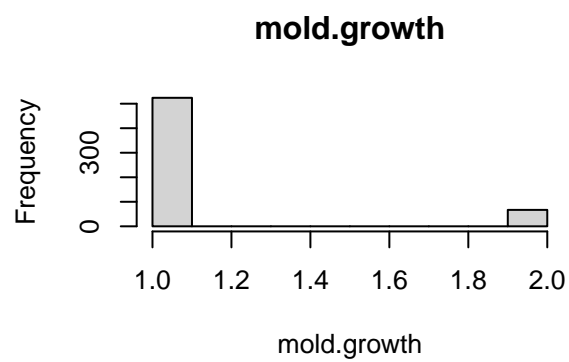
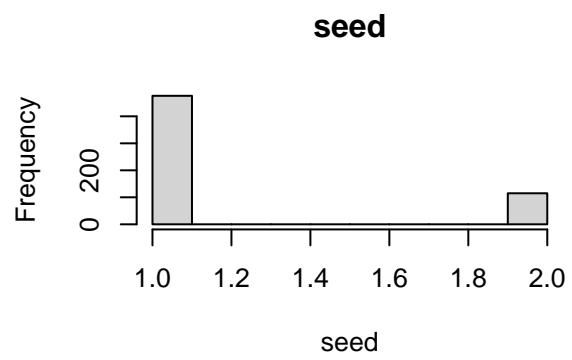
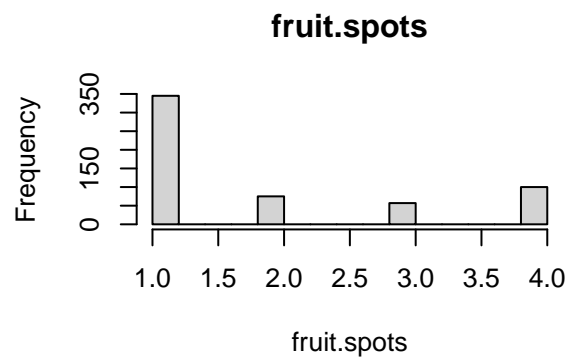


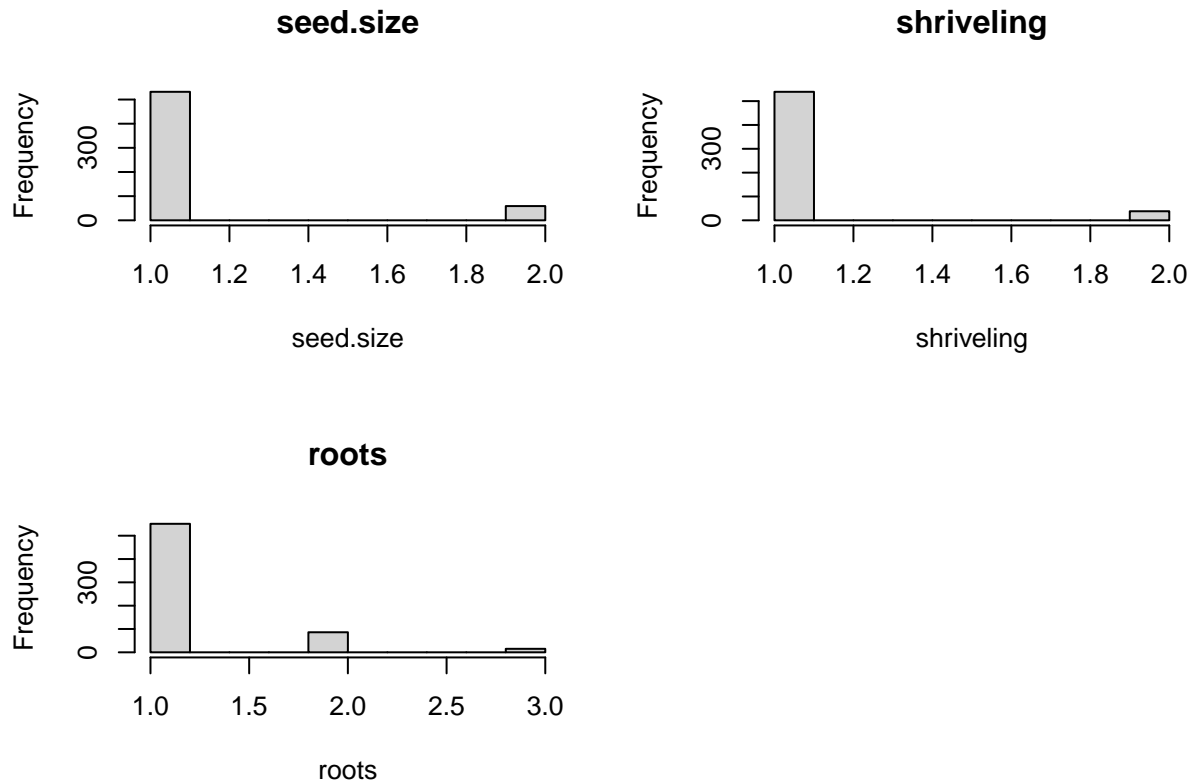












```
# Function to count distinct numeric values, including NAs, in a column
count_distinct_numeric <- function(column) {
  n_distinct(na.omit(column))
}

# Apply the function to each column of the data frame 'B'
distinct_counts <- sapply(Soybean, count_distinct_numeric)

# Reorder distinct counts in ascending order
distinct_counts <- distinct_counts[order(distinct_counts)]

# Remove columns with NA counts from the print output
distinct_counts <- distinct_counts[!is.na(distinct_counts)]

# Print the distinct counts for each column
print(distinct_counts)
```

```
##      plant.stand      hail  plant.growth      leaves  leaf.shread
##           2           2           2           2           2
##      leaf.malf      stem      lodging fruiting.bodies      mycelium
##           2           2           2           2           2
##      sclerotia      seed      mold.growth  seed.discolor      seed.size
##           2           2           2           2           2
##      shriveling      precip      temp      sever      seed.tmt
##           2           3           3           3           3
```

##	germ	leaf.halo	leaf.marg	leaf.size	leaf.mild
##	3	3	3	3	3
##	ext.decay	int.discolor	roots	crop.hist	area.dam
##	3	3	3	4	4
##	stem.cankers	canker.lesion	fruit.pods	fruit.spots	date
##	4	4	4	4	7
##	Class				
##	19				

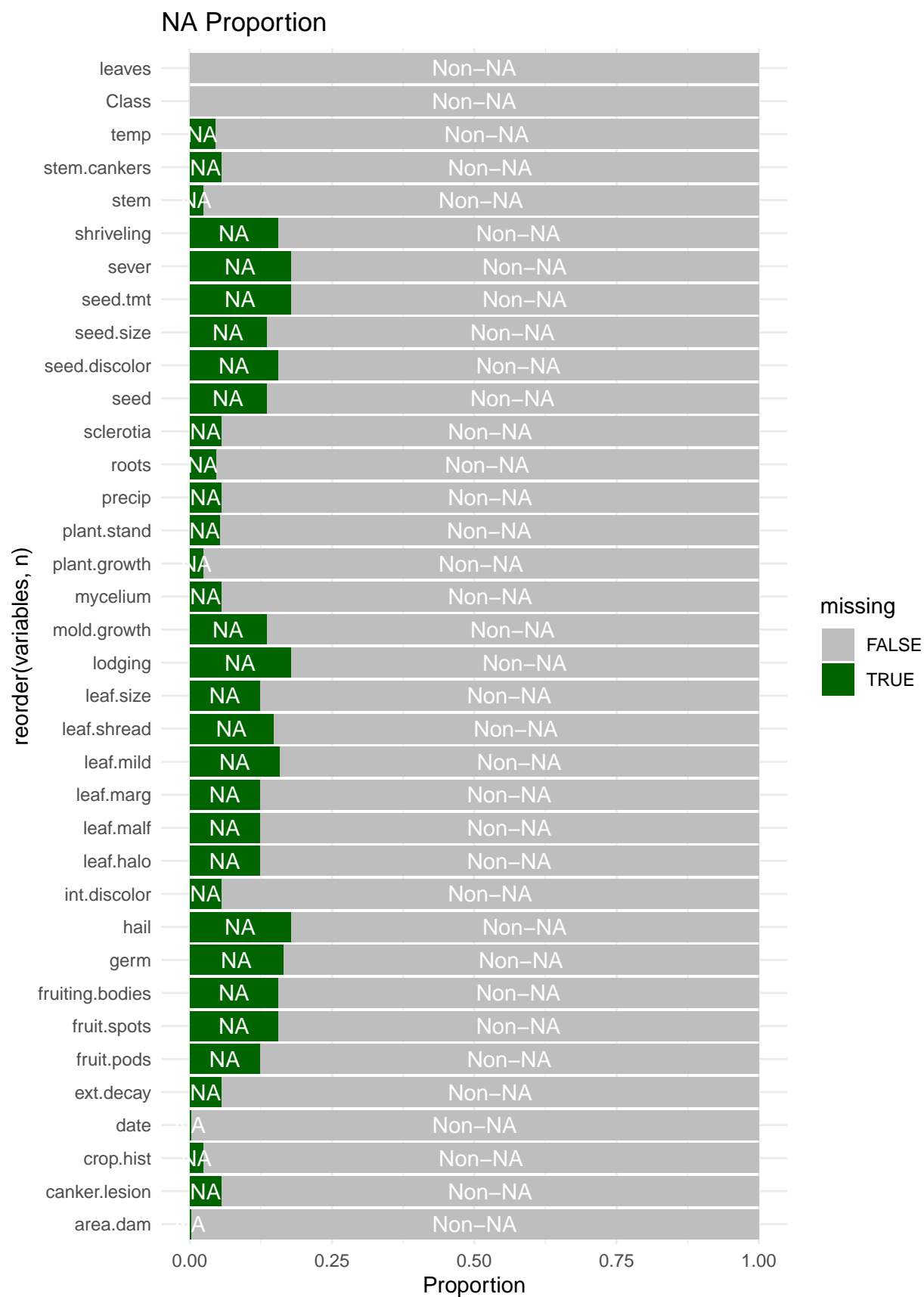
The distribution of `mycelium` and `sclerotia` appears to be degenerate, considering the low frequency count and minimal distinct values. They are significantly less than the other attributes to where visually `mycelium` almost appeared to have just 1 value.

(b)

Roughly 18 % of the data are missing. Are there particular predictors that are more likely to be missing? Is the pattern of missing data related to the classes?

```
df_soybean%>%
  summarise_all(list(~is.na(.))) %>%
  pivot_longer(everything(), names_to = "variables", values_to = "missing") %>%
  count(variables, missing) %>%
  ggplot(aes(y = reorder(variables, n), x = n, fill = missing)) +
  geom_col(position = "fill") +
  geom_text(aes(label = ifelse(missing, "NA", "Non-NA")),
            position = position_fill(vjust = 0.5),
            color = "white", size = 4) + # Add data labels
  labs(title = "NA Proportion",
       x = "Proportion") +
  scale_fill_manual(values = c("grey", "darkgreen")) +
  theme_minimal()
```

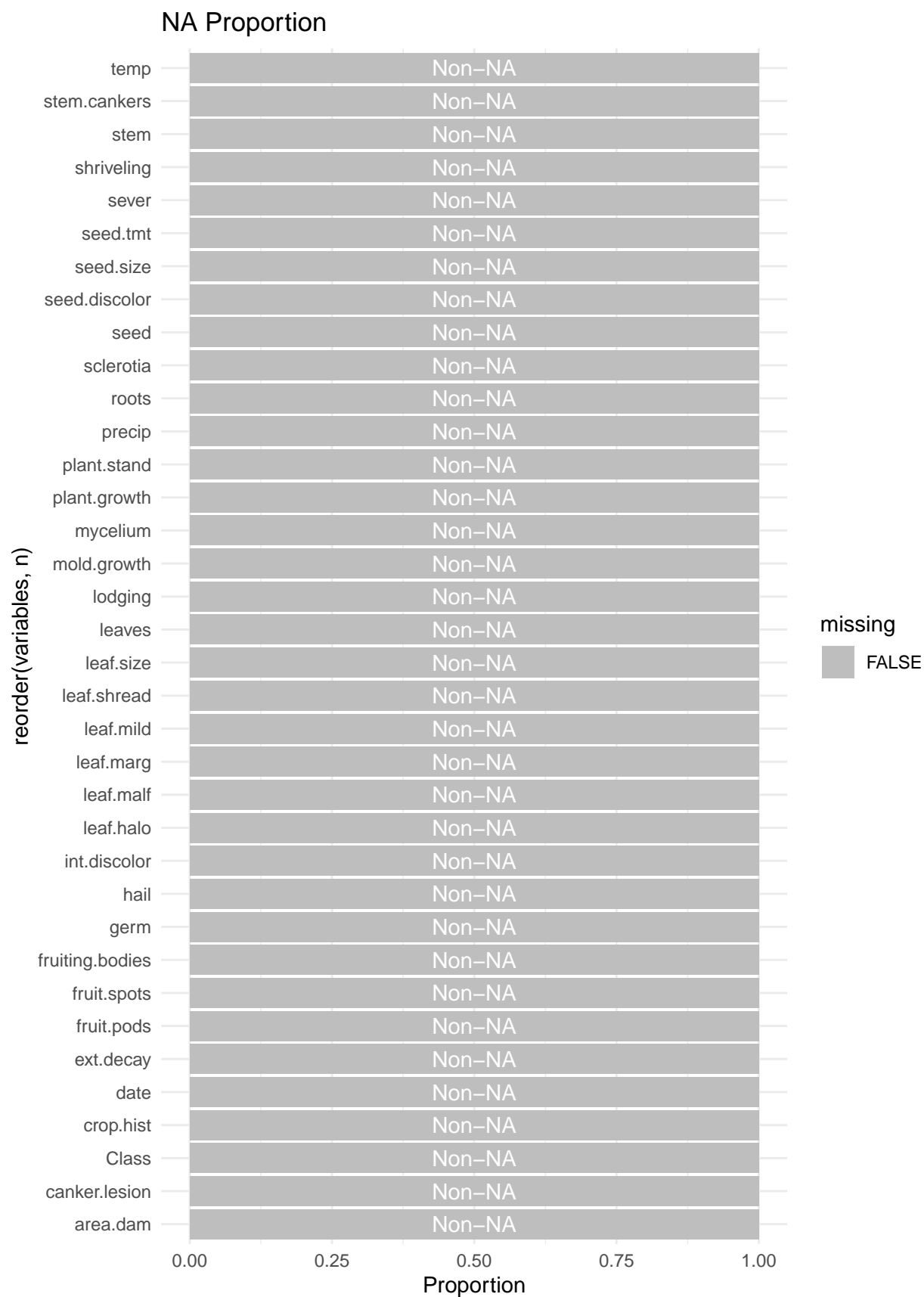
```
## Warning: Returning more (or less) than 1 row per `summarise()` group was deprecated in
## dplyr 1.1.0.
## i Please use `reframe()` instead.
## i When switching from `summarise()` to `reframe()`, remember that `reframe()`
## always returns an ungrouped data frame and adjust accordingly.
## i The deprecated feature was likely used in the dplyr package.
## Please report the issue at <https://github.com/tidyverse/dplyr/issues>.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.
```



```
df_incomplete <- df_soybean[!complete.cases(df_soybean),]
(df_incomplete %>%
  group_by(Class) %>%
  tally())
```

```
## # A tibble: 5 x 2
##   Class                      n
##   <fct>                  <int>
## 1 2-4-d-injury            16
## 2 cyst-nematode          14
## 3 diaporthes-pod-&-stem-blight 15
## 4 herbicide-injury        8
## 5 phytophthora-rot        68
```

```
df_soybean%>%
  filter(!Class %in% c("2-4-d-injury", "cyst-nematode",
    "diaporthes-pod-&-stem-blight",
    "herbicide-injury", "phytophthora-rot"))%>%
  summarise_all(list(~is.na(.))) %>%
  pivot_longer(everything(),
    names_to = "variables",
    values_to = "missing") %>%
  count(variables, missing) %>%
  ggplot(aes(y = reorder(variables, n),
    x = n, fill = missing)) +
  geom_col(position = "fill") +
  geom_text(aes(label = ifelse(missing,
    "NA", "Non-NA")),
    position = position_fill(vjust = 0.5),
    color = "white", size = 4) + # Add data labels
  labs(title = "NA Proportion",
    x = "Proportion") +
  scale_fill_manual(values = c("grey", "darkgreen")) +
  theme_minimal()
```



(c)

Develop a strategy for handling missing data, either by eliminating predictors or imputation.

I wouldn't just remove the classes although it seems much easier to just do that. I would say replace with zero where it makes sense, for binary values like **hail** or **lodging** since it is more logical to default to "no" unless reason to believe otherwise. I say this assuming **hail**=yes likelihood being significantly smaller if presuming. For values like **severe** I'd much rather not put a value, unless an "unknown" metric is put in, as it's frequency is likely to be very low. For the remaining, I would likely want to get the frequency and substitute the categorical metric with its mode for normalization with box-cox, and see if it better fits the model we want to predict with.