Homework 1

PSTAT 131/231, Winter 2019

Due on January 26, 2018 at 11:55 pm

Note: If you are working with a partner, please submit only one homework per group with both names and whether you are taking the course for graduate credit or not. Submit your Rmarkdown (.Rmd) and the compiled pdf on Gauchospace.

Predicting Algae Blooms

Background High concentrations of certain harmful algae in rivers constitute a serious ecological problem with a strong impact not only on river lifeforms, but also on water quality. Being able to monitor and perform an early forecast of algae blooms is essential to improving the quality of rivers.

With the goal of addressing this prediction problem, several water samples were collected in different European rivers at different times during a period of approximately 1 year. For each water sample, different chemical properties were measured as well as the frequency of occurrence of seven harmful algae. Some other characteristics of the water collection process were also stored, such as the season of the year, the river size, and the river speed.

Goal We want to understand how these frequencies are related to certain chemical attributes of water samples as well as other characteristics of the samples (like season of the year, type of river, etc.)

Data Description The data set consists of data for 200 water samples and each observation in the available datasets is in effect an aggregation of several water samples collected from the same river over a period of 3 months, during the same season of the year. Each observation contains information on 11 variables. Three of these variables are nominal and describe the season of the year when the water samples to be aggregated were collected, as well as the size and speed of the river in question. The eight remaining variables are values of different chemical parameters measured in the water samples forming the aggregation, namely: Maximum pH value, Minimum value of O_2 (oxygen), Mean value of Cl (chloride), Mean value of NO_3^- (nitrates), Mean value of NH_4^+ (ammonium), Mean of PO_4^3 (orthophosphate), Mean of total PO_4 (phosphate) and Mean of chlorophyll.

Associated with each of these parameters are seven frequency numbers of different harmful algae found in the respective water samples. No information is given regarding the names of the algae that were identified.

We can start the analysis by loading into R the data from the "algaeBloom.txt" file (the training data, i.e. the data that will be used to obtain the predictive models). To read the data from the file it is sufficient to issue the following command:

```
algae <- read_table2("algaeBloom.txt", col_names=
                     c('season','size','speed','mxPH','mnO2','Cl','NO3','NH4',
                       'oPO4','PO4','Chla','a1','a2','a3','a4','a5','a6','a7'),
                     na="XXXXXXX")

glimpse(algae)
```

1. ***Descriptive summary statistics*** Given the lack of further information on the problem domain, it is wise to investigate some of the statistical properties of the data, so as to get a better grasp of the problem. It is always a good idea to start our analysis with some kind of exploratory data analysis. A first idea of the statistical properties of the data can be obtained through a summary of its descriptive statistics.

   (a) Count the number of observations in each season using `summarise()` in `dplyr`.

```
season_obs <- algae %>%
  group_by(season) %>%
  summarize(obs_count = n())
```

#. Are there missing values? Calculate the mean and variance of each chemical (Ignore a_1 through a_7). What do you notice about the magnitude of the two quantities for different chemicals?

```
algae_na <- algae %>%
  select(c('mxPH','mnO2','Cl','NO3','NH4', 'oPO4','PO4','Chla')) %>%
  summarise_all(function(x) sum(is.na(x)))
```

There are missing values for several variables. One value is missing for mxPH. NO3, NH4, oPO4, and PO4 are all missing two values. Cl and Chla are each missing 10 and 12 variables.

```
print('Mean')
```

```
## [1] "Mean"
```

```
chem_means <- algae %>%
  select(c('mxPH','mnO2','Cl','NO3','NH4', 'oPO4','PO4','Chla')) %>%
  summarise_all(function (x) mean(x, na.rm=TRUE))
```

```
print('Variance')
```

```
## [1] "Variance"
```

```
chem_vars <- algae %>%
  select(c('mxPH','mnO2','Cl','NO3','NH4', 'oPO4','PO4','Chla')) %>%
  summarise_all(function (x) var(x, na.rm=TRUE))
```

The mean for NH4 is the largest, but it also has a disproportionately large variance as compared to the mean and variance coupling of other variables.

#. Mean and Variance is one measure of central tendency and spread of data. Median and Median Absolute Deviation are alternative measures of central tendency and spread.

For a univariate data set $X_1, X_2, ..., X_n$, the Median Absolute Deviation (MAD) is defined as t

Compute median and MAD of each chemical and compare the two sets of quantities (i.e., mean & varian

```
print('Median')
```

```
## [1] "Median"
```

```
chem_medians <- algae %>%
  select(c('mxPH','mnO2','Cl','NO3','NH4', 'oPO4','PO4','Chla')) %>%
  summarise_all(function (x) median(x, na.rm=TRUE))
```

```
print('MADs')
```

```
## [1] "MADs"
```

```
chem_mads <- algae %>%
  select(c('mxPH','mnO2','Cl','NO3','NH4', 'oPO4','PO4','Chla')) %>%
  summarise_all(function (x) mad(x, na.rm=TRUE))
```

2. ***Data visualization*** Most of the time, the information in the data set is also well captured graphically. Histogram, scatter plot, boxplot, Q-Q plot are frequently used tools for data visualization. Use ggplot for all of these visualizations.

(a) Produce a histogram of $mxPH$ with the title 'Histogram of mxPH' based on algae data set. Use an appropriate argument to show the probability instead of the frequency as the vertical axis. (Hint: look at the examples in the help file for function `geom_histogram()`). Is the distribution skewed?

```
hist_mxPH <- ggplot(algae, aes(x = mxPH)) +
  geom_histogram(bins = 12)  + #2*(200)^1/3
  labs(title = 'Histogram of mxPH') +
  ylab('Probability') +
  scale_y_continuous(labels =scales::percent) +
  geom_density() +
  geom_rug()

hist_mxPH
```

```
## Warning: Removed 1 rows containing non-finite values (stat_bin).
```

```
## Warning: Removed 1 rows containing non-finite values (stat_density).
```
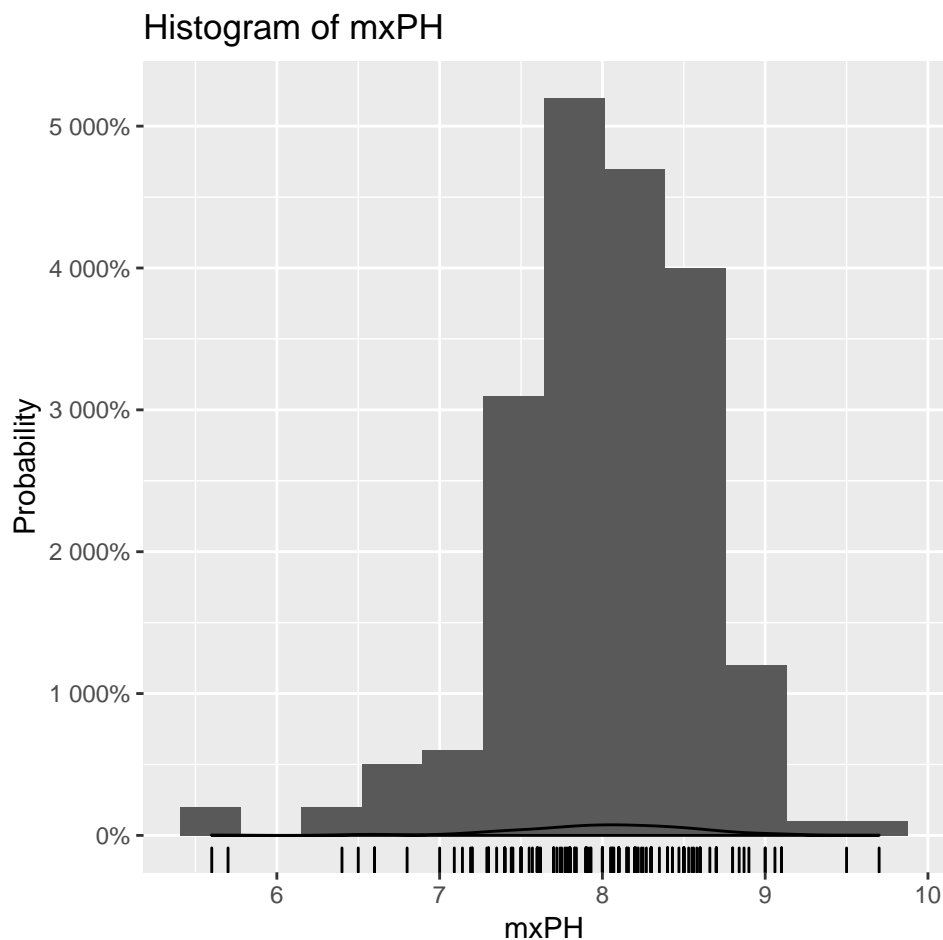

1. Add a density curve using `geom_density()` and rug plots using `geom_rug()` to above histogram.

(a) Create a boxplot with the title 'A conditioned Boxplot of Algal a_1' for a_1 grouped by *size*. (Refer

to help page for `geom_boxplot()`).

```
algae_boxplot <- ggplot(algae, aes(size, a1)) +
  geom_boxplot(outlier.color = 'orange') +
  labs(title = 'A conditioned Boxplot of Algal a1')

algae_boxplot
```
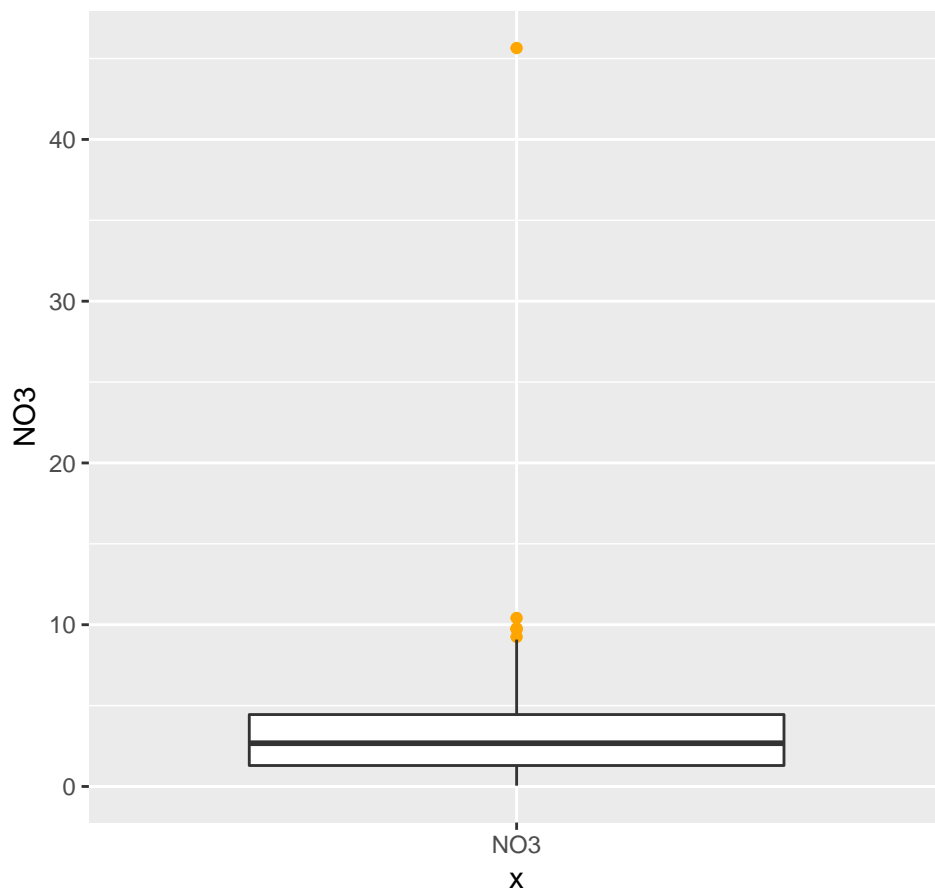
A conditioned Boxplot of Algal a1
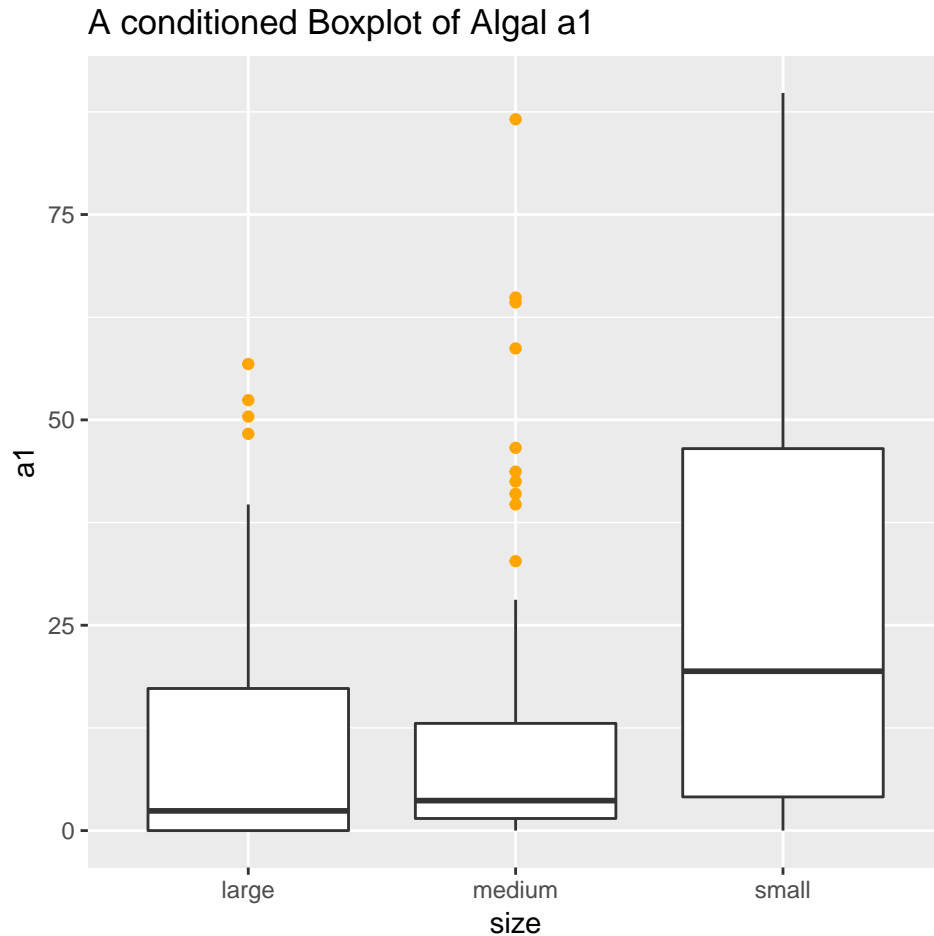
1. Are there any outliers for $NO3$ and $NH4$? How many observations would you consider as outliers? How did you arrive at this conclusion?

```
NO3_boxplot <- ggplot(algae, aes(x = 'NO3', y = NO3)) +
  geom_boxplot(outlier.color = 'orange') +
  labs(title = 'A conditioned Boxplot of NO3')

NO3_boxplot
```

```
## Warning: Removed 2 rows containing non-finite values (stat_boxplot).
```
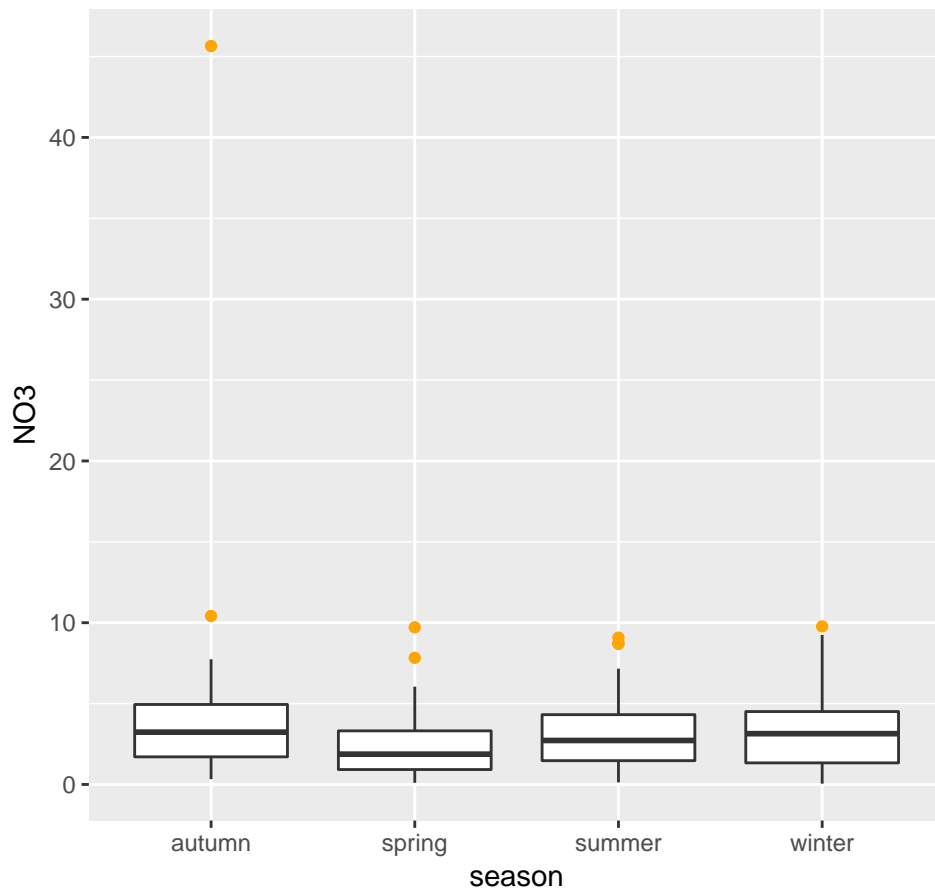
A conditioned Boxplot of NO3


```
NO3season_boxplot <- ggplot(algae, aes(season, y = NO3)) +
  geom_boxplot(outlier.color = 'orange') +
  labs(title = 'A conditioned Boxplot of NO3 by Season')

NO3season_boxplot
```

```
## Warning: Removed 2 rows containing non-finite values (stat_boxplot).
```
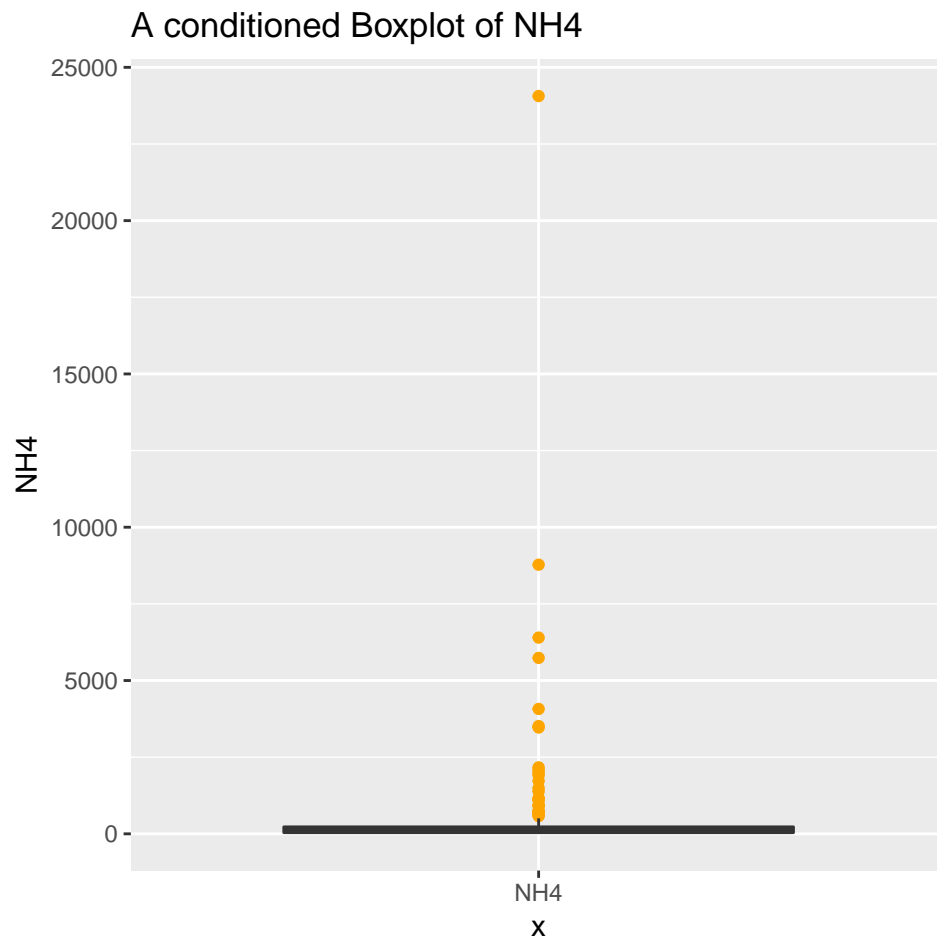
A conditioned Boxplot of NO3 by Season

By separating the NO3 data into seasons, we can see that there is a clear outlier in autumn that is significantly further from the Interquartile Range than outliers in other months. Note: outliers are indicated in orange. Thus, we will only consider this one autumn outlier as a true outlier.

```
NH4_boxplot <- ggplot(algae, aes(x = 'NH4', y = NH4)) +
  geom_boxplot(outlier.color = 'orange') +
  labs(title = 'A conditioned Boxplot of NH4')

NH4_boxplot
```

```
## Warning: Removed 2 rows containing non-finite values (stat_boxplot).
```

A conditioned Boxplot of NH4


```
NH4season_boxplot <- ggplot(algae, aes(season, y = NH4)) +
  geom_boxplot(outlier.color = 'orange') +
  labs(title = 'A conditioned Boxplot of NH4 by Season')

NH4season_boxplot
```
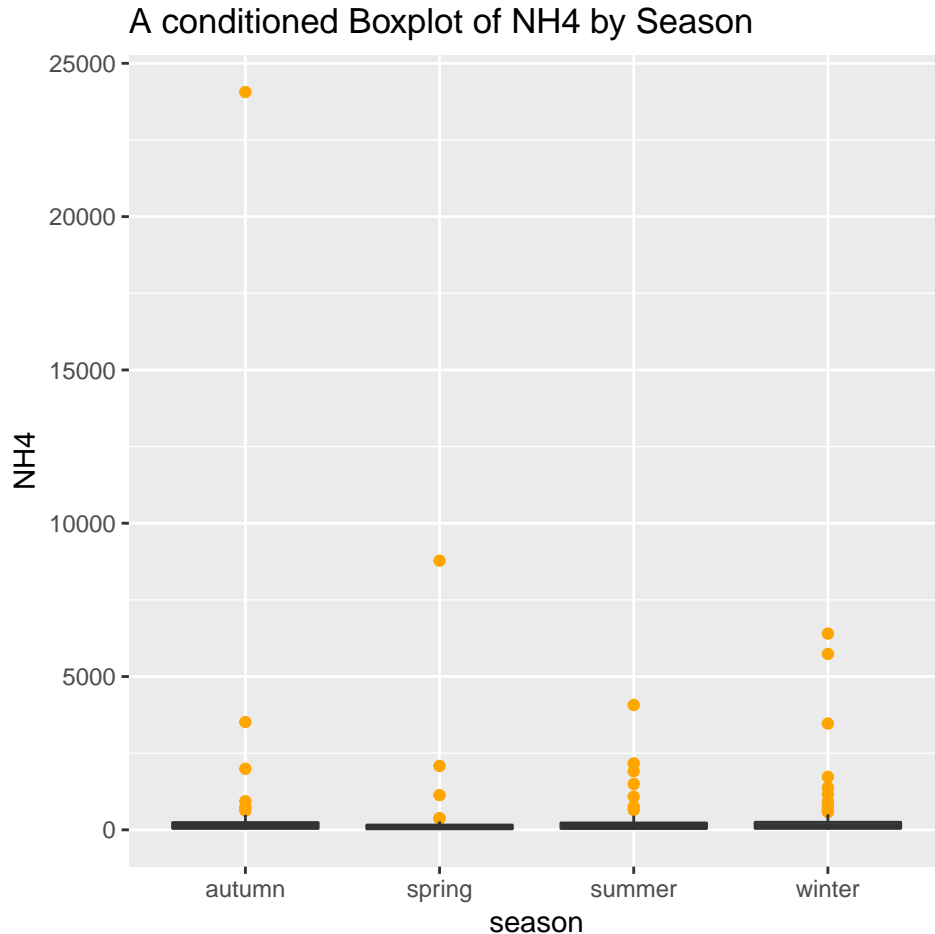
```
## Warning: Removed 2 rows containing non-finite values (stat_boxplot).
```

A conditioned Boxplot of NH4 by Season

1. Compare mean & variance vs. median & MAD for $NO3$ and $NH4$. What do you notice? Can you conclude which set of measures is more robust when outliers are present?

There is a larger difference between mean and median values for NH4 than NO3. The same pattern is true for variance and MAD, however the variance is much larger for NH4 than NO3. The median and MAD are a more appropriate measure when outliers are present because the value in autumn seems to skew our data when considered in parameters that average all values.

Predicting Algae Blooms

Some water samples contained unknown values in several chemicals. Missing data are very common in real-world problems, and may prevent the use of certain data mining techniques that are not able to handle missing values.

In this homework, we are going to introduce various ways to deal with missing values. After all the missing values have been taken care of, we will build a model to investigate the relationship between the variable `a1` and other 11 predictors (`season`, `size`, `speed`, `mxPH`, `mnO2`, `Cl`, `NO3`, `NH4`, `oPO4`, `PO4`, `Chla`) utilizing cross-validation in the next problem.

Dealing with missing values

3. (a) How many observations contain missing values? How many missing values are there in each variable?

```r
missingvalues <- algae %>%
  select(c('season','size','speed','mxPH','mnO2','Cl','NO3','NH4',
  'oPO4','PO4','Chla','a1','a2','a3','a4','a5', 'a6', 'a7')) %>%
  summarise_all(function(x) sum(is.na(x)))

sum(missingvalues>0)
```

[1] 8

There are 8 observations that contain missing values.

#. **Removing observations with missing values**: use `filter()` function in `dplyr` package to observations with any missing value, and save the resulting dataset (without missing values) as `algae.del`. Report how many observations are in `algae.del`.

   Hint: `complete.cases()` may be useful.

```r
algae.del <- algae %>%
  filter_all(all_vars(!is.na(.)))
```

#. \label{imputation} **Imputing unknowns with measures of central tendency**: the simplest and fastest way of filling in (imputing) missing values is to use some measures of central tendency such as mean, median and mode.

   Use `mutate_at()` and `ifelse()` in `dplyr` to fill in missing values for each chemical with its median, and save the imputed dataset as `algae.med`. Report the number of observations in `algae.med`. Display the values of each chemical for the 48th, 62th and 199th obsevation in `algae.med`.

```r
algae.med <- algae %>%
  mutate_at(.vars = c('mxPH','mnO2','Cl','NO3','NH4',
  'oPO4','PO4','Chla'), .funs = funs(ifelse(is.na(.), median(., na.rm = TRUE), .)))

algae.med.48 <- algae.med[48, 4:11]
algae.med.62 <- algae.med[62, 4:11]
algae.med.199 <- algae.med[199, 4:11]

algae.med.rows <- rbind(algae.med.48, algae.med.62, algae.med.199)
rownames(algae.med.rows) <- c("48", "62", "199")
```

Warning: Setting row names on a tibble is deprecated.

```r
kable(algae.med.rows, "latex", booktabs = T,
      caption = "Chemical Observations for Specific Rows After Imputing") %>%
      kable_styling(bootstrap_options = "striped", full_width = F, position = "center")
```

There are 200 observations in algae.med.

   This simple strategy, although extremely fast and thus appealing for large datasets, imputed values may have large bias that can influence our model fitting. An alternative for decreasing bias of imputed values is to use relationships between variables.

#. **Imputing unknowns using correlations**: another way to impute missing

Table 1: Chemical Observations for Specific Rows After Imputing

	mxPH	mnO2	Cl	NO3	NH4	oPO4	PO4	Chla
48	8.06	12.6	9.00	0.230	10.0000	5.00	6.0000	1.100
62	6.40	9.8	32.73	2.675	103.1665	40.15	14.0000	5.475
199	8.00	7.6	32.73	2.675	103.1665	40.15	103.2855	5.475

```
values is to use correlation with another variable. For a highly
correlated pair of variables, we can fill in the unknown values by
predicting one based on the other with a simple linear regression model,
provided the two variables are not both unknown.
```

```
    Compute pairwise correlation between the continuous (chemical) variables.
```

```
algae.cor = algae %>%
  select(c('mxPH','mnO2','Cl','NO3','NH4',
  'oPO4','PO4','Chla','a1','a2','a3','a4','a5', 'a6', 'a7')) %>%
  cor(use = "complete.obs")
```

```
    Then, fill in the missing value for `PO4` based on `oPO4` in the
    $28^{th}$ observation. What is the value you obtain?
```

```
    Hint: use `lm()` and `predict()` function.
```

```
PO.lm <- lm(PO4 ~ oPO4, data = algae %>%
            select(c('PO4','oPO4')))
oPO4 <- algae %>%
  select(c('oPO4'))
prediction28 = predict(PO.lm, oPO4[28,])

prediction28
```

```
##        1
## 48.06929
```

The model predicts a value of 48.07 units of P04 in the 28th observation.

```
#. **Questioning missing data assumptions**:  When might imputation using only the observed data lead y
```

Estimating the Test Error with Cross Validation (CV)

Using `algae.med` dataset obtained in (**??**), we will build a linear regression model to predict the levels of algae type `a1` based on 11 variables (`season, size, speed, mxPH, mnO2, Cl, NO3, NH4, oPO4, PO4, Chla`), and test generalization of model to data that have not been used for training.

4. **Cross-validation**: in class we talked about how to use cross-validation (CV) to estimate the "test error". In k-fold CV, each of k equally sized random~ partitions of data (chunks) are used in a heldout set (called validation set or test set). After k runs, we average the held-out error as our final estimate of the validation error. For this part, we will run cross-validation on only a single model, as a way to estimate our test error for future predictions (we are not using it here for model selection since we are considering only one model). Perform 5-fold cross-validation on this model to estimate the (average) test error.

   (a) First randomly partition data into 5 equal sized chunks.

   Hint: a simple way to randomly assign each observation to a chunk is to do the following. First, use `cut(..., label=FALSE)` to divide observation ids $(1, 2, \ldots)$ into equal numbers of chunk ids.

Then, randomize output of `cut()` by using `sample()`.

(b) Perform 5-fold cross-validation with training error and validation errors of each chunk determined from (4a).

Since same computation is repeated 5 times, we can define the following function for simplicity.

```r
do.chunk <- function(chunkid, chunkdef, dat){  # function argument

    train = (chunkdef != chunkid)

    Xtr = dat[train,1:11]   # get training set
    Ytr = dat[train,12]   # get true response values in trainig set

    Xvl = dat[!train,1:11]   # get validation set
    Yvl = dat[!train,12]   # get true response values in validation set

    lm.a1 <- lm(a1~., data = dat[train,1:12])
    predYtr = predict(lm.a1)   # predict training values
    predYvl = predict(lm.a1,Xvl)   # predict validation values

    data.frame(fold = chunkid,
               train.error = mean((predYtr - Ytr)^2), # compute and store training error
               val.error = mean((predYvl - Yvl)^2))   # compute and store test error

}
```

First argument `chunkid` indicates which chunk to use as validation set (one of 1:5). Second argument `chunkdef` is chunk assignments from (4a). Third argument `dat` will be `algae.med` dataset.

In order to repeatedly call `do.chunk()` for each value of `chunkid`, use functions `lapply()` or `ldply()`. Note that `chunkdef` and `dat` should be passed in as optional arguments (refer to help pages).

Write the code and print out the `train.error` and `val.error` five times (e.g. for each chunk).

5. **Test error on additional data**: now imagine that you actually get *new* data that wasn't available when you first fit the model.

(a) Additional data can be found in the file `algaeTest.txt`.

```r
algae.Test <- read_table2('algaeTest.txt',
                   col_names=c('season','size','speed','mxPH','mnO2','Cl','NO3',
                                   'NH4','oPO4','PO4','Chla','a1'),
                   na=c('XXXXXXX'))
```

This data was not used to train the model and was not (e.g. wasn't used in the CV procedure to estimate the test error). We can get a more accurate measure of true test error by evaluating the model fit on this held out set of data. Using the same linear regression model from part 4 (fit to all of the training data), calculate the "true" test error of your predictions based on the newly collected measurements in `algaeTest.txt`. Is this roughly what you expected based on the CV estimated test error from part 4?

Cross Validation (CV) for Model Selection

In this problem, we will be exploring a dataset of wages from a group of 3000 workers. The goal in this part is to identify a relationship between wages and age.

6. First, install the `ISLR` package, which includes many of the datasets used in the ISLR textbook. Look at the variables defined in the `Wage` dataset. We will be using the `wage` and `age` variables for this problem.

```
library(ISLR)
head(Wage)
```

(a) Plot wages as a function of age using `ggplot`. Your plot should include the datapoints (`geom_point()`) as well as a smooth fit to the data (`geom_smooth()`). Based on your visualization, what is the general pattern of wages as a function of age? Does this match what you expect?

(b) In this part of the problem, we will find a polynomial function of age that best fits the wage data. For each polynomial function between $p = 0, 1, 2, ...10$:

   i. Fit a linear regression to predict wages as a function of age, age^2, ... age^p (you should include an intercept as well). Note that $p = 0$ model is an "intercept-only" model.
   ii. Use 5-fold cross validation to estimate the test error for this model. Save both the test error and the training error.

(c) Plot both the test error and training error (on the same plot) for each of the models estimated above as a function of p. What do you observe about the training error as p increases? What about the test error? Based on your results, which model should you select and why?

Note: `poly(age, degree=p, raw=TRUE)` will return a matrix with p columns, where the p-th column is age^p. For the predictors in your regression use `poly(age, degree=p, raw=FALSE)`. The `raw=FALSE` option returns predictors which are numerically more stable (it returns a matrix of "orthogonal polynomials"). Numerical stability can be an issue because age^p can be very very large if p is large. The orthogonal polynomials returned when `raw=FALSE` are rescaled to account for this so please use the `raw=FALSE` option.

Hint: A function similar to `do.chunk` from problem 4 will be helpful here as well.

---

7. **(231 Only) The bias-variance tradeoff**. Prove that the mean squared error can be decomposed into the variance plus bias squared. That is, who $E[(\hat{\theta} - \theta)^2] = \text{Var}(\hat{\theta}) + \text{Bias}(\hat{\theta})^2$ where $\text{Bias}(\hat{\theta}) = E[\hat{\theta} - \theta]$. Here $\hat{\theta}$ is an estimator (a random variable) of the fixed unknown constant θ. Hint: reogranize terms in the MSE by adding and subtracting $E[\hat{\theta}]$.

8. **(231 Only)** As we discussed in class, distance metrics satisfy the following properties:

   - *Positivity*:
     - $d(x, y) \geq 0$
     - $d(x, y) = 0$ only if $x = y$

   - *Symmetry*:
     - $d(x, y) = d(y, x)$ for all x and y

   - *Triangle Inequality*:
     - $d(x, z) \leq d(x, y) + d(y, z)$ for x, y, and z

   Show that the following measures are distance metrics by showing the above properties hold:

   (a) $d(x, y) = \|x - y\|_2$

   (b) $d(x, y) = \|x - y\|_\infty$