MH3510 Assignment 1

Question

The following data indicate the relationship between the amount of β-erythroidine in an aqueous solution and the colorimeter reading of the turbidity:

Concentration	Colorimeter Reading
40	69
50	175
60	272
70	335
80	490
90	415
40	72
60	265
80	492
50	180

(a) Fit a simple regression to the data.

(b) Comments on the model adequacy using $\mathcal{F}$ test and $\mathcal{R}^2$ statistics.

Solution

Data Preparation

We saved the data in `data/data.csv`. Then we named the columns as X and y.

```
data <- read.csv("data/data.csv")
names(data) <- c("X", "y")
head(data)
```

```
##    X   y
## 1 40  69
## 2 50 175
## 3 60 272
## 4 70 335
## 5 80 490
## 6 90 415
```

Simple Linear Regression

We first fit the simple linear regression model using the `lm` function.

```
model <- lm(y ~ X, data = data)
summary(model)
```

```
##
## Call:
## lm(formula = y ~ X, data = data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -100.312  -15.080    3.203   10.880   61.978
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -252.2971    58.7508  -4.294  0.00264 **
## X              8.5290     0.9153   9.318 1.43e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 48.09 on 8 degrees of freedom
## Multiple R-squared:  0.9156, Adjusted R-squared:  0.9051
## F-statistic: 86.83 on 1 and 8 DF,  p-value: 1.434e-05
```

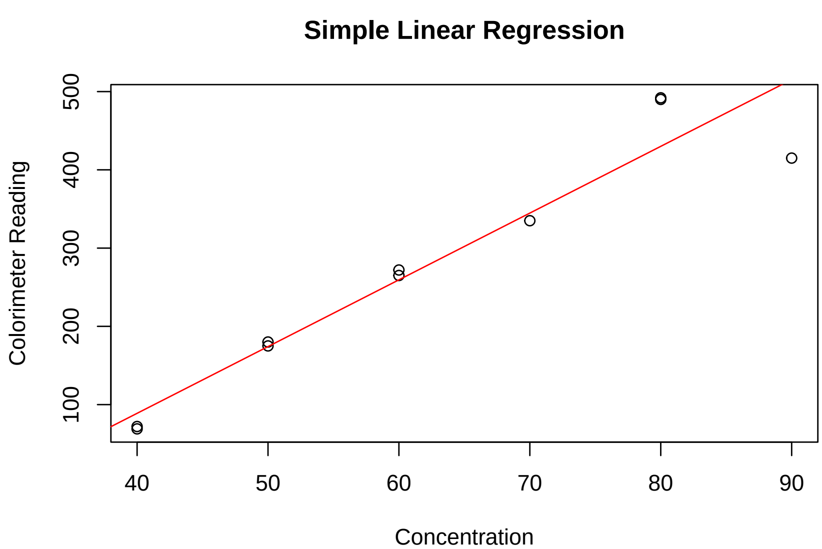
We can see that the estimated regression line is

$$\hat{y} = -252.2971 + 8.5290X$$

with $\mathcal{F} \approx 86.829$, $p \approx 1.434 \times 10^{-5}$ and $\mathcal{R}^2 \approx 0.9156$.

We can also plot the data and the regression line.

```
plot(data$X, data$y,
     xlab = "Concentration", ylab = "Colorimeter Reading",
     main = "Simple Linear Regression")
abline(model, col = "red")
```



We can also calculate the regression coefficients manually.

We can calculate $\overline{X}$, $\overline{y}$ first.

```r
X_bar <- mean(data$X)
y_bar <- mean(data$y)
cat(paste("X_bar =", X_bar, "\ny_bar =", y_bar))
```

```
## X_bar = 62
## y_bar = 276.5
```

Then we calculate S_{xx}, S_{xy} and S_{yy} by:

$$
\begin{aligned}
S_{xx} &= \sum_{i=1}^{n}(x_i - \overline{x})^2 \\
S_{xy} &= \sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y}) \\
S_{yy} &= \sum_{i=1}^{n}(y_i - \overline{y})^2
\end{aligned}
$$

```r
S_xx <- sum((data$X - X_bar)^2)
S_xy <- sum((data$X - X_bar) * (data$y - y_bar))
S_yy <- sum((data$y - y_bar)^2)
cat(paste("S_xx =", S_xx, "\nS_xy =", S_xy, "\nS_yy =", S_yy))
```

```
## S_xx = 2760
## S_xy = 23540
## S_yy = 219270.5
```

Then we can calculate the $\hat{\beta}_1$ and $\hat{\beta}_0$ by:

$$
\begin{cases}
\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} \\
\hat{\beta}_0 = \overline{y} - \hat{\beta}_1\overline{x}
\end{cases}
$$

```r
beta_1 <- S_xy / S_xx
beta_0 <- y_bar - beta_1 * X_bar
cat(paste("beta_1 =", beta_1, "\nbeta_0 =", beta_0))
```

```
## beta_1 = 8.52898550724638
## beta_0 = -252.297101449275
```

So we can write

$$\hat{y} = -252.2971 + 8.5290X$$

Which is the same as the result from `lm` function.

ANOVA Table

It is easy to see the $\mathcal{F}$ statistic and $\mathcal{R}^2$ statistic from the `summary` function. We can also calculate them manually.

We can calculate SSR and SSE by:

$$
\begin{aligned}
\mathrm{SSR} &= \sum_{i=1}^{n} (\hat{y}_i - \overline{y})^2 \\
\mathrm{SSE} &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2
\end{aligned}
$$

```r
y_hat <- beta_0 + beta_1 * data$X
SSR <- sum((y_hat - y_bar)^2)
SSE <- sum((data$y - y_hat)^2)
cat(paste("SSR =", SSR, "\nSSE =", SSE))
```

```
## SSR = 200772.31884058
## SSE = 18498.1811594203
```

And

$$
\begin{aligned}
\mathrm{MS}_{\mathrm{Reg}} &= \mathrm{SSR} \\
s^2 &= \frac{1}{n-2}\mathrm{SSE}
\end{aligned}
$$

```r
MS_Reg <- SSR
s2 <- SSE / 8
cat(paste("MS_Reg =", MS_Reg, "\ns^2 =", s2))
```

```
## MS_Reg = 200772.31884058
## s^2 = 2312.27264492754
```

After that, we can obtain the $\mathcal{F}$ statistic by

$$
\mathcal{F} = \frac{\mathrm{MS}_{\mathrm{Reg}}}{s^2}
$$

```r
F <- MS_Reg / s2
cat(paste("F =", F))
```

```
## F = 86.8289988557434
```

So we can calculate the p-value for $\mathcal{H}_0$ is $\beta_1 = 0$ is

$$
p = \mathbb{P}\left(X, y \mid \beta_1 = 0\right) = \int_{\mathcal{F}}^{+\infty} F_{1,8}(f)\mathrm{d}f \approx 1.434 \times 10^{-5}
$$

```r
p <- 1 - pf(86.829, 1, 8)
cat(paste("p =", p))
```

```
## p = 1.43437158113269e-05
```

The p value is quite small, so we can reject the null hypothesis and say that there is a significant relationship between X (concentration) and y (colorimeter reading).

For $\mathcal{R}^2$ statistic, we can calculate it by

$$
\mathcal{R}^2 = \frac{S_{xy}^2}{S_{xx}S_{yy}}
$$

```r
R2 <- S_xy^2 / (S_xx * S_yy)
cat(paste("R2 =", R2))
```

```
## R2 = 0.915637620384775
```

So the $\mathcal{R}^2$ statistic is about 0.9156. Which means that there is a strong linear relationship between X and y.

Conclusion

For question (a), we have fitted a simple linear regression model to the data by:

$$\hat{y} = -252.2971 + 8.5290X$$

For question (b), we have tested the model adequacy using $\mathcal{F}$ test and $\mathcal{R}^2$ statistics. The $\mathcal{F}$ statistic is 86.829 and the p value is 1.434×10^{-5}, which means that there is a significant relationship between X and y. The $\mathcal{R}^2$ statistic is 0.9156, which means that there is a strong linear relationship between X and y.