STAT 516 Lec 02

Review of simple linear regression

Karl Gregory

2025-01-28

Hemoglobin versus RBC count example

These data are a subset of the dataset Marcinkevičs et al. (2023)

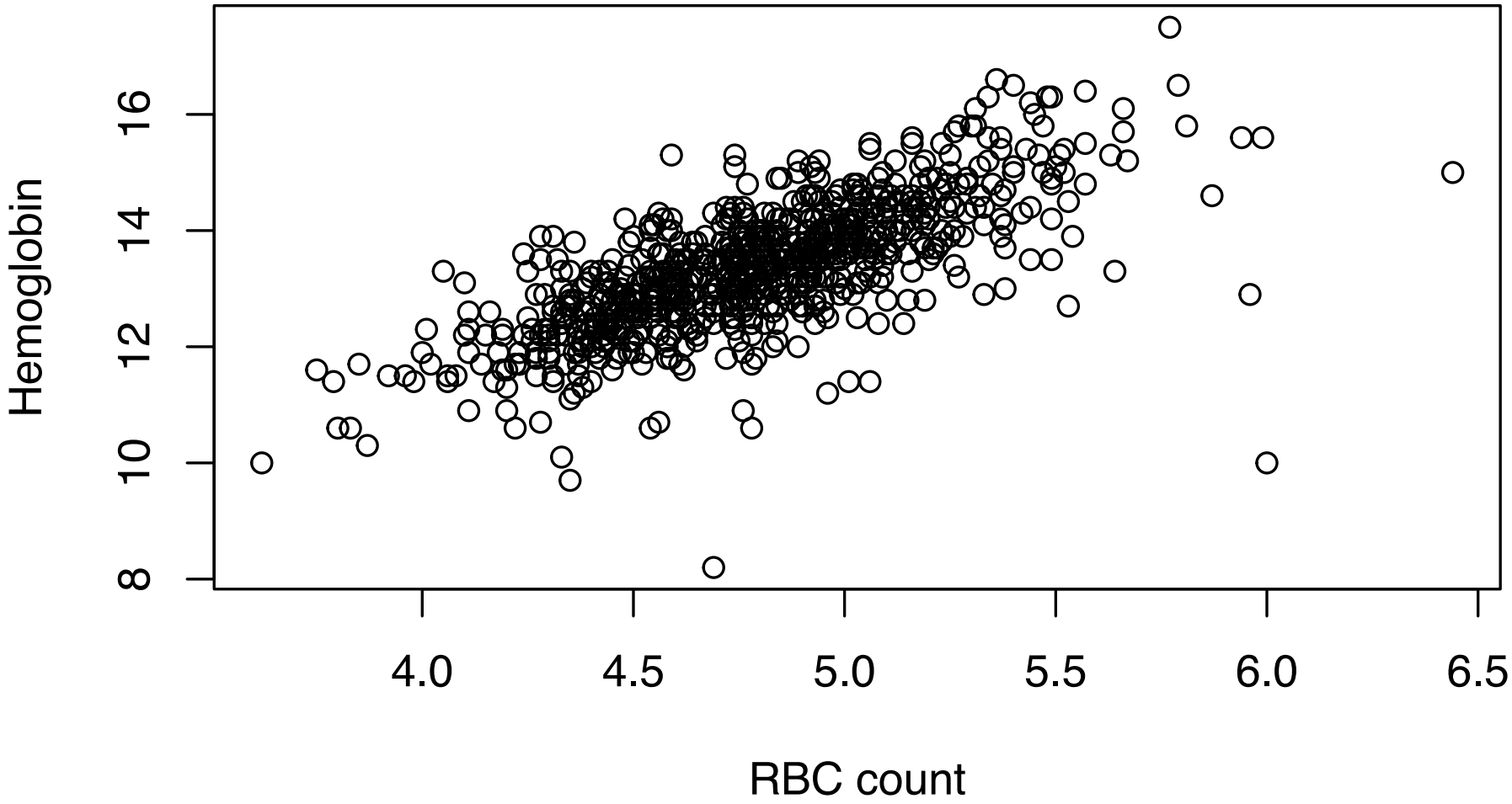
Some outliers and missing values were removed.

```
link <- url("https://people.stat.sc.edu/gregorkb/data/hrbc.csv")
data <- read.csv(link)
head(data)
```

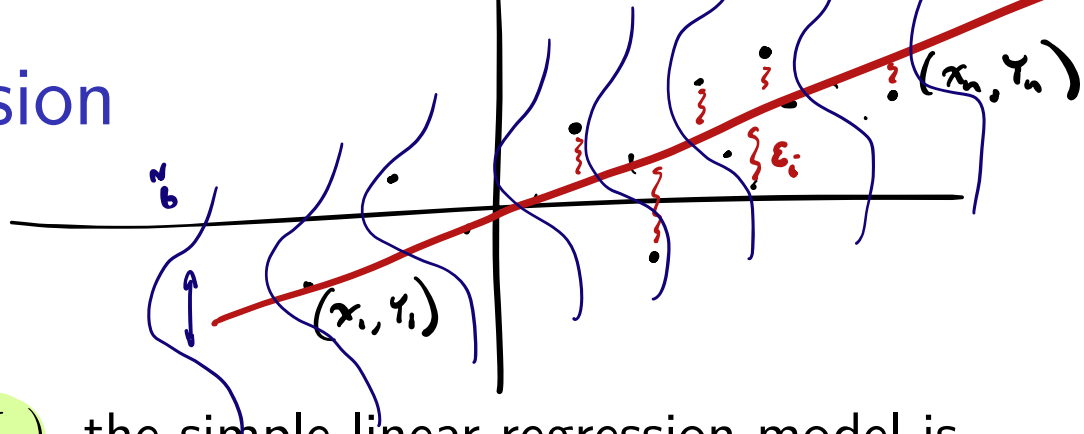
```
   hem  rbc    sex   age            diag
1 14.8 5.27 female 12.68    appendicitis
2 15.7 5.26   male 14.10 no appendicitis
3 11.4 3.98 female 14.14 no appendicitis
4 13.6 4.64 female 16.37 no appendicitis
5 12.6 4.44 female 11.08    appendicitis
6 12.5 4.96   male 11.05 no appendicitis
```

Hemoglobin level vs red blood cell count for $n = 762$ children.

```
plot(data$hem ~ data$rbc,
     ylab = "Hemoglobin",
     xlab = "RBC count")
```



Simple linear regression



For $(x_1, Y_1), \ldots, (x_n, Y_n)$, the simple linear regression model is

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad i = 1, \ldots, n$$

"epsilon"

"noise", "error term"

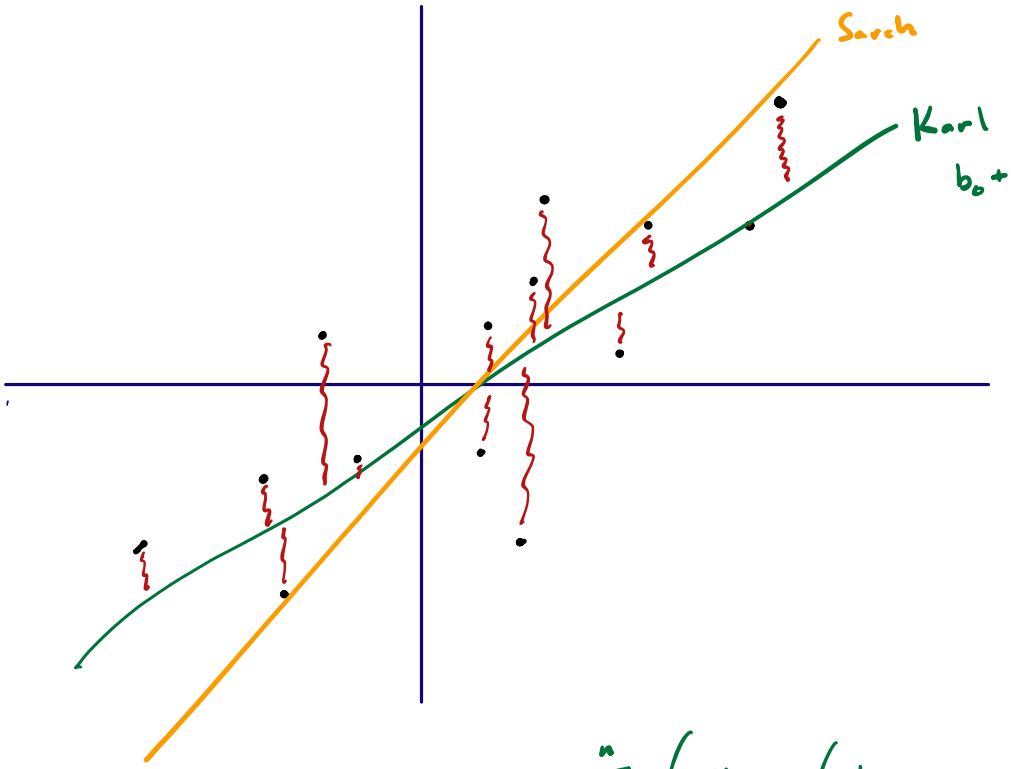
where

- $x_1, \ldots, x_n$ are the covariate or predictor values.
- $Y_1, \ldots, Y_n$ are the response values.
- β_0 and β_1 are the intercept and slope parameters, respectively.
- $\varepsilon_1, \ldots, \varepsilon_n$ are independent Normal$(0, \sigma^2)$ error terms.
- σ^2 is the error term variance.

Goals in simple linear regression

We will learn how to:

1. Estimate the intercept and slope parameters β_0 and β_1.
2. Estimate the error term variance σ^2.
3. Perform inference on β_1.
4. Build a confidence interval for $\beta_0 + \beta_1 x_{\text{new}}$ at any x_{new}.
5. Build a prediction interval for Y at any x_{new}.
6. Decompose the variation in Y into sums of squares.
7. Check whether the model assumptions are satisfied.
8. Identify outliers and understand their effects.



$$\sum_{i=1}^{n} \left(y_i - \left(b_0 + b_1 x_i \right) \right)^2$$

Least-squares estimation of slope and intercept

The squared error criterion given by the sum

$$Q(b_0, b_1) = \sum_{i=1}^{n} (Y_i - (b_0 + b_1 x_i))^2$$

of squared vertical distances of Y_i from the line $y = b_0 + b_1 x$.

We find $Q(b_0, b_1)$ is minimized at $(b_0, b_1) = (\hat{\beta}_0, \hat{\beta}_1)$, where

- $\hat{\beta}_0 = \bar{Y}_n - \hat{\beta}_1 \bar{x}_n$
- $\hat{\beta}_1 = \dfrac{\sum_{i=1}^{n} (x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{\sum_{i=1}^{n} (x_i - \bar{x}_n)^2}$

provided $\sum_{i=1}^{n} (x_i - \bar{x}_n)^2 > 0$.

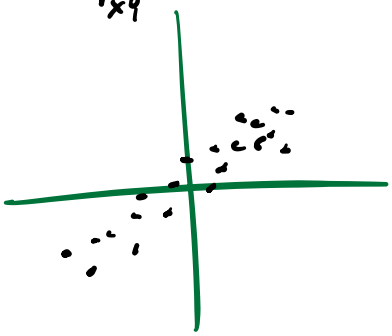
The least-squares line or fitted line is the line $y = \hat{\beta}_0 + \hat{\beta}_1 x$.

"Least-squares estimators"

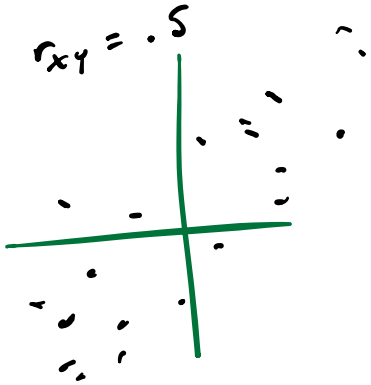
"in"

Pearson's Correlation Coef. $r_{xy} \in [-1, 1]$

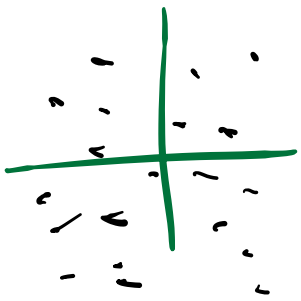
$r_{xy} = .8$



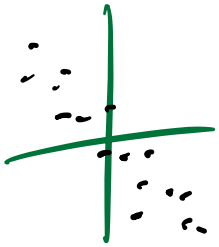
$r_{xy} = .5$



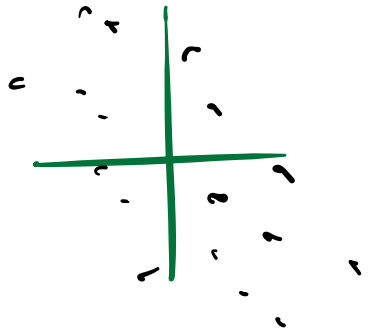
$r_{xy} = 0$



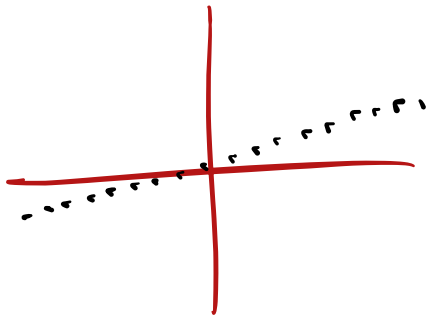
$r_{xy} = -.8$



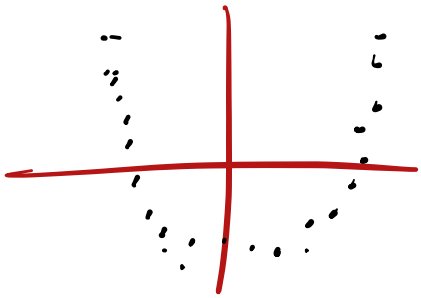
$r_{xy} = -.5$



$r_{xy} = 1$



$r_{xy} \approx 0$



Pearson's correlation coefficient

Given $(x_1, Y_n), \ldots, (x_n, Y_n)$, the quantity

$$r_{xY} = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2 \sum_{i=1}^{n}(Y_i - \bar{Y}_n)^2}}$$

is called Pearson's correlation coefficient.

- Describes strength and direction of *linear* relationships.
- Must satisfy $r_{xY} \in [-1, 1]$.
- Values close to zero indicate a weak linear relationship.
- Is related to $\hat{\beta}_1$ by

$$\hat{\beta}_1 = r_{xY} \frac{S_Y}{S_x}.$$

sd(Y) sd(x) cor(x,Y) = cor(Y,x)

where S_Y and S_x are the sample std devs of the Y and x values.

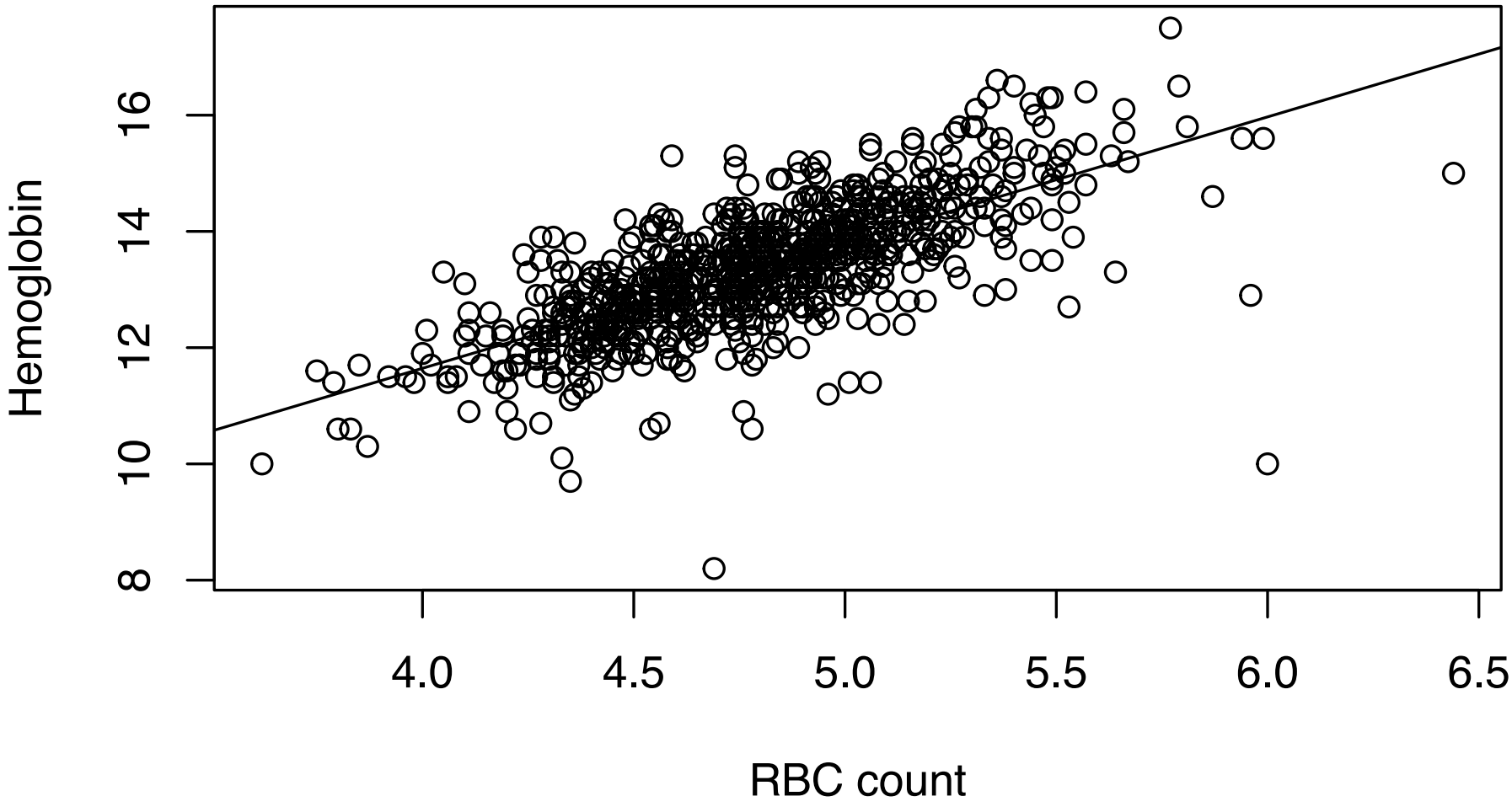
Hemoglobin versus RBC count example (cont)

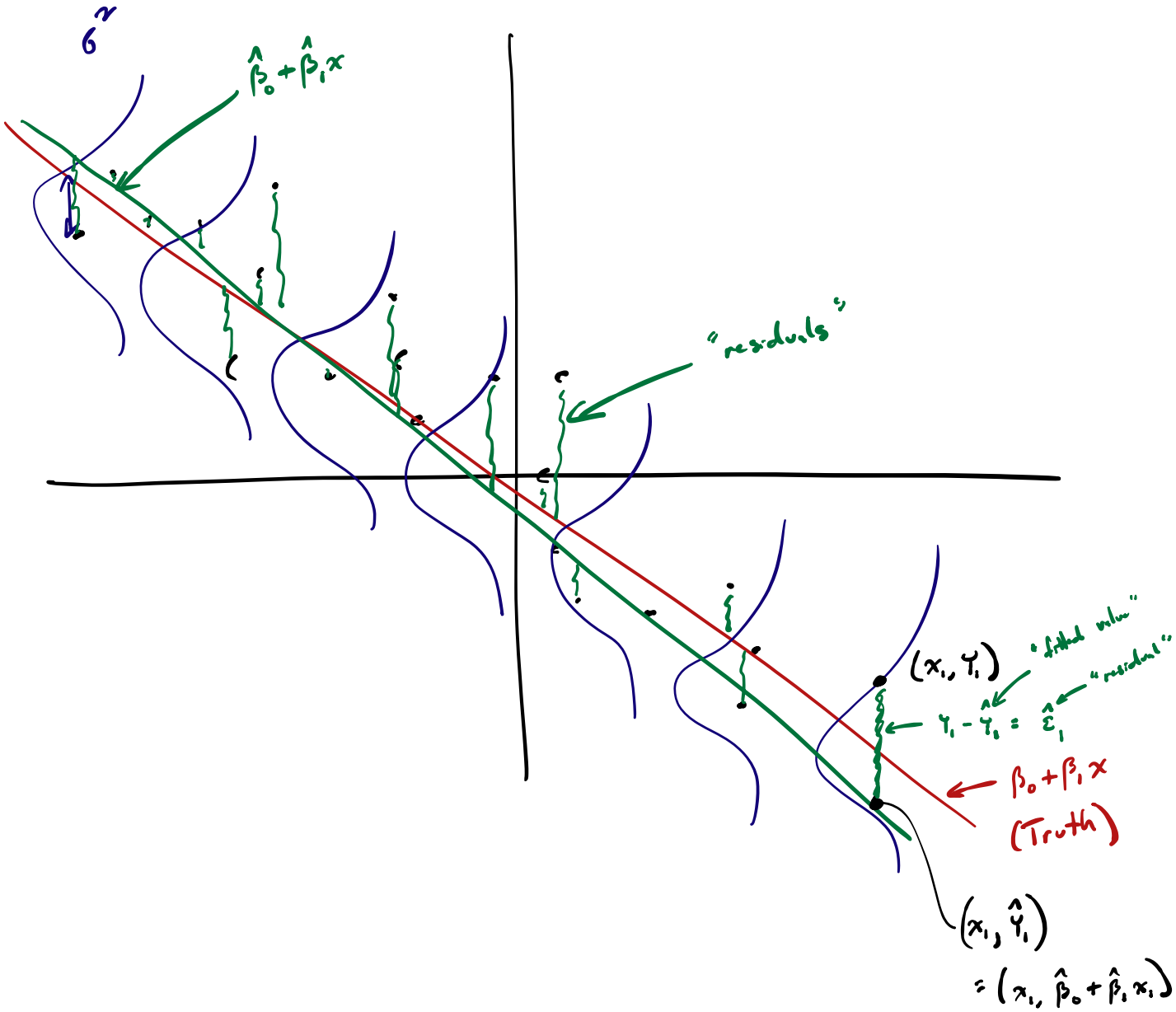
Find the least-squares line on the hemoglobin data.

```
Y <- data$hem
x <- data$rbc
n <- length(Y)
xbar <- mean(x)
Ybar <- mean(Y)

rxY <- cor(x,Y) # Pearson's correlation coefficient
b1hat <- rxY * sd(Y)/sd(x)
b0hat <- Ybar - b1hat * xbar
```

```r
plot(data$hem ~ data$rbc, ylab = "Hemoglobin", xlab = "RBC count")
abline(b0hat,b1hat)
```




$\hat{\beta}_0 + \hat{\beta}_1 x$
"residuals"
(x_i, y_i)
"fitted value"
"residual"
$y_i - \hat{y}_i = \hat{\varepsilon}_i$
$\beta_0 + \beta_1 x$
(Truth)
$(x_i, \hat{y}_i)$
$= (x_i, \hat{\beta}_0 + \hat{\beta}_1 x_i)$

Estimating the error term variance

After obtaining $\hat{\beta}_0$ and $\hat{\beta}_1$, define the

- fitted values as $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ ← Estimated line at the observed value of x.
- residuals as $\hat{\varepsilon}_i = Y_i - \hat{Y}_i$

for $i = 1, \ldots, n$.

Then an unbiased estimator of σ^2 is given by

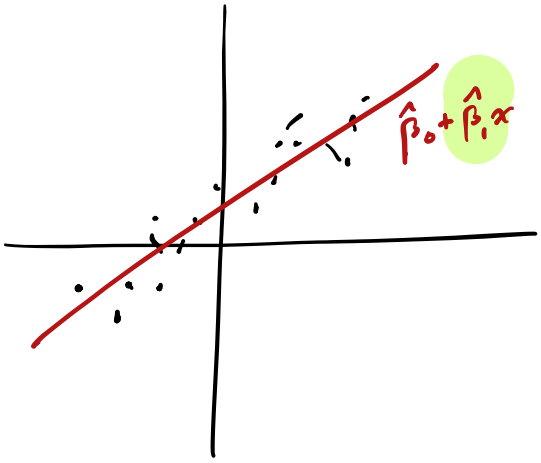
$$\hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^{n} \hat{\varepsilon}_i^2.$$

$= \frac{1}{n-2} \sum_{i=1}^{n} \left(\hat{\varepsilon}_i - \bar{\hat{\varepsilon}}_n \right)^2$

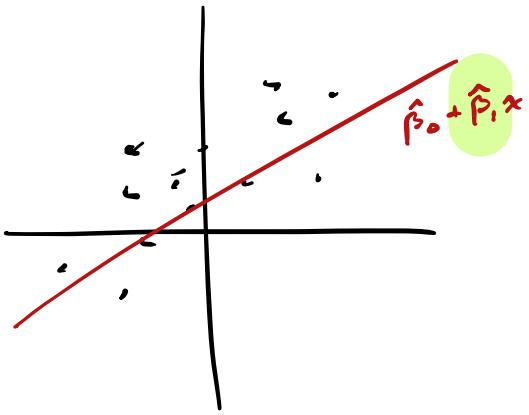
$n-2$ because we had n data points and estimated 2 things already.

mean of $\hat{\varepsilon}_1, \ldots, \hat{\varepsilon}_n$ is equal to zero

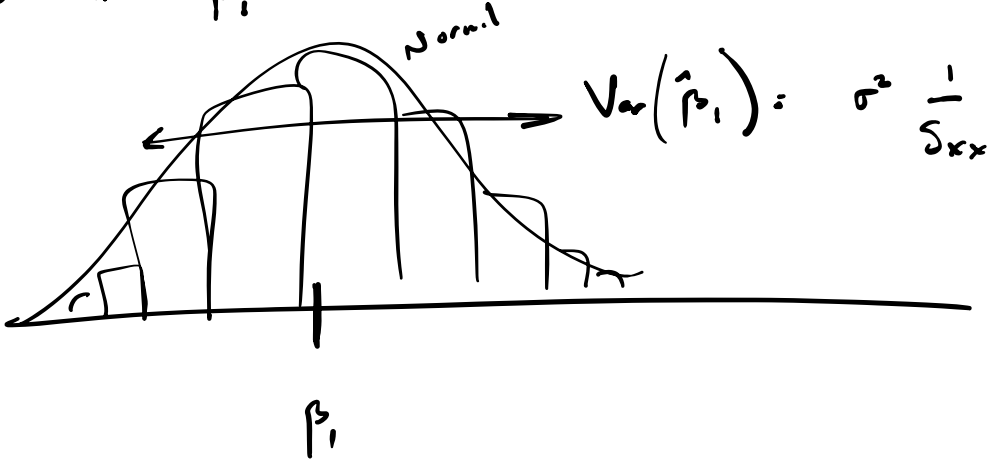
Collect data many times, compute LS estimates $\hat{\beta}_0, \hat{\beta}_1$



. . .



Many values of $\hat{\beta}_1$:



$$Var(\hat{\beta}_1) = \sigma^2 \frac{1}{S_{xx}}$$

$$S_{xx} = \sum_{i=1}^{n} (x_i - \bar{x}_n)^2$$

Confidence interval for the slope parameter

Assume $\varepsilon_1, \ldots, \varepsilon_n \overset{\text{ind}}{\sim} \text{Normal}(0, \sigma^2)$ and set $S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x}_n)^2$.

- The slope estimator $\hat{\beta}_1$ is distributed as

$$\hat{\beta}_1 \sim \text{Normal}(\beta_1, \sigma^2/S_{xx}).$$

- "Studentizing" the above gives

subtract the mean, divide by the estimated std. dev.

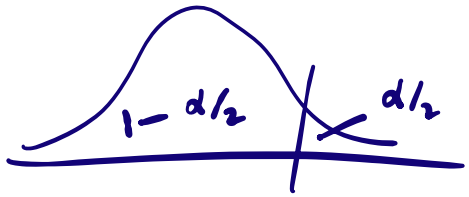
$$\frac{\hat{\beta}_1 - \beta_1}{\hat{\sigma}/\sqrt{S_{xx}}} \sim t_{n-2}.$$

- So a $(1-\alpha)100\%$ confidence interval for β_1 is

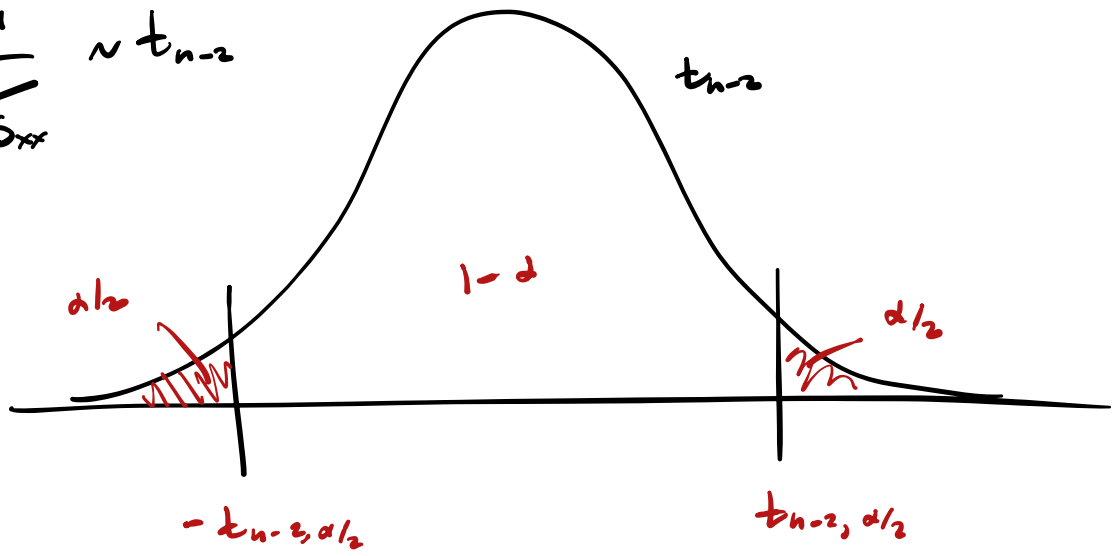
$t(1-\alpha/2, n-2)$

$$\hat{\beta}_1 \pm t_{n-2,\alpha/2}\hat{\sigma}/\sqrt{S_{xx}}.$$

Exercise: Justify the CI using the sampling distribution result.



$$\frac{\hat{\beta}_1 - \beta_1}{\hat{\sigma}/\sqrt{S_{xx}}} \sim t_{n-2}$$



$$\Rightarrow P\left(-t_{n-2,\alpha/2} < \frac{\hat{\beta}_1 - \beta_1}{\hat{\sigma}/\sqrt{S_{xx}}} < t_{n-2,\alpha/2}\right) = 1-\alpha$$

$\therefore$ Rearrange till β_1 is alone in middle

$$P\left(\hat{\beta}_1 - t_{n-2,\alpha/2}\frac{\hat{\sigma}}{\sqrt{S_{xx}}} < \beta_1 < \hat{\beta}_1 + t_{n-2,\alpha/2}\frac{\hat{\sigma}}{\sqrt{S_{xx}}}\right)$$

$\Rightarrow$ $(1-\alpha)\cdot 100\%$ C.I. for β_1 is

$$\hat{\beta}_1 \pm t_{n-2,\alpha/2}\frac{\hat{\sigma}}{\sqrt{S_{xx}}}.$$

Hemoglobin versus RBC count example (cont)

Obtain an estimate of the error term variance.

```
Yhat <- b0hat + b1hat * x
ehat <- Y - Yhat
sgsqhat <- sum(ehat^2)/(n-2)
```

We obtain $\hat{\sigma}^2 = 0.626$.

Now construct a 95% confidence interval for β_1.

```
alpha <- 0.05
Sxx <- sum((x - xbar)^2)
ta2 <- qt(1 - alpha/2, df = n - 2)
lo <- b1hat - ta2 * sqrt(sgsqhat / Sxx)
up <- b1hat + ta2 * sqrt(sgsqhat / Sxx)
```

The 95% CI is $(2.011, 2.314)$.

Note: can use `lm_out <- lm(Y ~ x)` `confint(lm_out)`

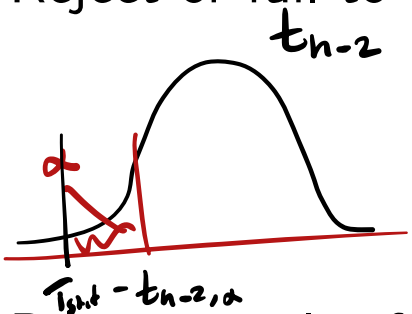
Tests of hypotheses about the slope

If $\beta_1 = 0$, then X and Y have no linear relationship

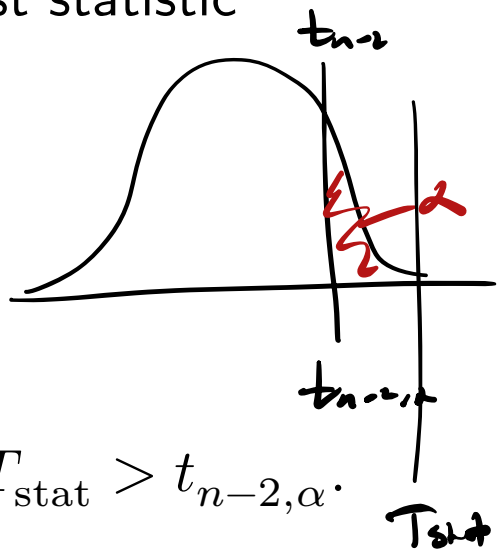
We most often test hypotheses about β_1 of the form

$$\begin{array}{l} H_0\colon \beta_1 \geq 0 \\ H_1\colon \beta_1 < 0 \end{array} \quad \text{or} \quad \begin{array}{l} H_0\colon \beta_1 = 0 \\ H_1\colon \beta_1 \neq 0 \end{array} \quad \text{or} \quad \begin{array}{l} H_0\colon \beta_1 \leq 0 \\ H_1\colon \beta_1 > 0. \end{array}$$

Reject or fail to reject H_0 based on the value of the test statistic



$$T_{\text{stat}} = \frac{\hat{\beta}_1 - 0}{\hat{\sigma}/\sqrt{S_{xx}}}.$$

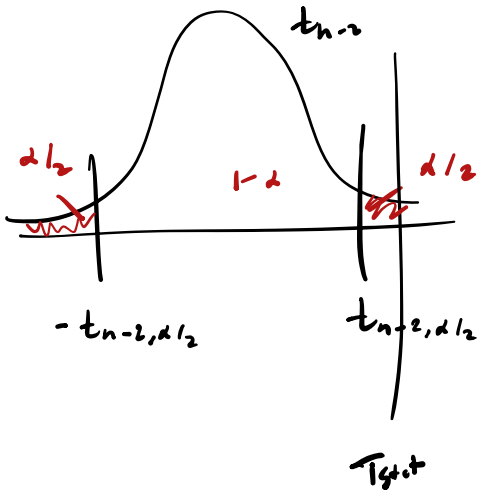


Rejection rules for the above at significance level α are

$$T_{\text{stat}} < -t_{n-2,\alpha} \quad \text{or} \quad |T_{\text{stat}}| > t_{n-2,\alpha/2} \quad \text{or} \quad T_{\text{stat}} > t_{n-2,\alpha}.$$

The corresponding p-values are, with $T \sim t_{n-2}$, the probabilities

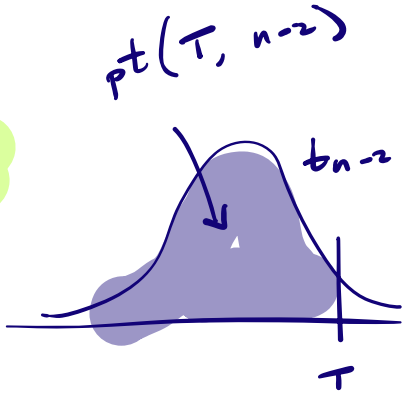
$$P(T < T_{\text{stat}}) \quad \text{or} \quad 2 \times P(T > |T_{\text{stat}}|) \quad \text{or} \quad P(T > T_{\text{stat}}).$$

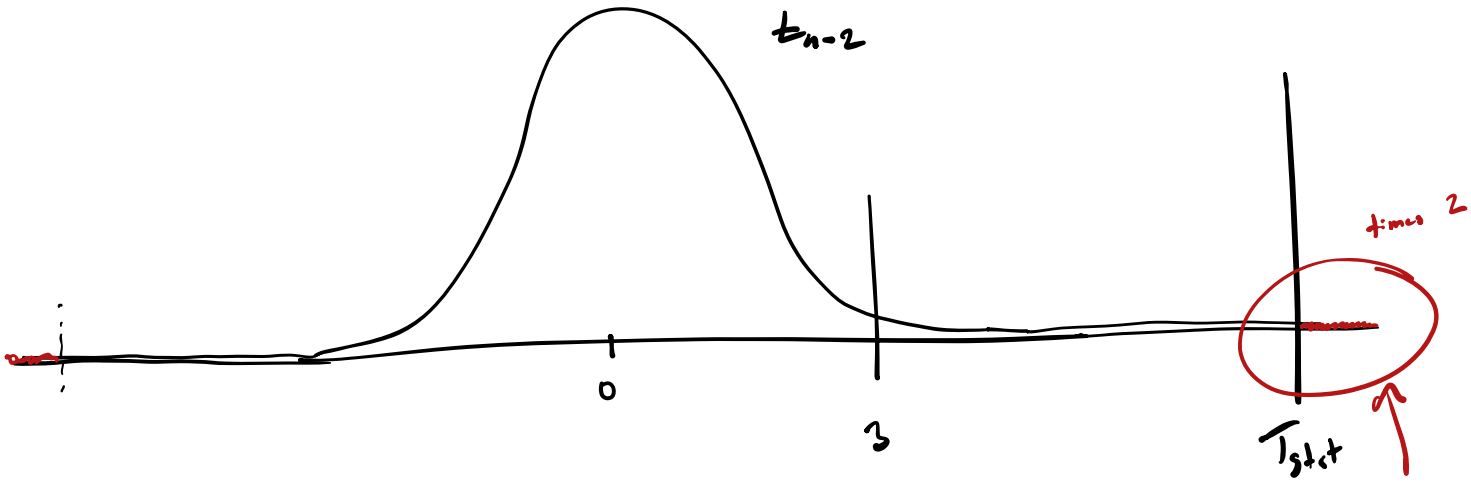


Test $H_0: \beta_1 = 0$ on RBC data

$H_1: \beta_1 \neq 0$ at $\alpha = 0.05$

$$T_{stat} = \frac{\hat{\beta}_1}{\hat{\sigma}/\sqrt{S_{xx}}} = 28.02$$





p-val ≈ 0

$2\,(1 - pt(|T_{stat}|, n-2))$

Hemoglobin versus RBC count example (cont)

Test the hypotheses H_0: $\beta_1 = 0$ vs H_1: $\beta_1 \neq 0$ at $\alpha = 0.05$.

```
alpha <- 0.05
Tstat <- b1hat / sqrt(sgsqhat/Sxx)
crit <-  qt(1-alpha/2, df = n - 2)
pval <- 2*(1 - pt(abs(Tstat), df = n - 2))
```

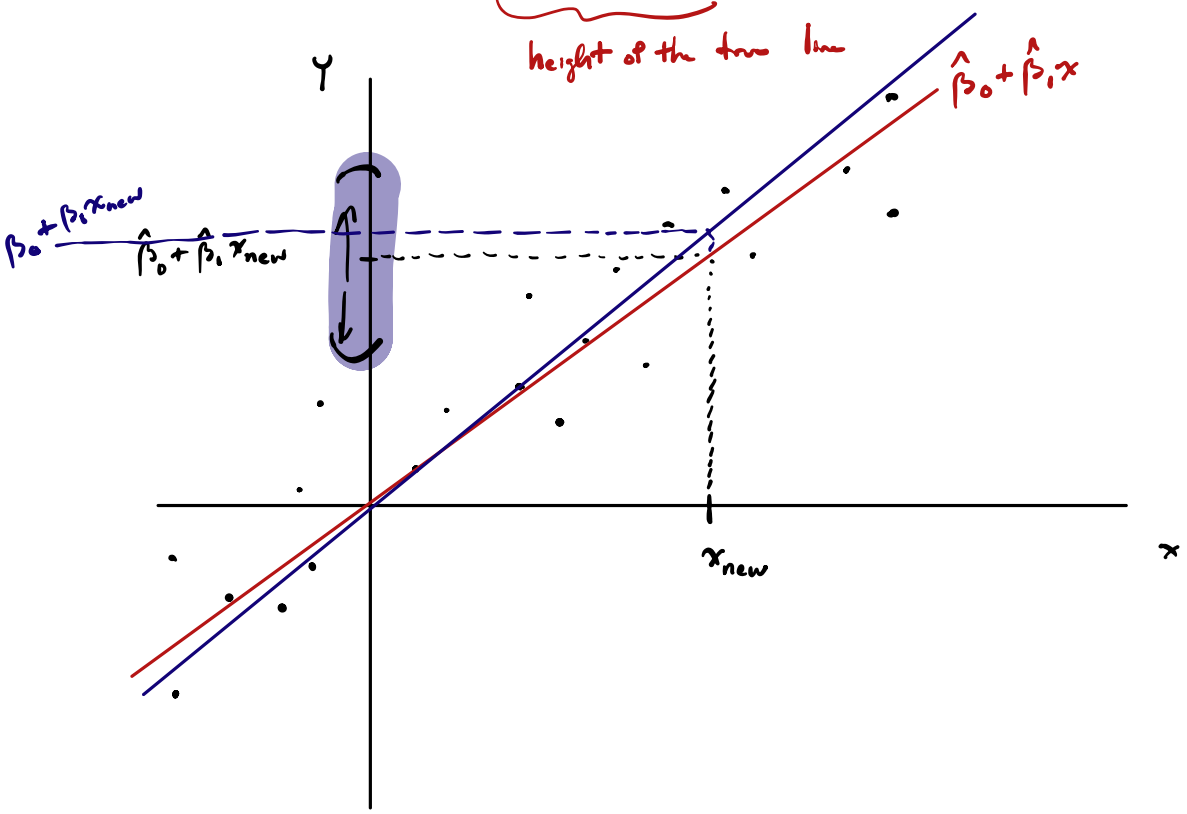
We get $T_{\text{stat}} = 28.021$, $t_{n-2,\alpha/2} = 1.963$, and p-value 0; we reject H_0.

Test the hypotheses H_0: $\beta_1 \leq 2$ vs H_1: $\beta_1 > 2$.

```
Tstat <- (b1hat - 2) / sqrt(sgsqhat/Sxx)
crit <-  qt(1-alpha, df = n - 2)
pval <- 1 - pt(Tstat, df = n - 2)
```

We get $T_{\text{stat}} = 2.107$, $t_{n-2,\alpha} = 1.647$, and p-value 0.018; we reject H_0.

Build C.I. for $\beta_0 + \beta_1 x_{new}$ at some x_{new}.



Confidence interval for the height of the line

Assume $\varepsilon_1, \ldots, \varepsilon_n \overset{\text{ind}}{\sim} \text{Normal}(0, \sigma^2)$. Then:

- The estimator $\hat{\beta}_0 + \hat{\beta}_1 x$ is distributed as

$$\hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}} \sim \text{Normal}\left(\beta_0 + \beta_1 x_{\text{new}}, \sigma^2 \left[\frac{1}{n} + \frac{(x_{\text{new}} - \bar{x}_n)^2}{S_{xx}}\right]\right).$$

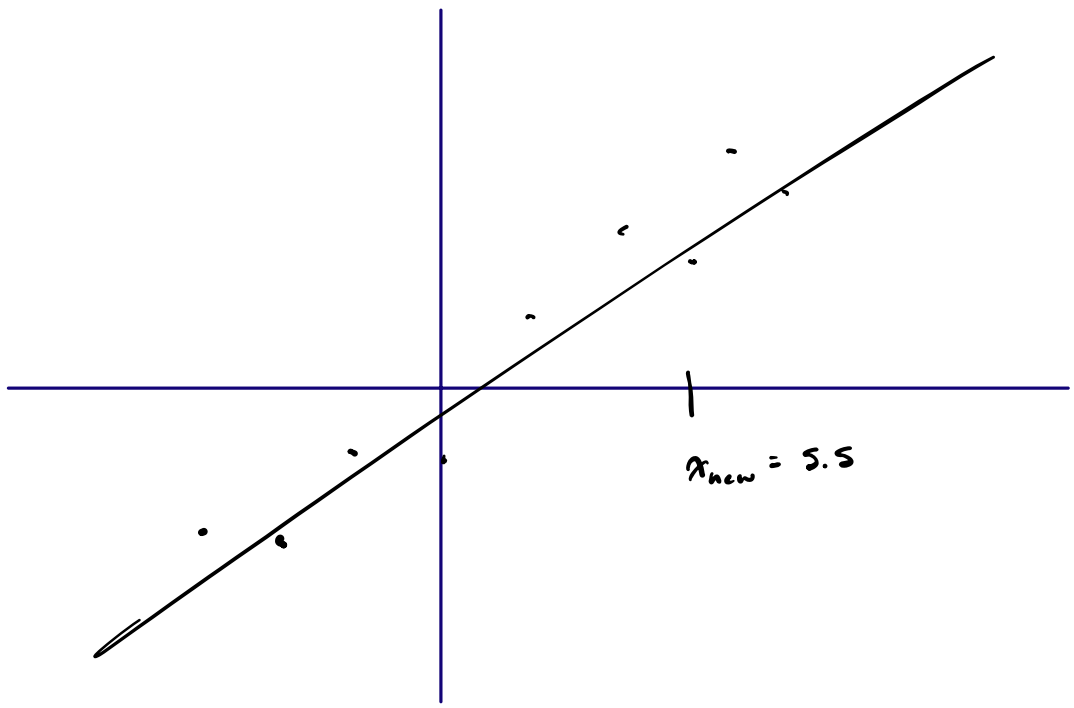
- "Studentizing" the above gives

$$\frac{\hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}} - (\beta_0 + \beta_1 x_{\text{new}})}{\hat{\sigma}\sqrt{\frac{1}{n} + \frac{(x_{\text{new}} - \bar{x}_n)^2}{S_{xx}}}} \sim t_{n-2}.$$

- So a $(1-\alpha)100\%$ confidence interval for $\beta_0 + \beta_1 x_{\text{new}}$ is

$$\hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}} \pm t_{n-2,\alpha/2}\hat{\sigma}\sqrt{\frac{1}{n} + \frac{(x_{\text{new}} - \bar{x}_n)^2}{S_{xx}}}.$$

$qt(1-\alpha/2, n-2)$ se


$x_{new} = 5.5$

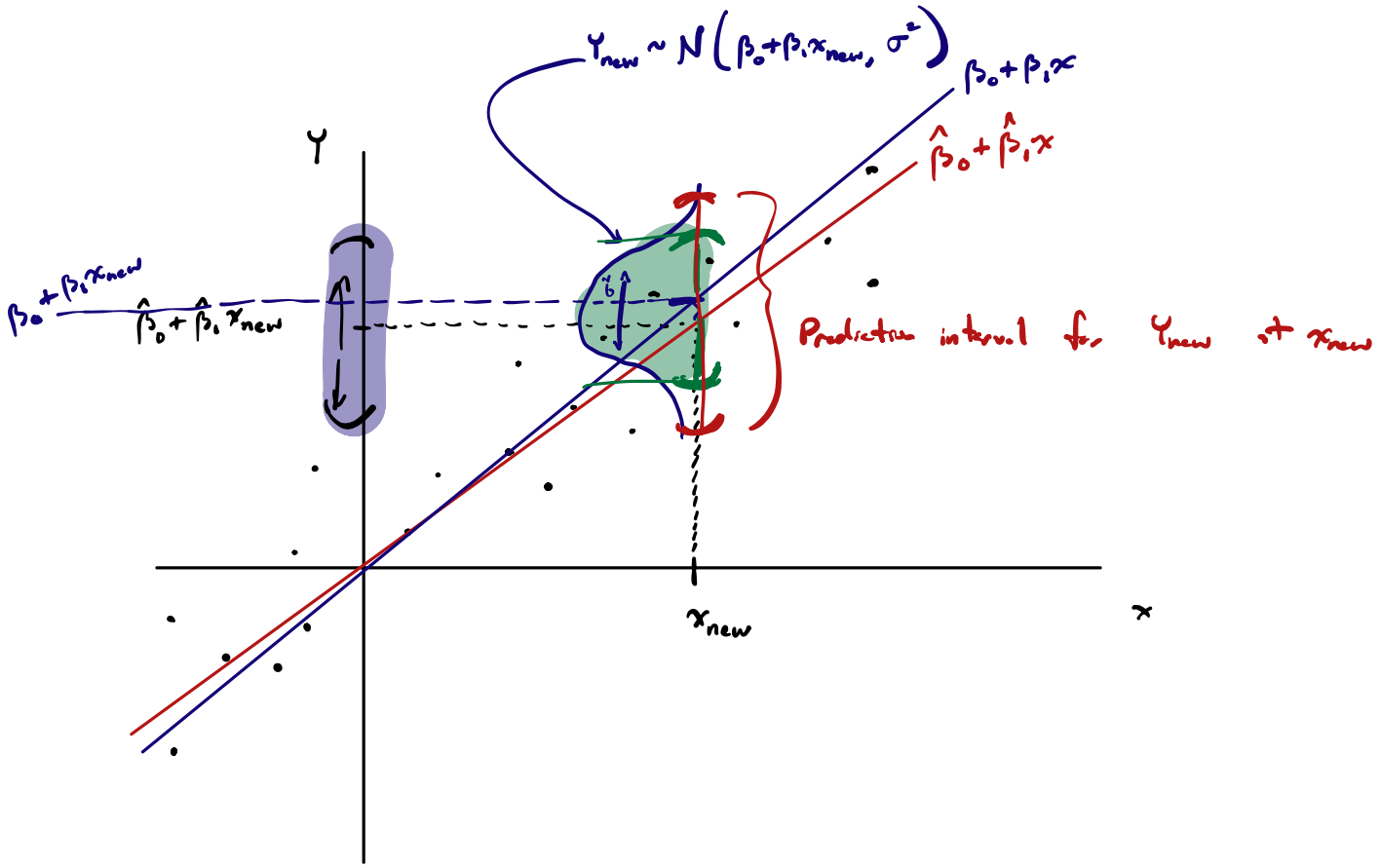
Hemoglobin versus RBC count example (cont)

Give a 95% CI for the mean hemoglobin level of individuals with RBC count 5.5.

```
alpha <- 0.05
xnew <- 5.5
xnew_se <- sqrt(sgsqhat)*sqrt(1/n+(xnew-xbar)^2/Sxx)
ta2 <- qt(1-alpha/2,n-2)
lo <- b0hat + b1hat * xnew - ta2 * xnew_se
up <- b0hat + b1hat * xnew + ta2 * xnew_se
```

We are 95% confident that the mean hemoglobin level of individuals with RBC count 5.5 lies in the interval $(14.767, 15.011)$.

Build a prediction interval for Y_{new} at some x_{new}.



The prediction interval should capture Y_{new} with prob. $1-\alpha$.

Prediction interval for a new value of the response

Assume $\varepsilon_1, \ldots, \varepsilon_n \overset{\text{ind}}{\sim} \text{Normal}(0, \sigma^2)$. Then:

- The new residual $Y_{\text{new}} - \hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}}$ is distributed as

$$\hat{\varepsilon}_{\text{new}} = Y_{\text{new}} - \hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}} \sim \text{Normal}\left(0, \sigma^2\left[1 + \frac{1}{n} + \frac{(x_{\text{new}} - \bar{x}_n)^2}{S_{xx}}\right]\right).$$

- "Studentizing" the above gives

$$\frac{Y_{\text{new}} - \hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}}}{\hat{\sigma}\sqrt{1 + \frac{1}{n} + \frac{(x_{\text{new}} - \bar{x}_n)^2}{S_{xx}}}} \sim t_{n-2}.$$

- So a $(1-\alpha)100\%$ prediction interval interval for Y_{new} is

$$\hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}} \pm t_{n-2,\alpha/2}\hat{\sigma}\sqrt{1 + \frac{1}{n} + \frac{(x_{\text{new}} - \bar{x}_n)^2}{S_{xx}}}.$$

only difference from the CI for $\beta_0 + \beta_1 x_{\text{new}}$

Hemoglobin versus RBC count example (cont)

Give a 95% prediction interval for the hemoglobin level when the RBC count is 5.5.

```
alpha <- 0.05
xnew <- 5.5
xnew_pse <- sqrt(sgsqhat)*sqrt(1+1/n+(xnew-xbar)^2/Sxx)
ta2 <- qt(1-alpha/2,n-2)
lo <- b0hat + b1hat * xnew - ta2 * xnew_pse
up <- b0hat + b1hat * xnew + ta2 * xnew_pse
```

We are 95% confident that an *individual* with RBC count 5.5 will have a hemoglobin level in the interval $(13.331, 16.447)$.

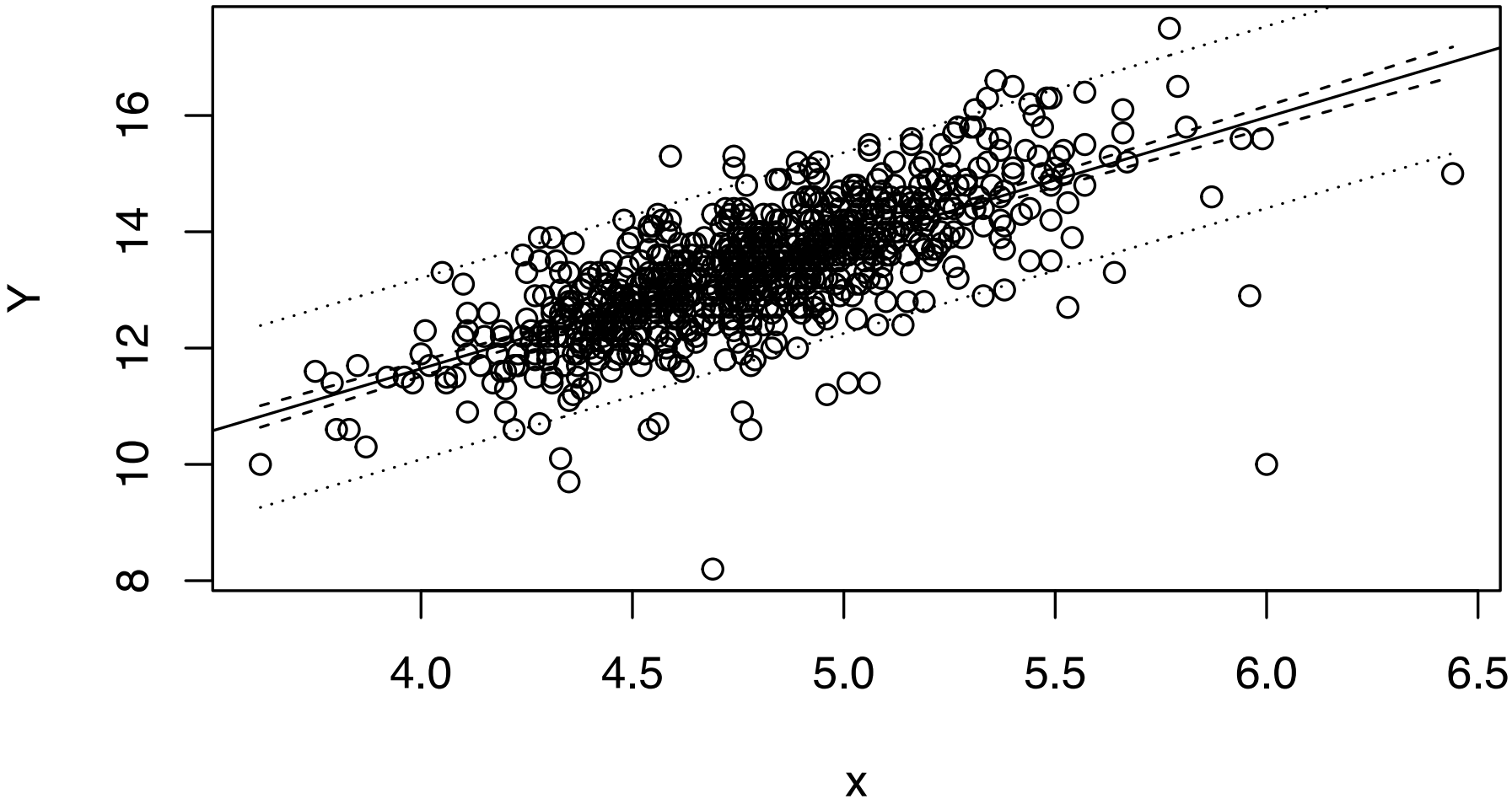
Plot confidence and prediction limits over the range of RBC counts.

```
alpha <- 0.05
ta2 <- qt(1-alpha/2,n-2)
xseq <- seq(min(x),max(x),length = 500)

xseq_se <- sqrt(sgsqhat)*sqrt(1/n+(xseq-xbar)^2/Sxx)
loci <- b0hat + b1hat * xseq - ta2 * xseq_se
upci <- b0hat + b1hat * xseq + ta2 * xseq_se

xseq_pse <- sqrt(sgsqhat)*sqrt(1+1/n+(xseq-xbar)^2/Sxx)
lopi <- b0hat + b1hat * xseq - ta2 * xseq_pse
uppi <- b0hat + b1hat * xseq + ta2 * xseq_pse
```

```r
plot(Y~x)
abline(b0hat,b1hat)
lines(loci ~ xseq, lty=2); lines(upci ~ xseq, lty=2)
lines(lopi ~ xseq, lty=3); lines(uppi ~ xseq, lty=3)
```



The predict() function in R

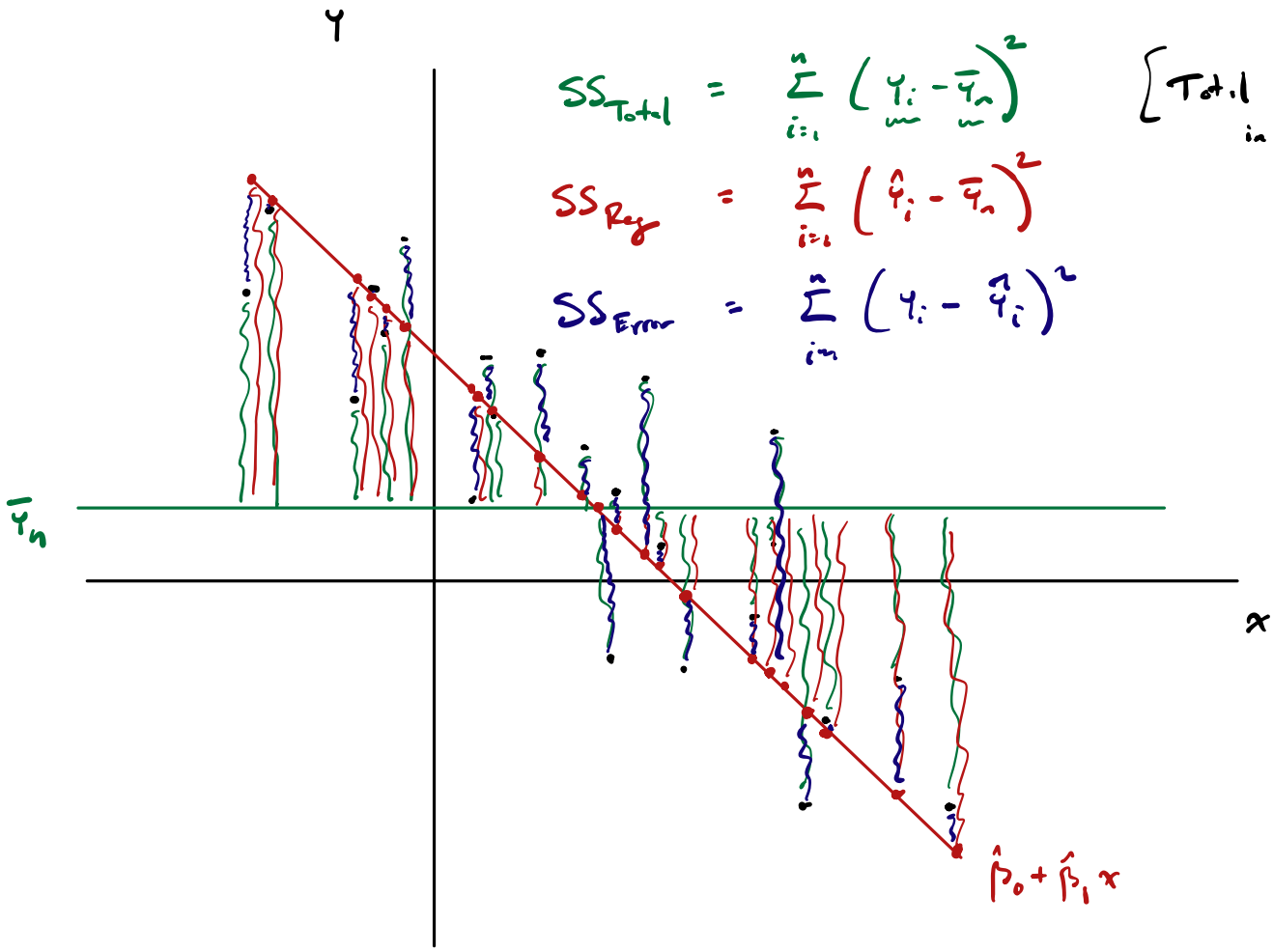
```
predict(lm_out, newdata = data.frame(x = 5.5), int = "conf")
```

```
       fit      lwr      upr
1 14.88892 14.76725 15.01059
```

```
predict(lm_out, newdata = data.frame(x = 5.5), int = "pred")
```

```
       fit      lwr      upr
1 14.88892 13.33117 16.44667
```

Sample variance of Y: $s_Y^2 = \frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y}_n)^2$



$SS_{Total} = \sum_{i=1}^{n} (y_i - \bar{y}_n)^2$ [Total variation in Y]

$SS_{Reg} = \sum_{i=1}^{n} (\hat{y}_i - \bar{y}_n)^2$

$SS_{Error} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$

$SS_{Total} = SS_{Reg} + SS_{Error}$

Sums of squares in simple linear regression

We decompose the variation in $Y_1, \ldots, Y_n$ by defining the:

- Total sum of squares: $\mathrm{SS}_{\mathrm{Tot}} = \sum_{i=1}^{n} (Y_i - \bar{Y}_n)^2$
- Regression sum of squares: $\mathrm{SS}_{\mathrm{Reg}} = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y}_n)^2$
- Error sum of squares: $\mathrm{SS}_{\mathrm{Error}} = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$

We have $\mathrm{SS}_{\mathrm{Tot}} = \mathrm{SS}_{\mathrm{Reg}} + \mathrm{SS}_{\mathrm{Error}}$.

The coefficient of determination is defined as $R^2 = \dfrac{\mathrm{SS}_{\mathrm{Reg}}}{\mathrm{SS}_{\mathrm{Tot}}}$.

Variation in $\hat{Y}$ / Total variation in Y

- $R^2 \in [0, 1]$
- Proportion of variation in Y "explained" by the covariate x.
- In simple linear regression we have $R^2 = r_{xY}^2$.

The mean squares in simple linear regression

The SS, appropriately scaled, follow chi-square distributions:

- $\frac{\mathrm{SS}_{\mathrm{Tot}}}{\sigma^2} \sim \chi^2_{n-1}(\phi_{\mathrm{Total}})$
- $\frac{\mathrm{SS}_{\mathrm{Reg}}}{\sigma^2} \sim \chi^2_{1}(\phi_{\mathrm{Reg}})$
- $\frac{\mathrm{SS}_{\mathrm{Error}}}{\sigma^2} \sim \chi^2_{n-2}$

The quantities ϕ_{Tot} and ϕ_{Reg} are called noncentrality parameters.

Dividing $\mathrm{SS}_{\mathrm{Reg}}$ and $\mathrm{SS}_{\mathrm{Error}}$ by their dfs, we define:

- Regression mean square: $\mathrm{MS}_{\mathrm{Reg}} = \frac{\mathrm{SS}_{\mathrm{Reg}}}{1}$
- Error mean square: $\mathrm{MS}_{\mathrm{Error}} = \frac{\mathrm{SS}_{\mathrm{Error}}}{n-2}$

The Analysis of Variance (ANOVA) table

We often present the SS, df, and MS values in a table like this:

Source	Df	SS	MS	F value	p-value
Regression	1	$\mathrm{SS}_{\mathrm{Reg}}$	$\mathrm{MS}_{\mathrm{Reg}}$	F_{stat}	$P(F > F_{\mathrm{stat}})$
Error	$n-2$	$\mathrm{SS}_{\mathrm{Error}}$	$\mathrm{MS}_{\mathrm{Error}}$		
Total	$n-1$	$\mathrm{SS}_{\mathrm{Tot}}$			

This is an example of an ANOVA table.

Overall F test

In addition to the SS, df, and MS value, the ANOVA table presents

- $F_{\text{stat}} = \dfrac{\text{MS}_{\text{Reg}}}{\text{MS}_{\text{Error}}}$
- $P(F > F_{\text{stat}})$, where this is computed under $F \sim F_{1,n-2}$

These are the test statistic and p-value of the overall F test.

In simple linear regression this p-value is the same as the one for testing H_0: $\beta_1 = 0$ versus H_1: $\beta_1 \neq 0$ with the t test; moreover $F_{\text{stat}} = T_{\text{stat}}^2$.

For what it's worth, one can show $F_{\text{stat}} = \dfrac{(n-2)r_{xY}^2}{1 - r_{xY}^2}$ in SLR.

We will discuss the overall F test in greater detail later.

Building the ANOVA table

```
SST <- sum((Y - Ybar)^2)
SSR <- sum((Yhat - Ybar)^2)
SSE <- sum((Y - Yhat)^2)
MSR <- SSR / 1
MSE <- SSE / (n-2)
Fstat <- MSR / MSE # same as (n-2)*rxY^2/(1 - rxY^2)
pval <- 1 - pf(Fstat,1,n-2)
```

Source	Df	SS	MS	F value	p-value
x	1	491.37	491.37	785.15	0
Error	760	475.63	0.63		
Total	761	967			

The lm(), summary(), and anova() functions in R

```
lm_out <- lm(Y~x)
lm_out
```

```
Call:
lm(formula = Y ~ x)

Coefficients:
(Intercept)            x
      2.994        2.163
```

```
summary(lm_out)
```

```
Call:
lm(formula = Y ~ x)

Residuals:
    Min      1Q  Median      3Q     Max
-5.9702 -0.4232  0.0074  0.4645  2.3791

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.99447    0.37065   8.079 2.56e-15 ***
x            2.16263    0.07718  28.021  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.7911 on 760 degrees of freedom
Multiple R-squared:  0.5081,    Adjusted R-squared:  0.5075
F-statistic: 785.1 on 1 and 760 DF,  p-value: < 2.2e-16
```

```r
anova(lm_out)
```

```
Analysis of Variance Table

Response: Y
           Df Sum Sq Mean Sq F value    Pr(>F)
x           1 491.37  491.37  785.15 < 2.2e-16 ***
Residuals 760 475.63    0.63
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

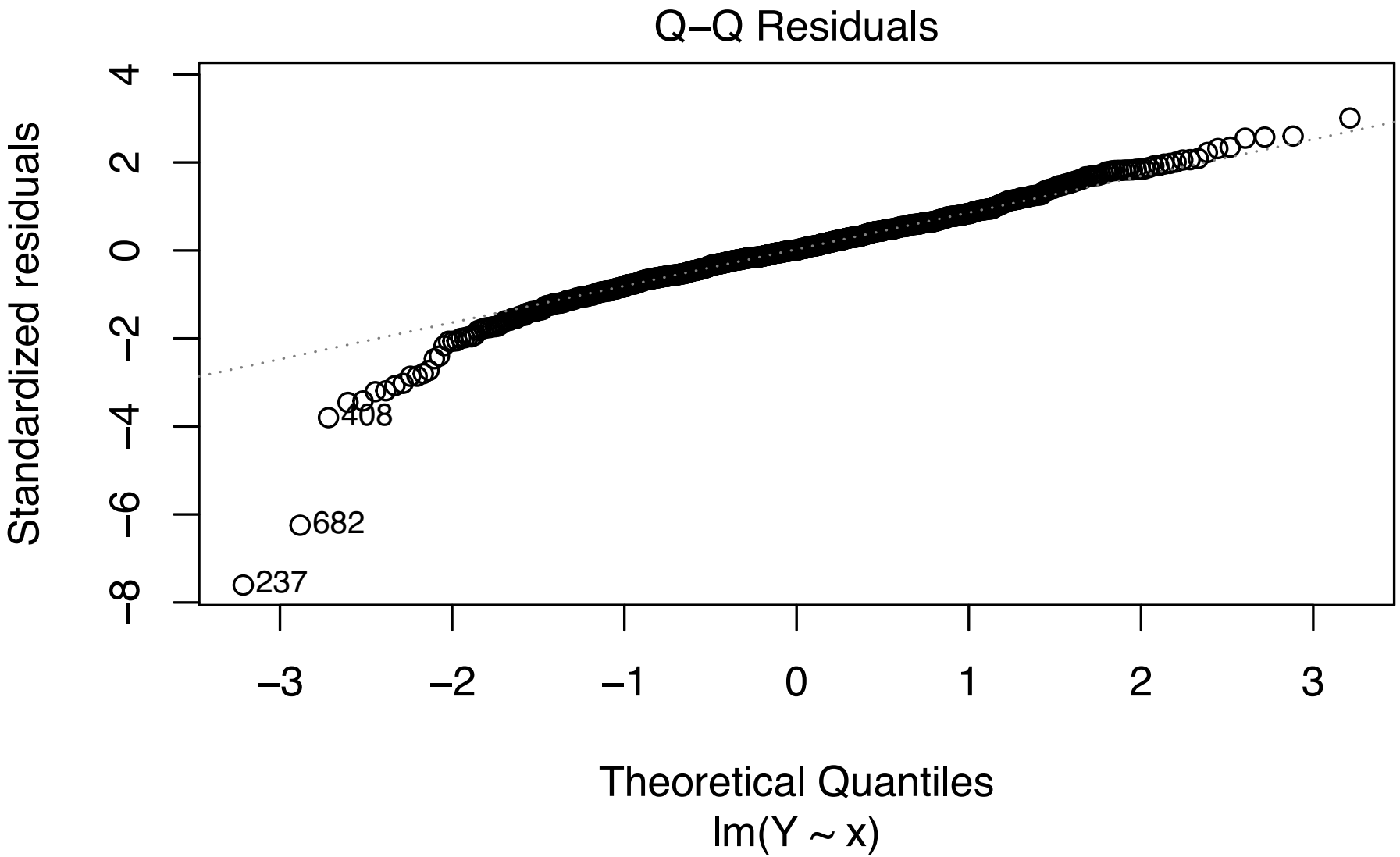
Checking model assumptions

Validity of the foregoing analyses depends on these assumptions:

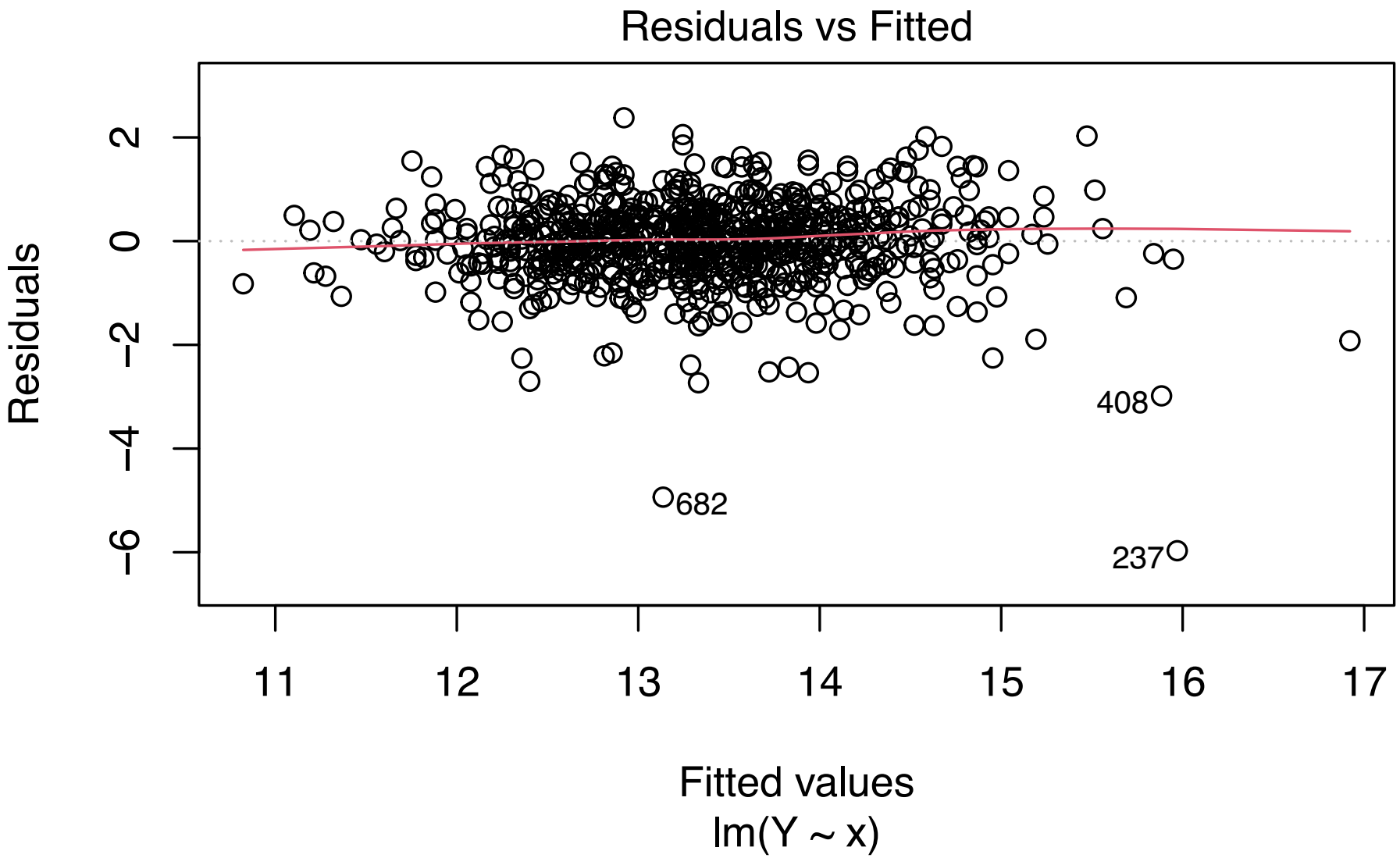
1. The responses are normally distributed around the regression line (Check QQ plot of residuals). *If n is large this doesn't matter.*
2. The response has the same variance for all values of the covariate (Check residuals vs fitted values plot).
3. The covariate and the response are linearly related (Check residuals vs fitted values plot).
4. The response values are independent of each other (No way to check; must trust experimental design).

Generating diagnostic plots from `lm()` with `plot()`

```
plot(lm_out,which = 2)
```



```r
plot(lm_out,which = 1)
```



The abalone...

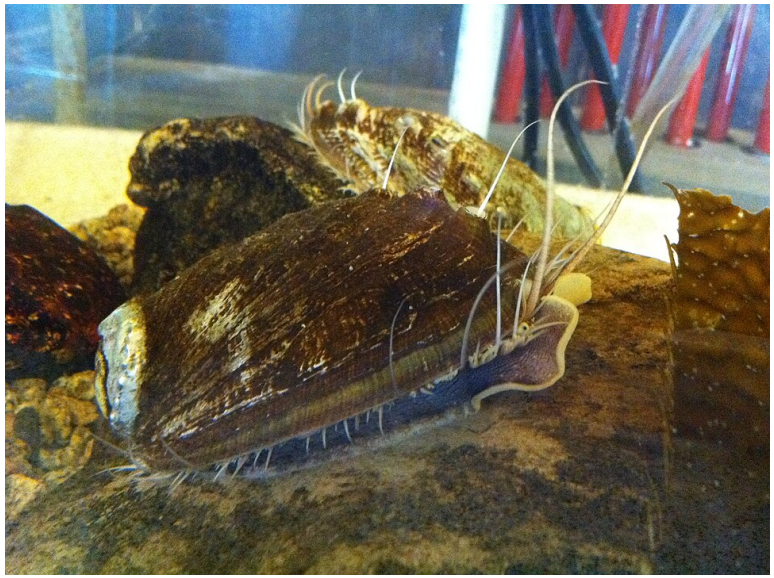


Photo on the left by Sharktopus - Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=14082271

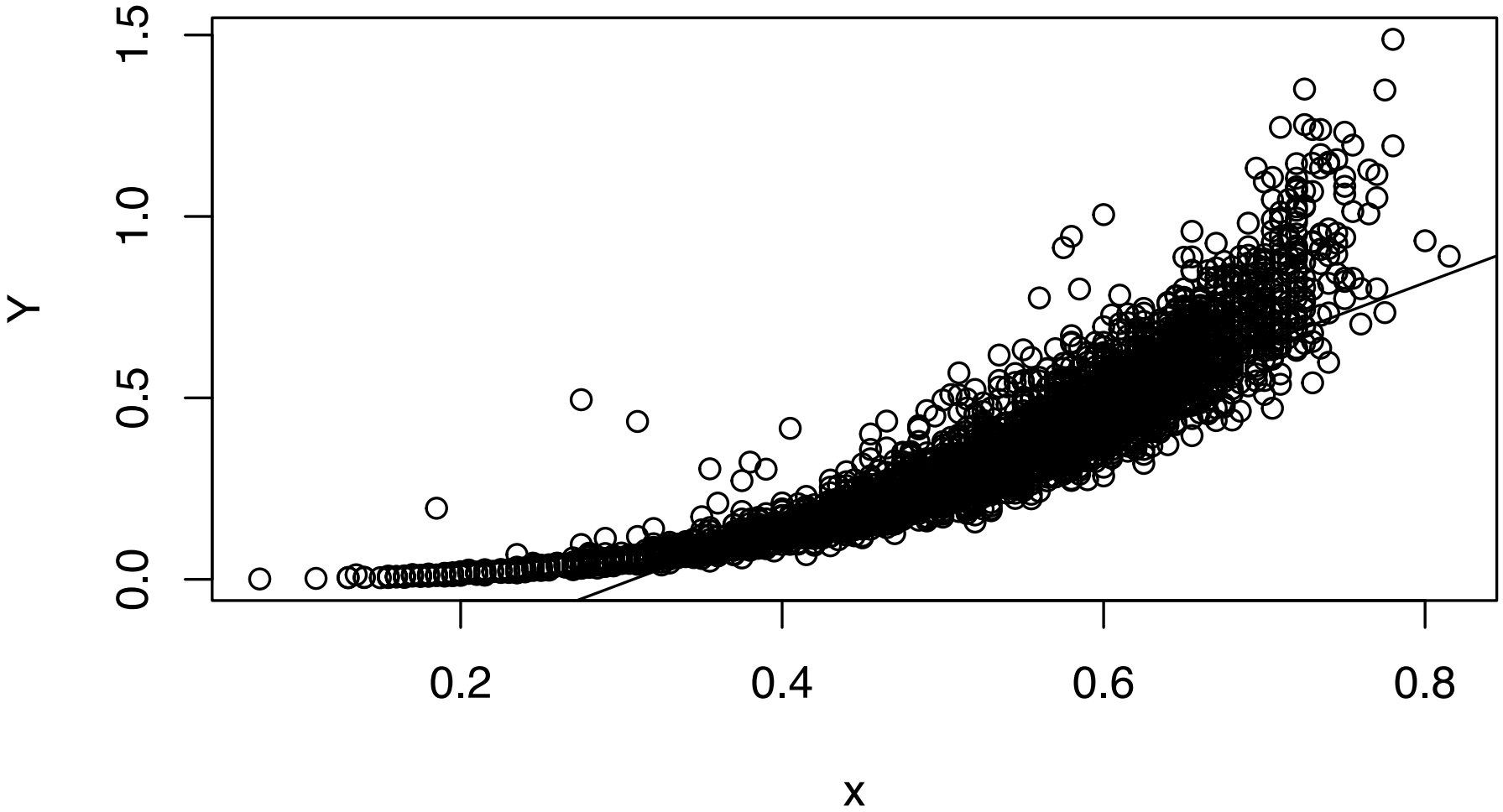
Abalone data example

Predict shucked weight of an abalone by its length.

```
csv <- url("https://people.stat.sc.edu/gregorkb/data/abalone.csv")
abalone <- read.csv(csv,col.names = c("Sex",
                                      "Length",
                                      "Diameter",
                                      "Height",
                                      "Whole_Wt",
                                      "Shucked_Wt",
                                      "Viscera_Wt",
                                      "Shell_Wt",
                                      "Rings"))
Y <- abalone$Shucked_Wt
x <- abalone$Length
n <- length(Y)
```

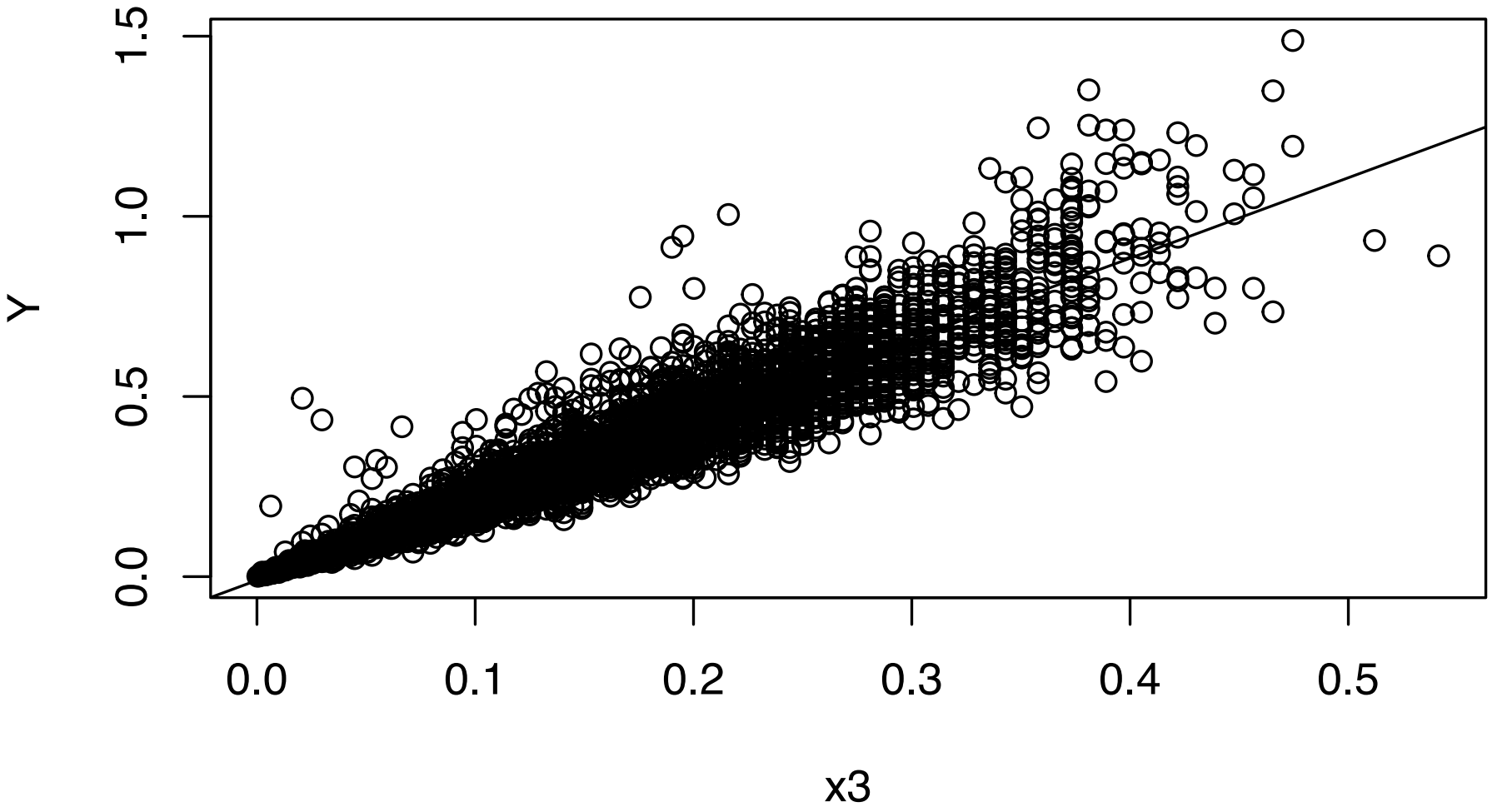
There are $n = 4176$ records. Data come from Nash and Ford (1995).

```r
lm1 <- lm(Y~x)
plot(Y~x)
abline(lm1)
```

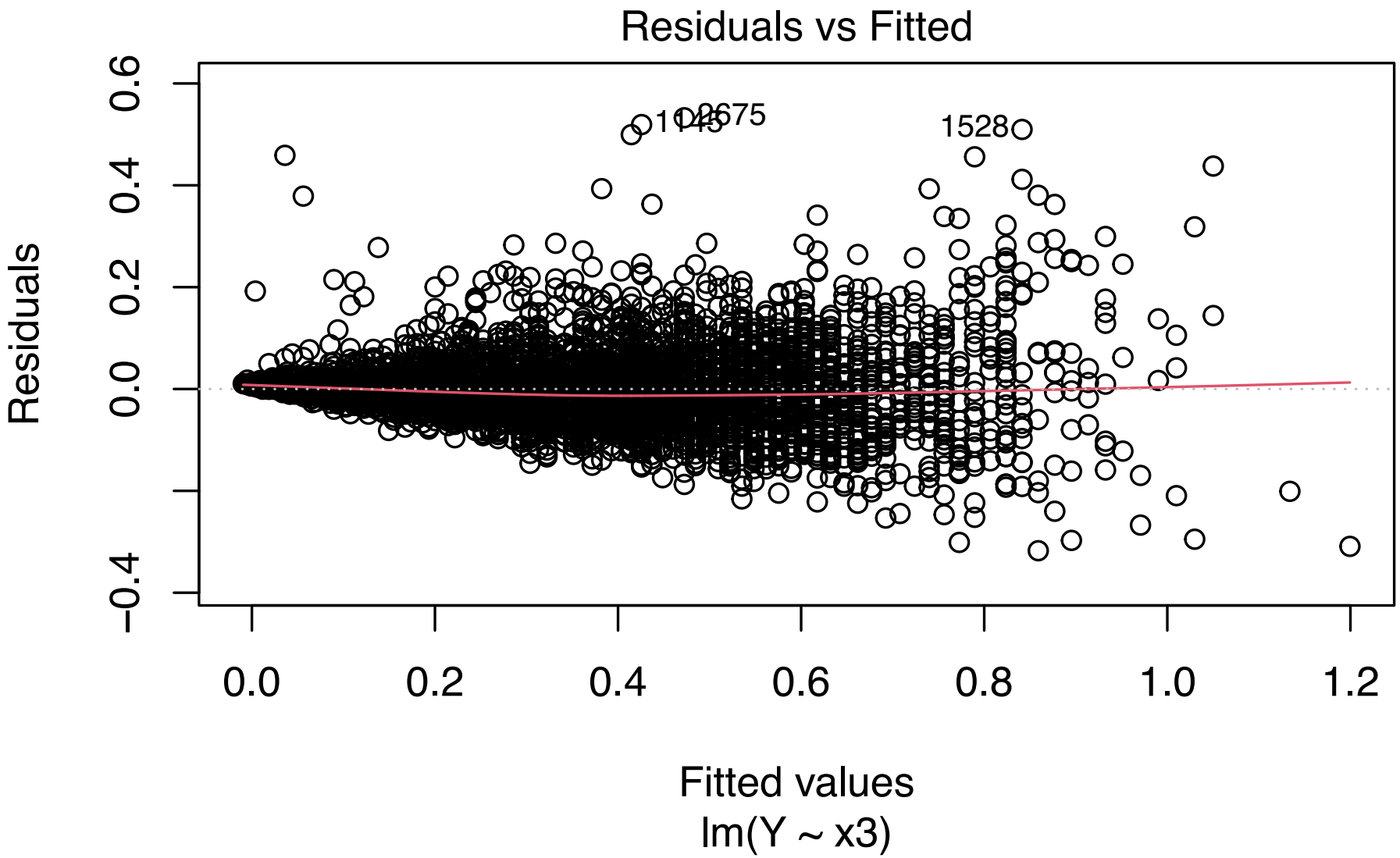


Try transforming x:

```
x3 <- x**3
lm2 <- lm(Y ~ x3)
plot(Y ~ x3); abline(lm2)
```

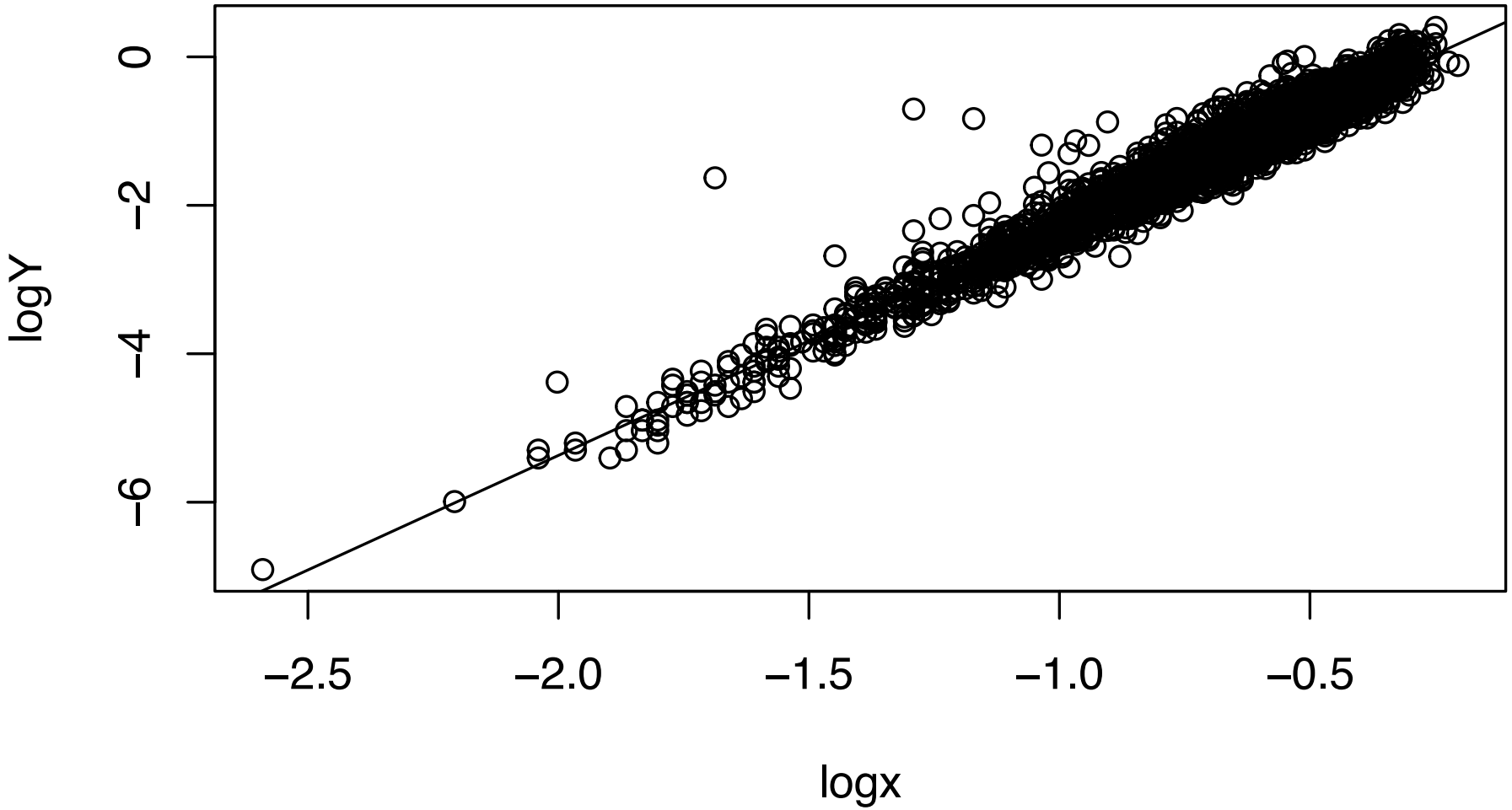


```r
plot(lm2,which = 1)
```

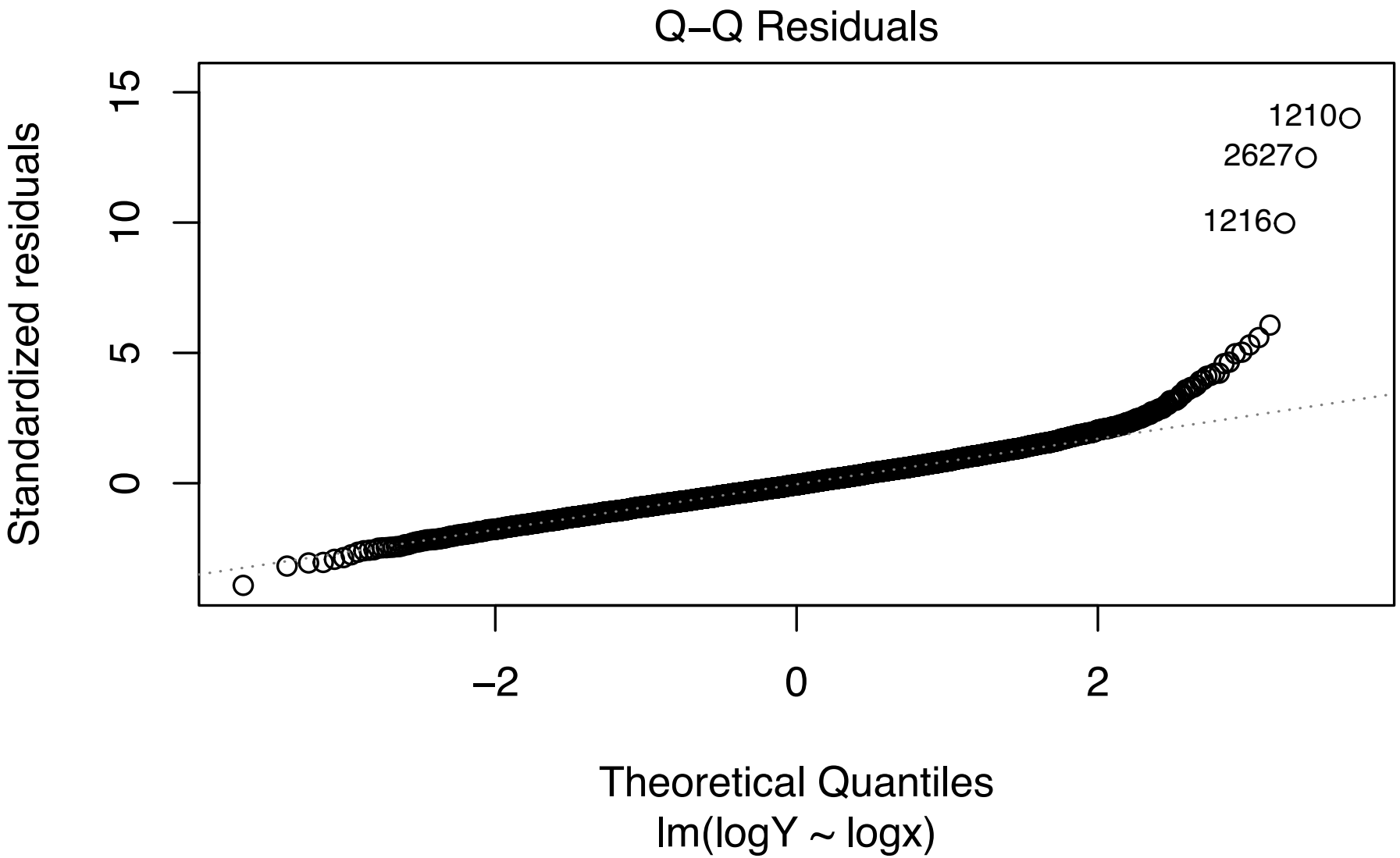


Could transform both Y and x:

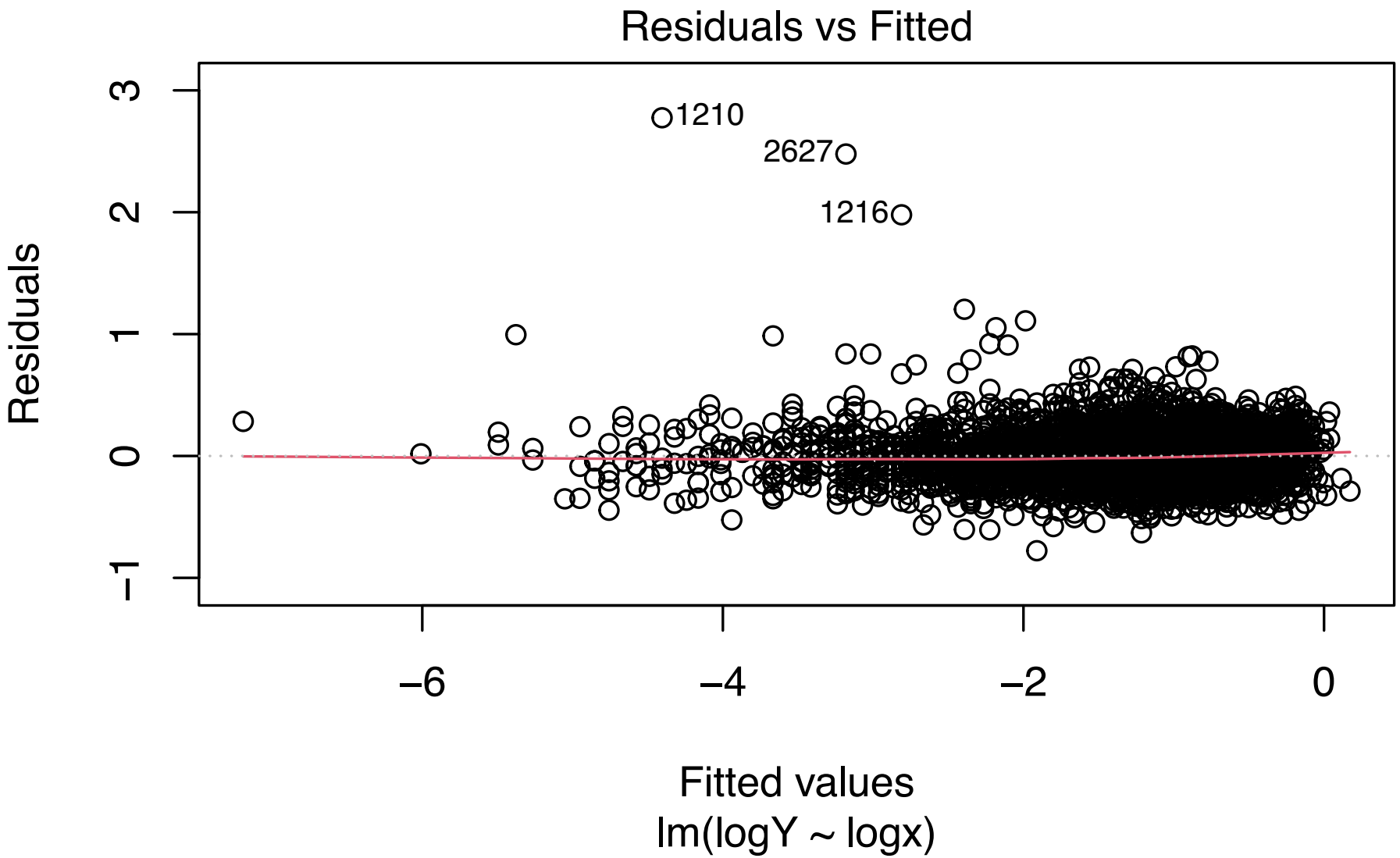
```
logY <- log(Y); logx <- log(x)
lm3 <- lm(logY ~ logx)
plot(logY~logx); abline(lm3)
```



```r
plot(lm3,which = 2)
```



```r
plot(lm3,which = 1)
```



Transforming variables to obtain a linear relationship

Take care how to interpret β_1 after transforming the data.

Example: Log transforming x and Y gives β_1 a %-change interpretation:

$$\log y = \beta_0 + \beta_1 \log x \iff \frac{d \log y}{dx} = \beta_1 \frac{1}{x} \iff \frac{dy}{y} = \beta_1 \frac{dx}{x}$$

Abalone data example (cont)

We must back-transform prediction intervals if we have transformed Y.

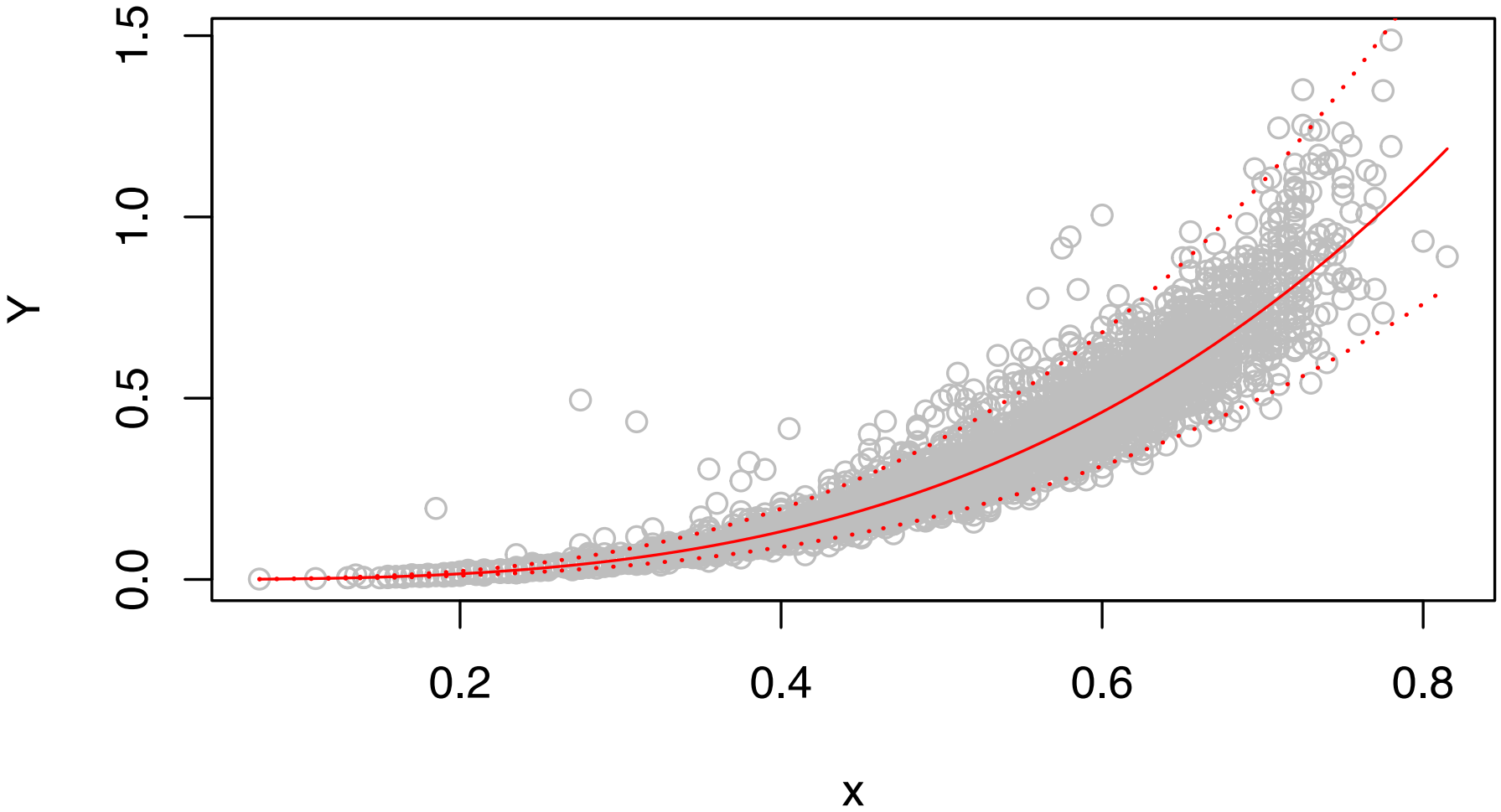
```
xnew <- 0.5
newdata <- data.frame( logx = log(xnew))
pi_logY <- predict(lm3,newdata = newdata, int = "pred")
pi_logY
```

```
        fit       lwr       upr
1 -1.335636 -1.724831 -0.946441
```

```
pi <- exp(pi_logY)
pi
```

```
        fit       lwr       upr
1 0.2629909 0.1782032 0.3881199
```

```r
plot(Y~x,col="gray"); logx <- seq(min(logx),max(logx),length=500)
newdata <- data.frame(logx = logx)
logy_hat <- predict(lm3,newdata = newdata,int = "pred")
lines(exp(logy_hat[,1]) ~ exp(logx), col = "red")
lines(exp(logy_hat[,2]) ~ exp(logx), col = "red", lty = 3,lwd=1.5)
lines(exp(logy_hat[,3]) ~ exp(logx), col = "red", lty = 3,lwd=1.5)
```



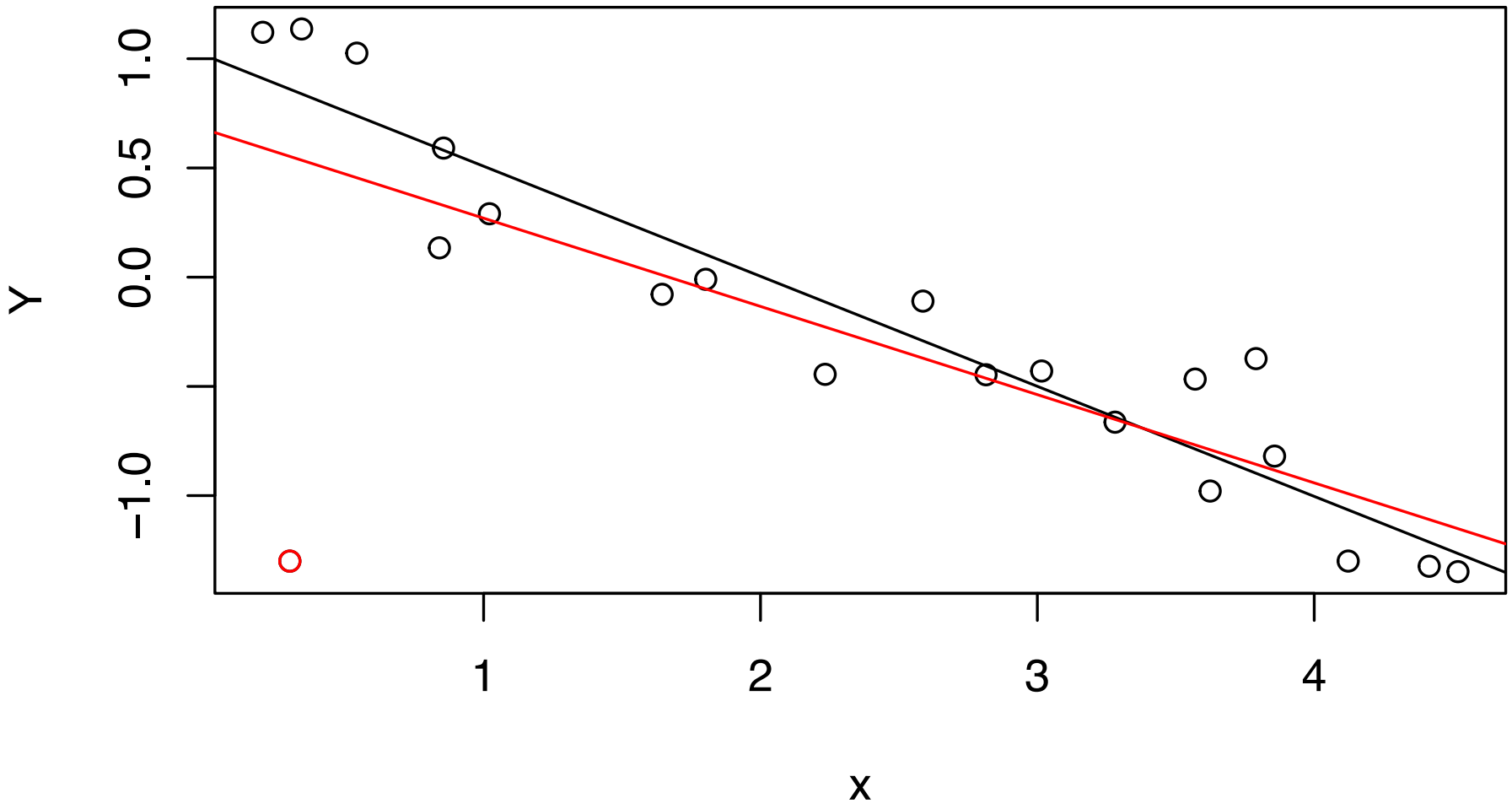
Outliers in simple linear regression

Outlying data points can have a large influence on the estimated regression function.

Let's generate some data and then add an outlier:

```
n <- 20
b0 <- 1
b1 <- -1/2
sg <- .2
x0 <- runif(n,0,5)
e <- rnorm(n,0,sg)
Y0 <- b0 + b1 * x0 + e
x <- c(x0,.3)
Y <- c(Y0,-1.3)
```

```r
plot(Y~x);points(Y[n+1]~x[n+1], col = "red")
abline(lm(Y0~x0))
abline(lm(Y~x), col = "red")
```



The red data point appears to exert an undue influence over the fit.

Leverage and Cook's distance

The leverage of a point (x_i, Y_i) among $(x_1, Y_1), \ldots, (x_n, Y_n)$ is

$$\text{lev}_i = \frac{1}{n} + \frac{(x_i - \bar{x}_n)^2}{S_{xx}}$$

Leverage only shows outlying-ness in the x direction.

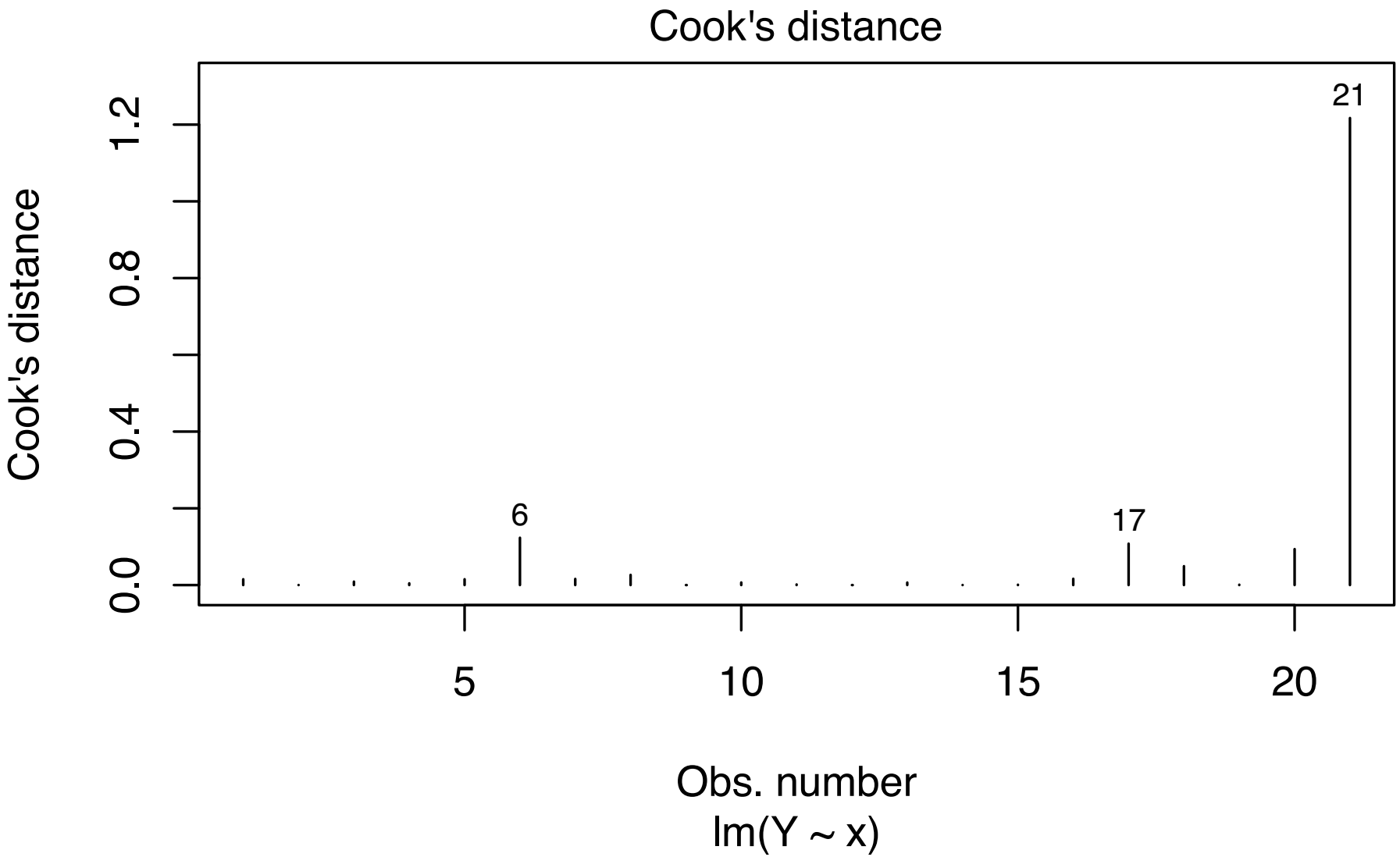
Cook's Distance measures how much each data point changes the fit:

$$D_i = \frac{1}{2\hat{\sigma}^2} \sum_{j=1}^{n} (\hat{Y}_j - \hat{Y}_{j(i)})^2 = \frac{\hat{e}_i^2}{2\hat{\sigma}^2} \frac{\text{lev}_i}{(1 - \text{lev}_i)^2} \quad \text{for } i = 1, \ldots, n,$$

where $\hat{Y}_{j(i)}$ is the jth fitted value from the model fitted without obs i.

Make a plot of the Cook's distances

```
plot(lm(Y~x),which = 4)
```



Code to compute Cook's distances

```
n <- length(Y)
xbar <- mean(x)
Ybar <- mean(Y)
rxY <- cor(x,Y) # Pearson's correlation coefficient
b1hat <- rxY * sd(Y)/sd(x)
b0hat <- Ybar - b1hat * xbar
Sxx <- sum((x - xbar)^2)
lev <- 1/n + (x - xbar)^2/Sxx
Yhat <- b0hat + b1hat * x
ehat <- Y - Yhat
sgsqhat <- sum(ehat^2)/(n-2)

cooksD <- ehat^2 / (2*sgsqhat) * lev / (1 - lev)^2
```

Two-sample t-test by simple linear regression

Let $Y_{ij} \overset{\text{ind}}{\sim} \text{Normal}(\mu_i, \sigma^2)$, $j = 1, \ldots, n_i$, $i = 1, 2$ and consider

$$H_0\colon\ \mu_2 - \mu_1 = 0 \text{ versus } H_1\colon\ \mu_2 - \mu_1 \neq 0.$$

The (equal-variances) two-sample t-test uses the test statistic

$$T_{\text{stat}} = \frac{\bar{Y}_2 - \bar{Y}_1}{S_{\text{pooled}}\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}},$$

where $\bar{y}_i = n_i^{-1} \sum_{j=1}^{n_i} Y_{ij}$, $i = 1, 2$ and

$$S^2_{\text{pooled}} = \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{n_1 + n_2 - 2}, \quad S_i = \frac{1}{n_i - 1}\sum_{j=1}^{n_i}(Y_{ij} - \bar{Y}_i)^2.$$

We reject H_0 at significance level α if $|T_{\text{stat}}| > t_{n-2,\alpha/2}$.

Appendicitis example

Look again at the data from Marcinkevičs et al. (2023).

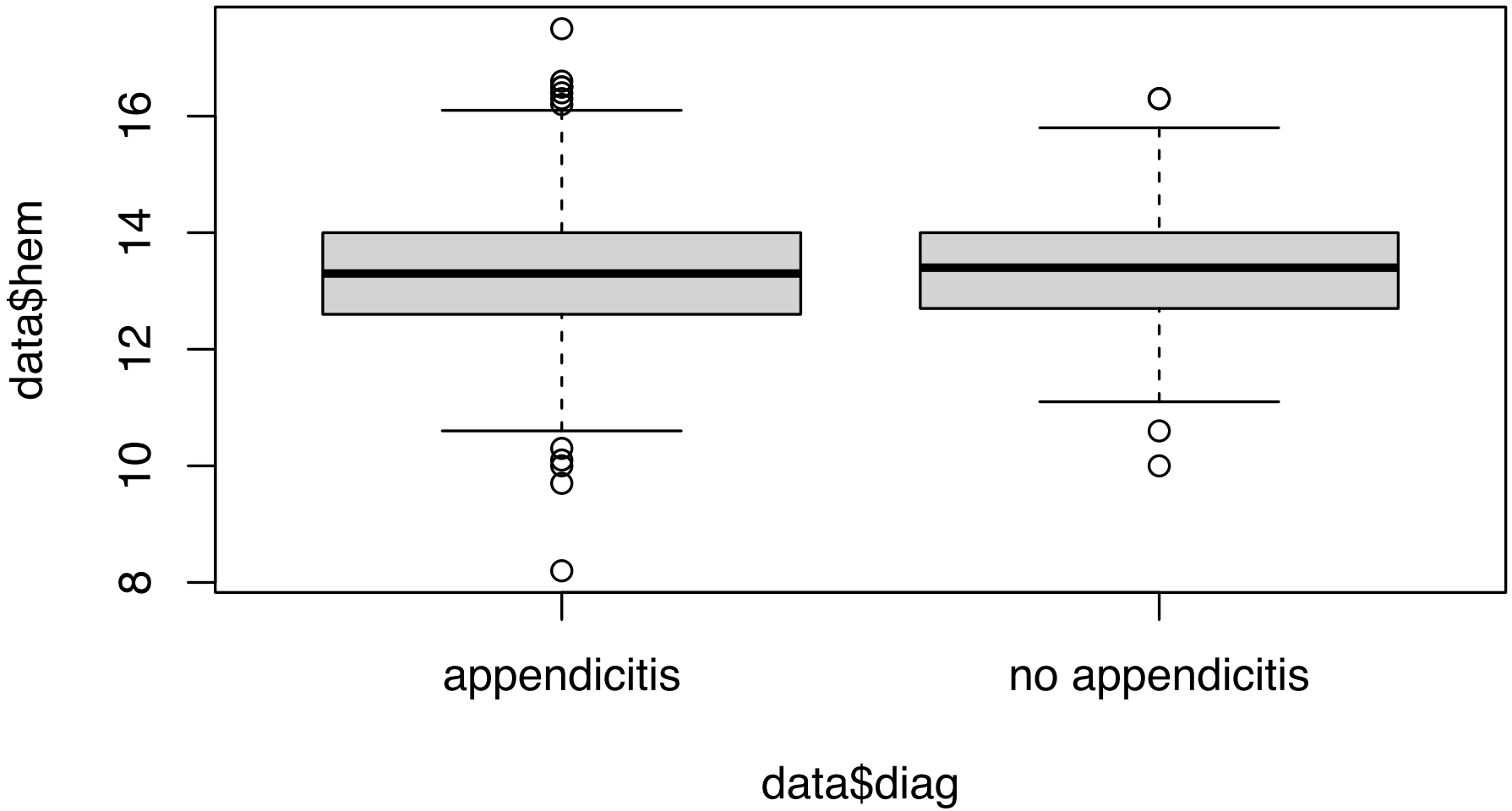
```
link <- url("https://people.stat.sc.edu/gregorkb/data/hrbc.csv")
data <- read.csv(link)
head(data)
```

```
   hem  rbc    sex   age            diag
1 14.8 5.27 female 12.68    appendicitis
2 15.7 5.26   male 14.10 no appendicitis
3 11.4 3.98 female 14.14 no appendicitis
4 13.6 4.64 female 16.37 no appendicitis
5 12.6 4.44 female 11.08    appendicitis
6 12.5 4.96   male 11.05 no appendicitis
```

Is the mean hemaglobin level the same in children with and without appendicitis (ignoring rbc, age, and sex)?

Appendicitis example (cont)

```
boxplot(data$hem ~ data$diag)
```



Appendicitis example (cont)

```r
t.test(data$hem ~ data$diag, var.equal = TRUE)
```

```
    Two Sample t-test

data:  data$hem by data$diag
t = -0.49212, df = 760, p-value = 0.6228
alternative hypothesis: true difference in means between group appendicitis and
95 percent confidence interval:
 -0.2038964  0.1221585
sample estimates:
   mean in group appendicitis mean in group no appendicitis
                     13.33229                      13.37316
```

Appendicitis example (cont)

Let the Y_i be the hemaglobin values and define an indicator variable as

$$x_i = \begin{cases} 0 & \text{if no appendicitis} \\ 1 & \text{if appendicitis} \end{cases} \qquad \text{for } i = 1, \ldots, n.$$

Then in the SLR model $Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$ we have

- $\beta_0 = \mu_{\text{no app}}$
- $\beta_0 + \beta_1 = \mu_{\text{app}}$
- $\beta_1 = \mu_{\text{app}} - \mu_{\text{no app}}$

The t test in the simple linear regression setup of

$$H_0\colon\ \beta_1 = 0 \text{ versus } H_1\colon\ \beta_1 \neq 0$$

will give the same p value as the equal-variances two-sample t test of

$$H_0\colon\ \mu_{\text{app}} - \mu_{\text{no app}} = 0 \text{ versus } H_1\colon\ \mu_{\text{app}} - \mu_{\text{no app}} \neq 0. \quad \text{Cool!}$$

Exercise: Show that in the above setup we have

$$\frac{\bar{Y}_2 - \bar{Y}_1}{S_{\text{pooled}}\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} = \frac{\hat{\beta}_1}{\hat{\sigma}/\sqrt{S_{xx}}}.$$

Do it in steps, showing:

1. $\hat{\beta}_0 = \bar{Y}_1$
2. $\hat{\beta}_1 = \bar{Y}_2 - \bar{Y}_1$
3. $\hat{\sigma} = S_{\text{pooled}}$
4. $1/\sqrt{S_{xx}} = \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}$

Appendicitis example (cont)

Prepare the data:

```
Y <- data$hem
x <- as.numeric(data$diag == "appendicitis")
head(cbind(Y,x))
```

```
        Y x
[1,] 14.8 1
[2,] 15.7 0
[3,] 11.4 0
[4,] 13.6 0
[5,] 12.6 1
[6,] 12.5 0
```

```r
summary(lm(Y~x))
```

```
Call:
lm(formula = Y ~ x)

Residuals:
    Min      1Q  Median      3Q     Max
-5.1323 -0.7323 -0.0323  0.6677  4.1677

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 13.37316    0.06375 209.782   <2e-16 ***
x           -0.04087    0.08305  -0.492    0.623
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.128 on 760 degrees of freedom
Multiple R-squared:  0.0003186, Adjusted R-squared:  -0.0009968
F-statistic: 0.2422 on 1 and 760 DF,  p-value: 0.6228
```

Automatic if we designate the predictor as a "factor" (but watch sign!).

```
x <- as.factor(data$diag)
summary(lm(data$hem ~ x))
```

```
Call:
lm(formula = data$hem ~ x)

Residuals:
    Min      1Q  Median      3Q     Max
-5.1323 -0.7323 -0.0323  0.6677  4.1677

Coefficients:
                 Estimate Std. Error t value Pr(>|t|)
(Intercept)      13.33229    0.05322 250.490   <2e-16 ***
xno appendicitis  0.04087    0.08305   0.492    0.623
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.128 on 760 degrees of freedom
Multiple R-squared:  0.0003186, Adjusted R-squared:  -0.0009968
F-statistic: 0.2422 on 1 and 760 DF,  p-value: 0.6228
```

References

Marcinkevičs, Ričards, Patricia Reis Wolfertstetter, Ugne Klimiene, Ece Ozkan, Kieran Chin-Cheong, Alyssia Paschke, Julia Zerres, et al. 2023. "Regensburg Pediatric Appendicitis Dataset." Zenodo. https://doi.org/10.5281/zenodo.7711412.

Nash, Sellers, Warwick, and Wes Ford. 1995. "Abalone." UCI Machine Learning Repository. https://doi.org/10.24432/C55C7W.