4 Describing relationships between variables

This chapter provides methods that address a more involved problem of describing relationships between variables and require more computation. We start with relationships between two variables and move on to more.

4.1 Fitting a line by least squares

Goal: Notice a relationship between 2 quantitative variables

We would like to use an equation to describe how a dependent (response) variable, y, changes in response to a change in one or more independent (experimental) variable(s), x.

4.1.1 Line review

Recall a linear equation of the form $y = mx + b$

m: slope

b: y-intercept

In statistics, we use the notation $y = \beta_0 + \beta_1 x + \epsilon$ where we assume β_0 and β_1 are unknown parameters and ϵ is some error.

β_0: intercept　　ε: error

β_1: slope

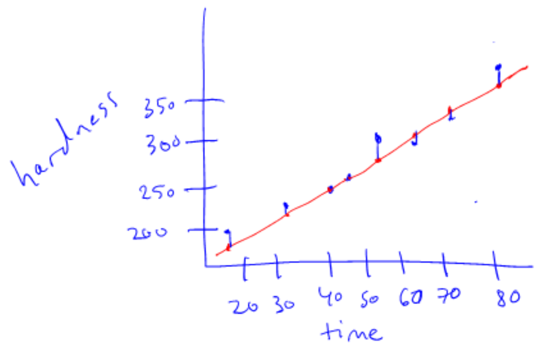
The goal is to find estimates b_0 and b_1 for the parameters. (sometimes $\hat{\beta}_0$ and $\hat{\beta}_1$)

b_0: intercept　　b_1: slope

Example 4.1 (Plastic hardness)**.** Eight batches of plastic are made. From each batch one test item is molded and its hardness, y, is measured at time x. The following are the 8 measurements and times:

time	32	72	64	48	16	40	80	56
hardness	230	323	298	255	199	248	359	305

Step 1: look at a scatterplot to determine if a linear relationship seems appropriate.



- describe strength, direction, and form:

There is a strong, positive, linear relationship between time and hardness.

How do we find an equation for the line that best fits the data?

A straight line will not pass through every data point, so when we estimate a line, we will have predicted values ($\hat{y}$) instead of the observed data (y)

The fitted equation is then $\hat{y} = b_0 + b_1 x$

Definition 4.1. A *residual* is the vertical distance between the actual data point and a fitted line, $e = y - \hat{y}$.

$= y - b_0 - b_1 x$

We choose the line that has the smallest residuals.

The *principle of least squares* provides a method of choosing a "best" line to describe the data.

Definition 4.2. To apply the *principle of least squares* in the fitting of an equation for y to an n-point data set, values of the equation parameters are chosen to minimize

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

where $y_1, y_2, \ldots, y_n$ are the observed responses and $\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n$ are corresponding responses predicted or fitted by the equation.

We want to choose b_0 and b_1 to minimize

$$\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)^2$$

Take derivatives and set them to zero:

$$0 = \frac{\partial}{\partial b_0}\sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)^2 = -2\sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)$$

$$0 = \sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)$$

AND

$$0 = \frac{\partial}{\partial b_1}\sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)^2 = -2\sum_{i=1}^{n}x_i(y_i - b_0 - b_1 x_i)$$

$$0 = \sum_{i=1}^{n}x_i(y_i - b_0 - b_1 x_i)$$

Solving for b_0 and b_1, we get

$$b_0 = \overline{y} - b_1\overline{x}$$

$$b_1 = \frac{\sum(x_i - \overline{x})(y_i - \overline{x})}{\sum(x_i - \overline{x})^2} = \frac{\sum x_i y_i - \frac{1}{n}\sum x_i \sum y_i}{\sum x_i^2 - \frac{1}{n}(\sum x_i)^2}$$

start here — easier to remember — easier to compute

Example 4.2 (Plastic hardness, cont'd)**.** Compute the least squares line for the data in Example 4.1.

x	y	xy	x^2	y^2
32	230	7360	1024	52900
72	323	23256	5184	104329
64	298	19072	4096	88804
48	255	12240	2304	65025
16	199	3184	256	39601
40	248	9920	1600	61504
80	359	28720	6400	128881
56	305	17080	3136	93025
sum 408	2217	120832	24000	634069

$n = 8$

$$b_1 = \frac{\sum x_i y_i - \frac{1}{n}\sum x_i \sum y_i}{\sum x_i^2 - \frac{1}{n}(\sum x_i)^2} = \frac{120832 - \frac{1}{8}(408)(2217)}{24000 - \frac{1}{8}(408)^2} = 2.433$$

$$b_0 = \bar{y} - b_1\bar{x} = \frac{2217}{8} - 2.433\,\frac{408}{8} = 153.06$$

Now we have the fitted line: $\hat{y} = 153.06 + 2.433x$

We can use this to ① get interpretations of estimates and ② compute a predicted/fitted value for a given x:

Q: What is the predicted hardness for time $x = 24$?

$$\hat{y} = 153.06 + 2.433(24) = 211.452$$

ALWAYS to put interpretations in context of the problem
=> replace everything in parentheses w/ actual problem context.

4.1.2 Interpreting slope and intercept

- Slope: For every 1 (unit) increase in (x) we expect a (b_1) → increase/decrease in (y)
  (if $b_1 \geq 0$ / $b_1 < 0$) (b_1 positive) (b_1 negative)
- Intercept

  When (x) is 0 (units), we expect (y) to be (b_0).

Interpreting the intercept is nonsense when

1. A value of 0 for x is not practical (i.e. measuring heights of adult humans)
2. Extrapolation would have to be used to get the predicted value of y (i.e. get a negative intercept for any measurement).

Note: this doesn't mean the intercept is wrong! It's just not interpretable.

Example 4.3 (Plastic hardness, cont'd)**.** Interpret the coefficients in the plastic hardness example. Is the interpretation of the intercept reasonable?

Slope: ($b_1 = 2.433$)

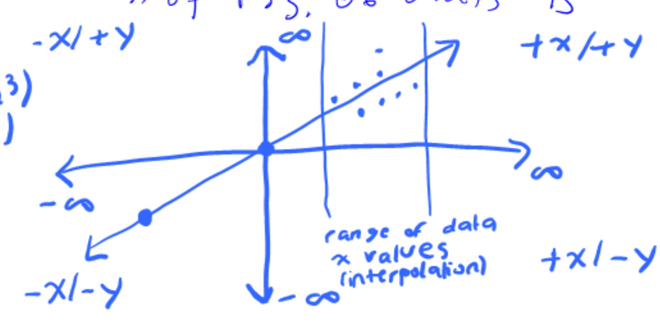
For every 1 hour (units) increase in time (x), we expect the hardness (y) to increase (b_1 positive) by 2.433 (b_1) units (units).

Intercept: ($b_0 = 153.06$)

At time (x) 0, we expect the hardness (y) to be 153.06 (b_0) units (units).

The intercept interpretation is NOT reasonable, because at time 0, the plastic is molten so expecting a hardness of 153.06 units is unrealistic.

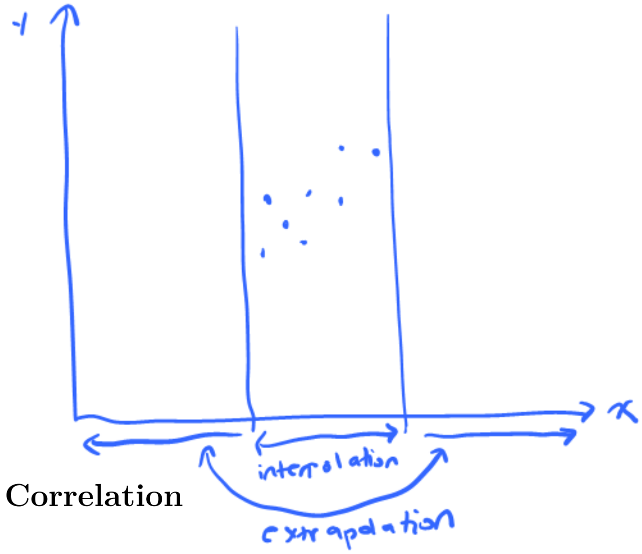
x = size of house (m^3)
y = cost of house ($)



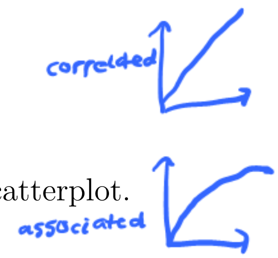
When making predictions, don't *extrapolate*.

Definition 4.3. *Extrapolation* is when a value of x beyond the range of our actual observations is used to find a predicted value for y. We don't know the behavior of the line beyond our collected data.

Definition 4.4. *Interpolation* is when a value of x within the range of our observations is used to find a predicted value for y.



4.1.3 Correlation

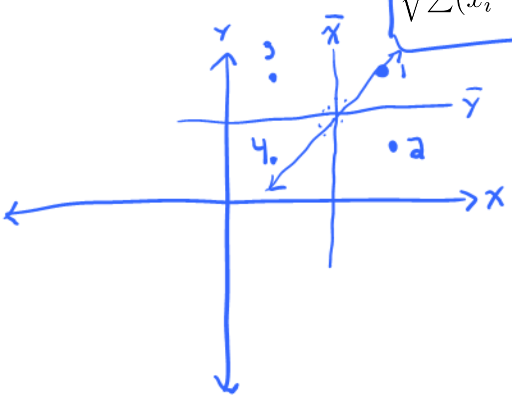


Visually we can assess if a fitted line does a good job of fitting the data using a scatterplot. However, it is also helpful to have methods of quantifying the quality of that fit.

Definition 4.5. *Correlation* gives the strength and direction of the linear relationship between two variables.

Definition 4.6. The *sample correlation* between x and y in a sample of n data points (x_i, y_i) is

$$r = \frac{\sum(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum(x_i - \overline{x})^2 \sum(y_i - \overline{y})^2}} = \frac{\sum x_i y_i - \frac{1}{n}\sum x_i \sum y_i}{\sqrt{\sum x_i^2 - \frac{1}{n}(\sum x_i)^2}\sqrt{\sum y_i^2 - \frac{1}{n}(\sum y_i)^2}}$$



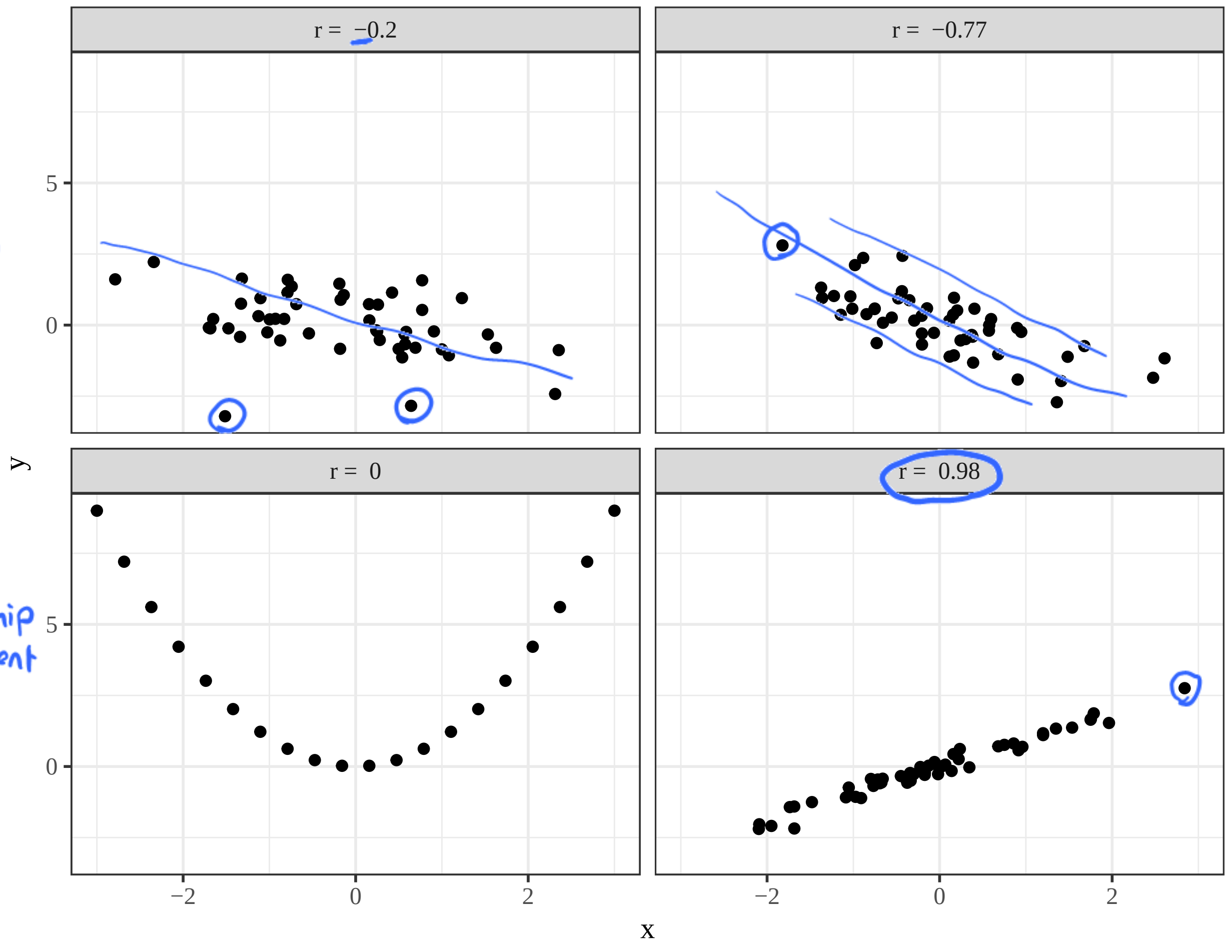
Properties of the sample correlation:

- $-1 \leq r \leq 1$
- $r = -1$ or $r = 1$ if all points lie exactly on the fitted line
- The closer r is to 0, the weaker the linear relationship; the closer it is to 1 or -1, the stronger the linear relationship.
- Negative r indications negative linear relationship (linear slope); Positive r indications positive linear relationship (linear slope, b_1)
- Interpretation always need 3 things
  1. Strength (strong, moderate, weak)
  2. Direction (positive or negative)
  3. Form (linear relationship or no linear relationship) ⟹ looking at scatterplot & residual plots

Note:

① strong ≡ $0.7 \leq r \leq 1$ or $-1 \leq r \leq -0.7$
moderate ≡ $0.3 \leq r < 0.7$ or $-0.7 < r \leq -0.3$
weak ≡ $-0.3 < r < 0.3$

② $r = 0 \Rightarrow$ No linear relationship btwn x and y.
(there could be some other form of relationship btwn x and y)



weak negative linear (possibly 2 outliers)

strong negative linear (probably no outliers)

No linear relationship (no apparent outliers)

strong positive linear (possibly 1 outlier)

Example 4.4 (Plastic hardness, cont'd)**.** Compute and interpret the sample correlation for the plastic hardness example. Recall,

$\sum X$ is a short-cut for $\sum_{i=1}^{n} X_i$

$$\sum x = 408, \sum y = 2217, \sum xy = 120832, \sum x^2 = 24000, \sum y^2 = 634069 \quad n = 8$$

$$r = \frac{\sum x_i y_i - \frac{1}{n}\sum x_i \sum y_i}{\sqrt{\sum x_i^2 - \frac{1}{n}(\sum x_i)^2}\sqrt{\sum y_i^2 - \frac{1}{n}(\sum y_i)^2}} = \frac{120,832 - \frac{1}{8}(408 \cdot 2,217)}{\sqrt{(24,000) - \frac{1}{8}(408)^2} \cdot \sqrt{(634,069 - \frac{1}{8}(2217)^2}}$$

$$= 0.9796$$

There is a ① strong, ② positive, ③ linear relationship btwn time and hardness of plastic.

If linear model is appropriate, y_i's should look like $\hat{y}_i$'s except for small fluctuations explainable only as random variation

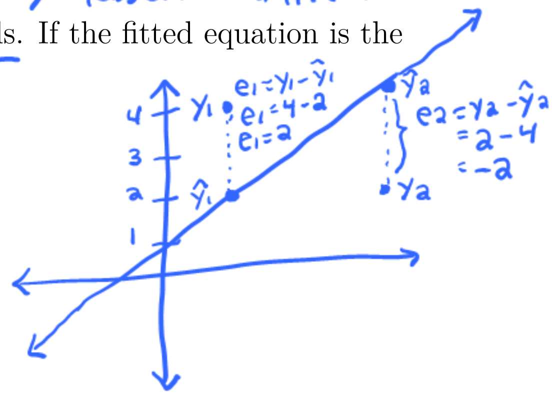
4.1.4 Assessing models

"predicted"/"estimation"

When modeling, it's important to assess the (1) **validity** and (2) **usefulness** of your model.

$e = y - \hat{y}$ = (observed y) − (predicted y)

To assess the validity of the model, we will look to the residuals. If the fitted equation is the good one, the residuals will be:



1. patternless (cloud-like, random scatter)

2. centered at zero

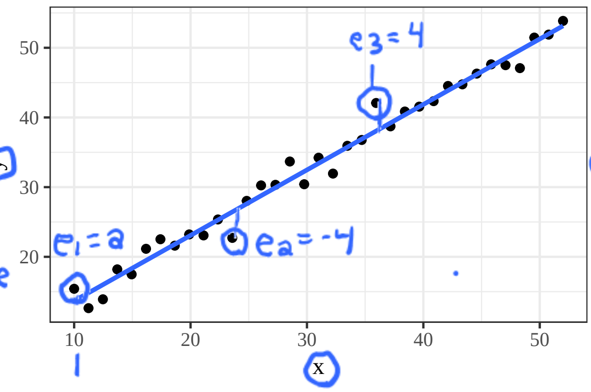
3. Bell shaped

To check if these three things hold, we will use two plotting methods.

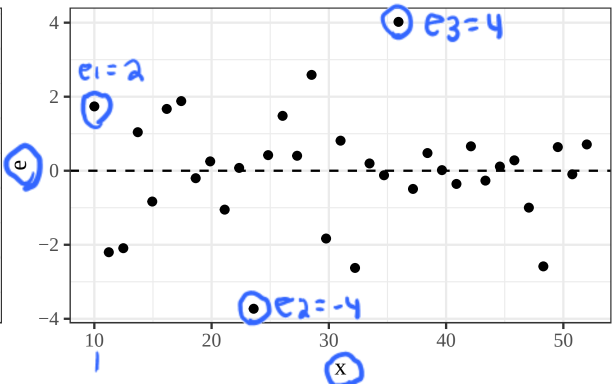
Definition 4.7. A *residual plot* is a plot of the residuals, $e = y - \hat{y}$ vs. x (or $\hat{y}$ in the case of multiple regression, Section 4.2).

Scatterplot | Residual Plots

Ideal scatterplot and its ideal residual plot (linear fit is appropriate as seen in both plots)

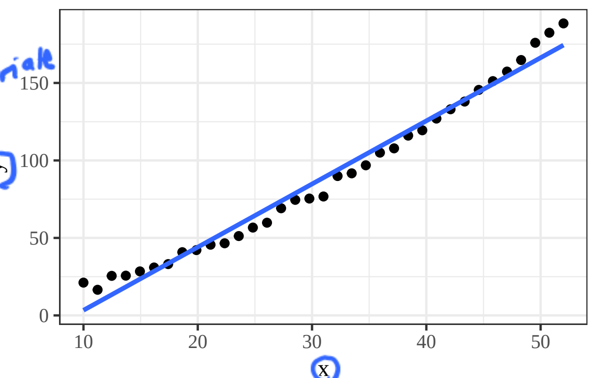


Looks linear

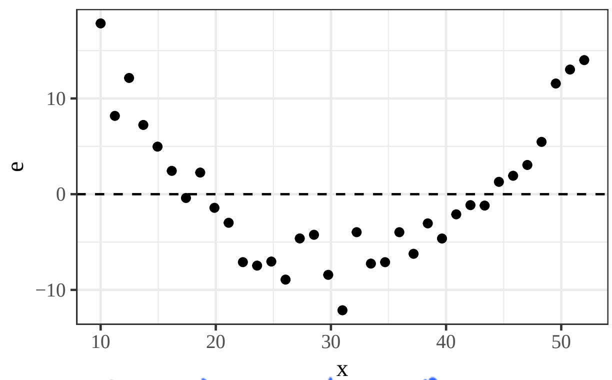


1. centered at zero
2. random scatter

Linear fit is not appropriate (residual plot has a pattern)

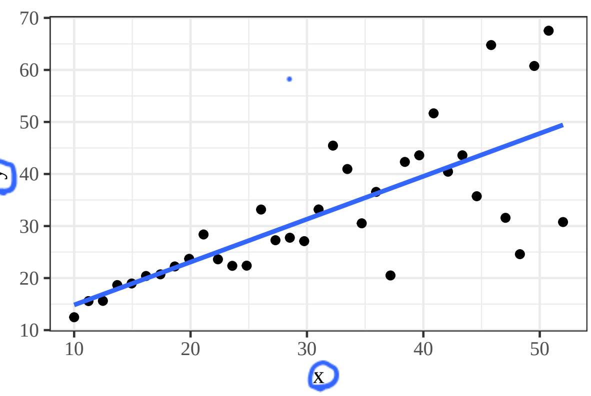


Looks quadratic

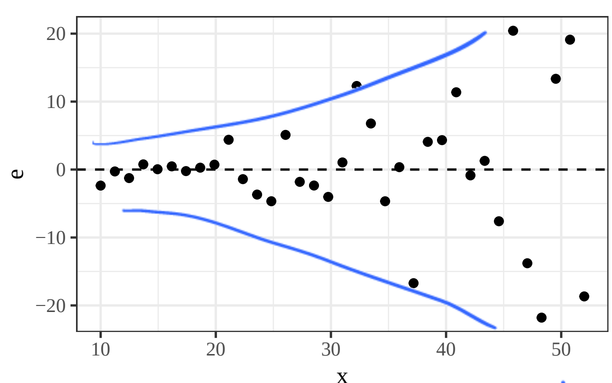


1. centered at zero
2. NOT random scatter (above- below - above) pattern

Residual plot shows a pattern (linear fit is not appropriate)



(Heteroscedasticity)
(Megaphone-shape)



As x increases, so does the variance giving a "fan" shape

$\hat{y} = \alpha x^{\beta} \Rightarrow \log(\hat{y}) = \log\alpha + \beta\log x$

non-linear rltnshp btwn x and y (rearrangement of Taylor series).

linear relationship btwn log(x) and log(y)

Solutions:
① investigate measurement process
② transform the data! (use log transformation)

variables / constants

so, $\tilde{y} = \hat{\gamma}_0 + \hat{\gamma}_1\tilde{x}$ where $\tilde{y} = \log(\hat{y})$, $\tilde{x} = \log(x)$, $\hat{\gamma}_0 = \log\alpha$, $\hat{\gamma}_1 = \hat{\beta}$

$\hat{\gamma}_0$ and $\hat{\gamma}_1$ can be obtained using simple linear regression of log(y) on log(x)

$\hat{\alpha} = e^{\hat{\gamma}_0}$ and $\hat{\beta} = \hat{\gamma}_1$, $\hat{y} = e^{\hat{\gamma}_0 + \hat{\gamma}_1\tilde{x}} = e^{\log\hat{\alpha}} e^{\hat{\beta}\log x} = \hat{\alpha} x^{\hat{\beta}}$ ← relationship btwn x and y for a linear rltnshp btwn log(x) and log(y)

To check if residuals have a Normal distribution,

To assess the usefulness of the model, we use R^2, the *coefficient of determination*.

Definition 4.8. The *coefficient of determination*, R^2, is the proportion of variation in the response that is explained by the model.

Total amount of variation in the response

$$Var(y) =$$

Sum of squares breakdown:

Properties of R^2:

- R^2 is used to assess the fit of other types of relationships as well (not just linear).
- Interpretation - fraction of raw variation in y accounted for by the fitted equation.
- $0 \leq R^2 \leq 1$
- The closer R^2 is to 1, the better the model.
- For SLR, $R^2 = (r)^2$

Example 4.5 (Plastic hardness, contd)**.** Compute and interpret R^2 for the example of the relationship between plastic hardness and time.

4.1.5 Precautions

Precautions about Simple Linear Regression (SLR)

- r only measures linear relationships
- R^2 and r can be drastically affected by a few unusual data points.

4.1.6 Using a computer

You can use JMP (or `R`) to fit a linear model. See BlackBoard for videos on fitting a model using JMP.

4.2 Fitting curves and surfaces by least squares

The basic ideas in Section 4.1 can be generalized to produce a powerful tool: **multiple linear regression**.

4.2.1 Polynomial regression

In the previous section, a straight line did a reasonable job of describing the relationship between time and plastic hardness. But what to do when there is not a linear relationship between variables?

Example 4.6 (Cylinders, pg. 132)**.** B. Roth studied the compressive strength of concrete-like fly ash cylinders. These were made using various amounts of ammonium phosphate as an additive.

ammonium.phosphate	strength	ammonium.phosphate	strength
0	1221	3	1609
0	1207	3	1627
0	1187	3	1642
1	1555	4	1451
1	1562	4	1472
1	1575	4	1465
2	1827	5	1321
2	1839	5	1289
2	1802	5	1292

Table 1: Additive concentrations and compressive strengths for fly ash cylinders.

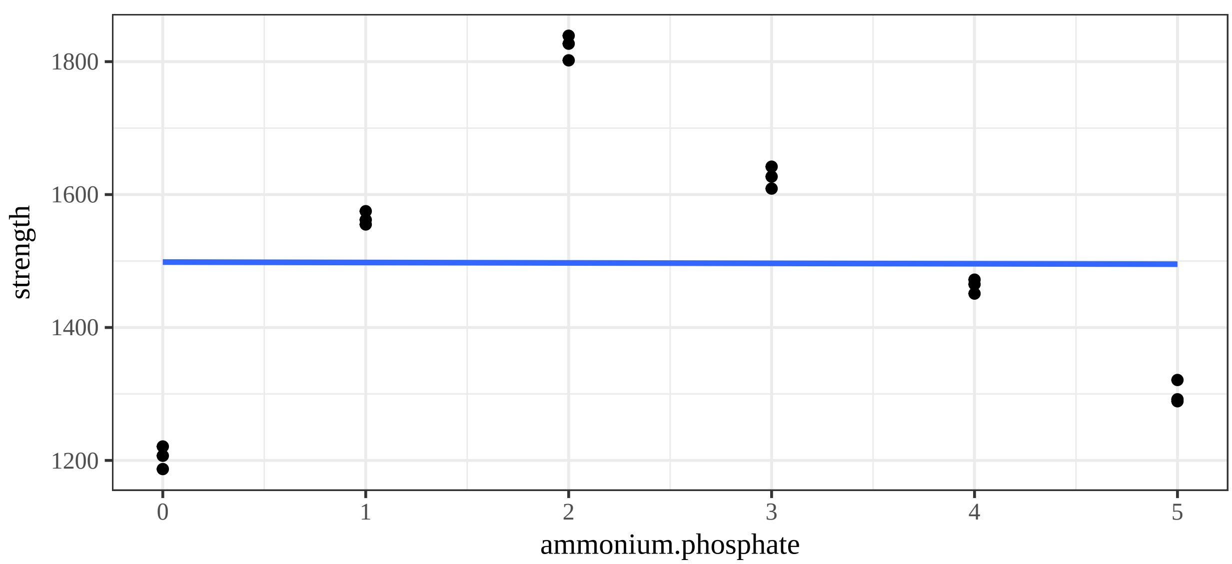


Figure 1: Scatterplot of compressive strength of concrete-like fly ash cylinders for various amounts of ammonium phosphate as an additive with a fitted line.

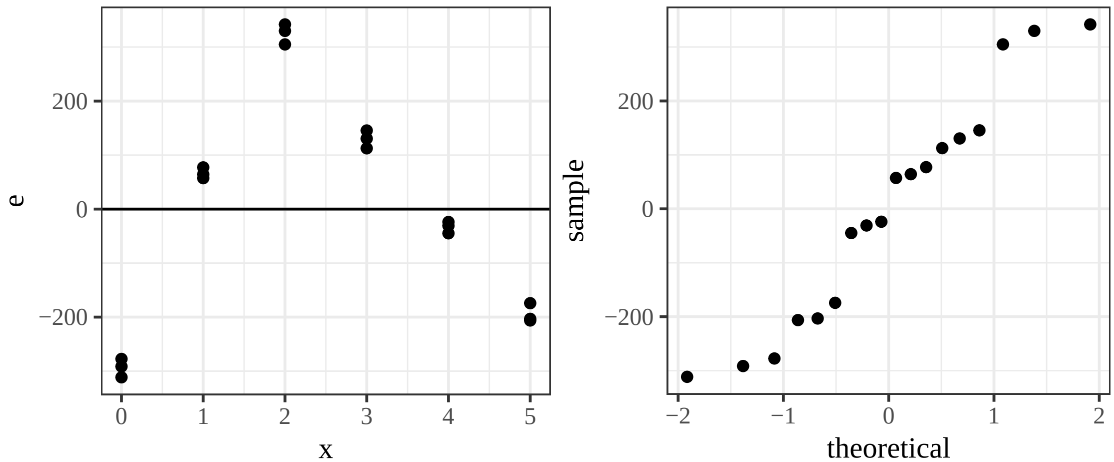


Figure 2: Residual plots for linear fit of cylinder compressive strength on amounts of ammonium phosphate.

A natural generalization of the linear equation

$$y \approx \beta_0 + \beta_1 x$$

is the **polynomial equation**

$$y \approx \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_{p-1} x^{p-1}.$$

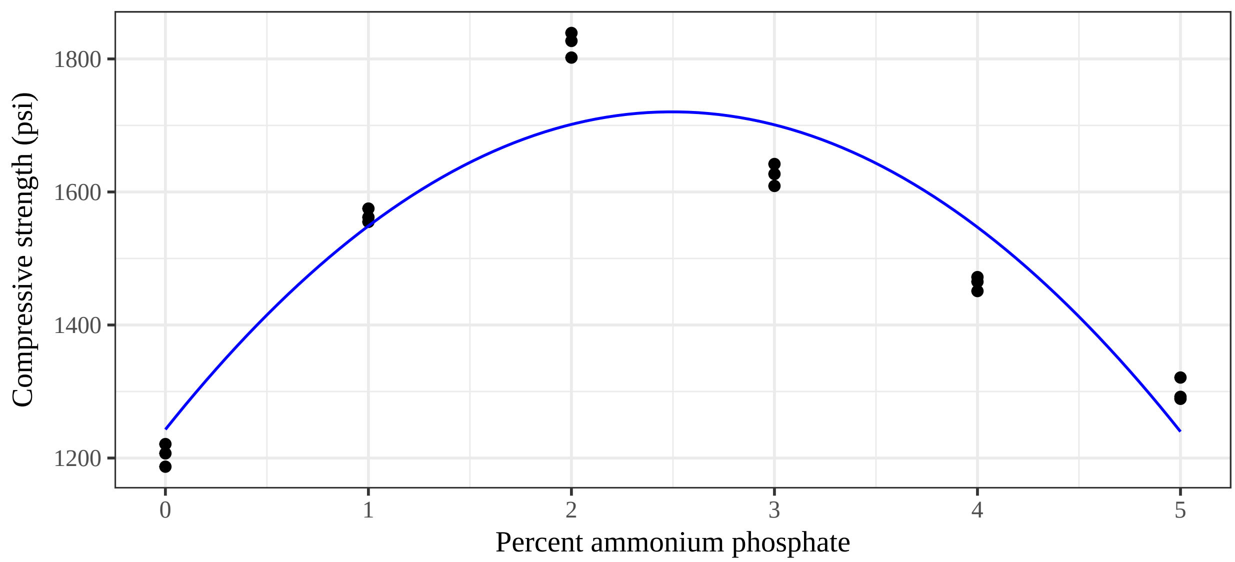
The p coefficients are again estimated using the *principle of least squares*, where the function

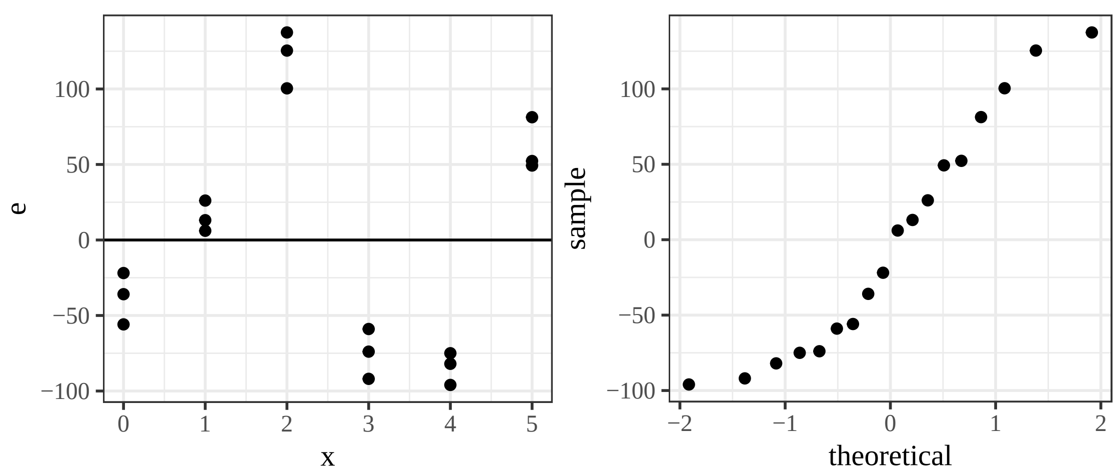
$$S(b_0, \ldots, b_{p-1}) = \sum_{i=1}^{n} (y_i - \hat{y})^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i - \cdots - \beta_{p-1} x_i^{p-1})^2$$

must be minimized to find the estimates $b_0, \ldots, b_{p-1}$.

Example 4.7 (Cylinders, cont'd)**.** The linear fit for the relationship between ammonium phosphate and compressive strength of cylinders was not great ($R^2 = 2.8147436 \times 10^{-5}$). We can fit a quadratic model.

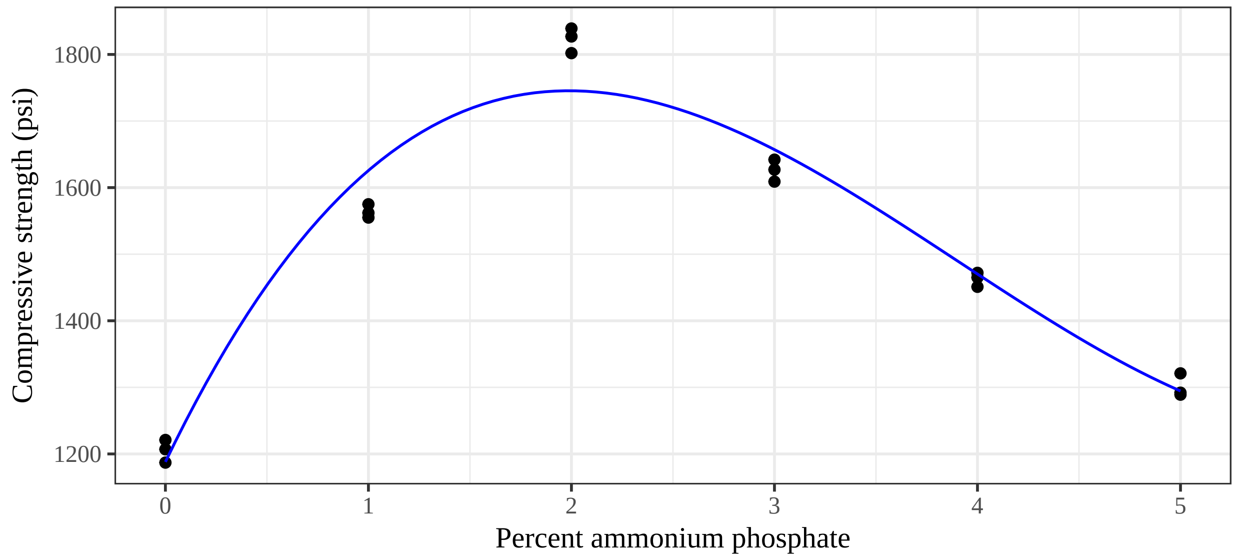
```
Call:
lm(formula = strength ~ ammonium.phosphate + I(ammonium.phosphate^2),
    data = cylinders)

Residuals:
    Min      1Q  Median      3Q     Max
-95.983 -70.193  -7.895  51.548 137.419

Coefficients:
                        Estimate Std. Error t value Pr(>|t|)
(Intercept)             1242.893     42.982  28.917 1.43e-14 ***
ammonium.phosphate       382.665     40.430   9.465 1.03e-07 ***
I(ammonium.phosphate^2)  -76.661      7.762  -9.877 5.88e-08 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 82.14 on 15 degrees of freedom
Multiple R-squared:  0.8667,    Adjusted R-squared:  0.849
F-statistic: 48.78 on 2 and 15 DF,  p-value: 2.725e-07
```

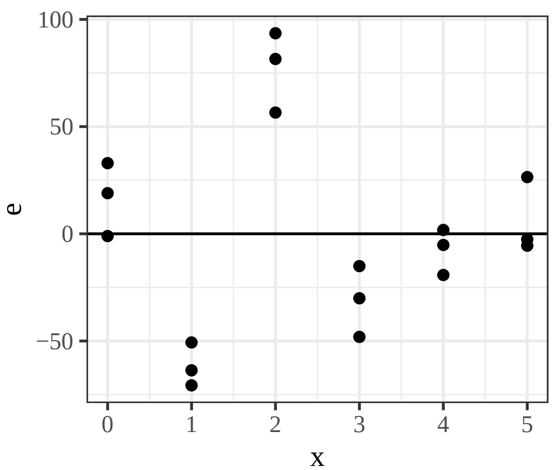

Compressive strength (psi)
1800
1600
1400
1200
0
1
2
3
4
5
Percent ammonium phosphate

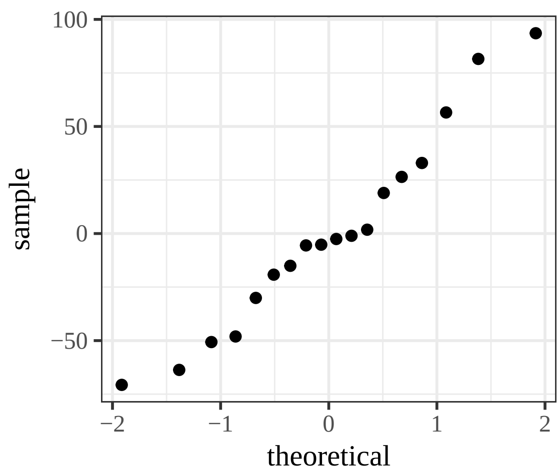

e
100
50
0
−50
−100
x
sample
theoretical
−2
−1
0
1
2

Example 4.8 (Cylinders, cont'd)**.** How about a cubic model.

```
Call:
lm(formula = strength ~ ammonium.phosphate + I(ammonium.phosphate^2) +
    I(ammonium.phosphate^3), data = cylinders)

Residuals:
    Min      1Q  Median      3Q     Max
-70.677 -27.353  -3.874  24.579  93.545

Coefficients:
                        Estimate Std. Error t value Pr(>|t|)
(Intercept)             1188.050     28.786  41.272 5.03e-16 ***
ammonium.phosphate       633.113     55.913  11.323 1.96e-08 ***
I(ammonium.phosphate^2) -213.767     27.787  -7.693 2.15e-06 ***
I(ammonium.phosphate^3)   18.281      3.649   5.010 0.000191 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 50.88 on 14 degrees of freedom
Multiple R-squared:  0.9523,    Adjusted R-squared:  0.9421
F-statistic: 93.13 on 3 and 14 DF,  p-value: 1.733e-09
```


1800
1600
1400
1200
Compressive strength (psi)
0
1
2
3
4
5
Percent ammonium phosphate


100
50
0
−50
e
0
1
2
3
4
5
x


100
50
0
−50
sample
−2
−1
0
1
2
theoretical

4.2.2 Multiple regression (surface fitting)

The next generalization from fitting a line or a polynomial curve is to use the same methods to summarize the effects of several different quantitative variables $x_1, \ldots, x_{p-1}$ on a response y.

$$y \approx \beta_0 + \beta_1 x_1 + \cdots \beta_{p-1} x_{p-1}$$

Where we estimate $\beta_0, \ldots, \beta_{p-1}$ using the *least squares principle.* The function

$$S(b_0, \ldots, b_{p-1}) = \sum_{i=1}^{n} (y_i - \hat{y})^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{1,i} - \cdots - \beta_{p-1} x_{p-1,i})^2$$

must be minimized to find the estimates $b_0, \ldots, b_{p-1}$.

Example 4.9 (New York rivers)**.** Nitrogen content is a measure of river pollution. We have data from 20 New York state rivers concerning their nitrogen content as well as other characteristics. The goal is to find a relationship that explains the variability in nitrogen content for rivers in New York state.

Variable	Description
Y	Mean nitrogen concentration (mg/liter) based on samples taken at regular intervals during the spring, summer, and fall months
X_1	Agriculture: percentage of land area currently in agricultural use
X_2	Forest: percentage of forest land
X_3	Residential: percentage of land area in residential use
X_4	Commercial/Industrial: percentage of land area in either commercial or industrial use

Table 2: Variables present in the New York rivers dataset.

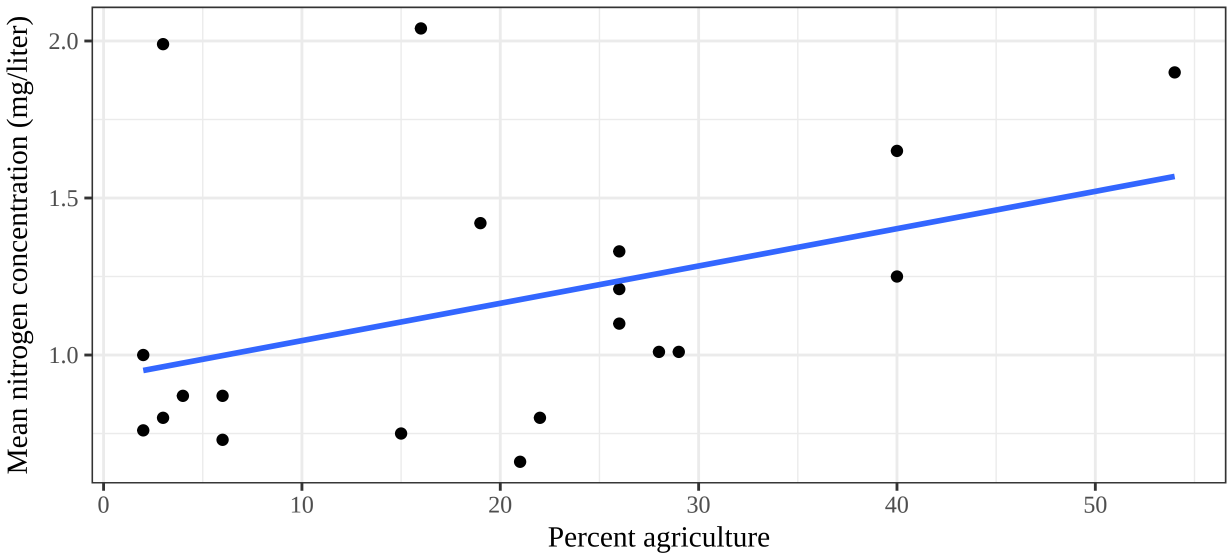
We will fit each of

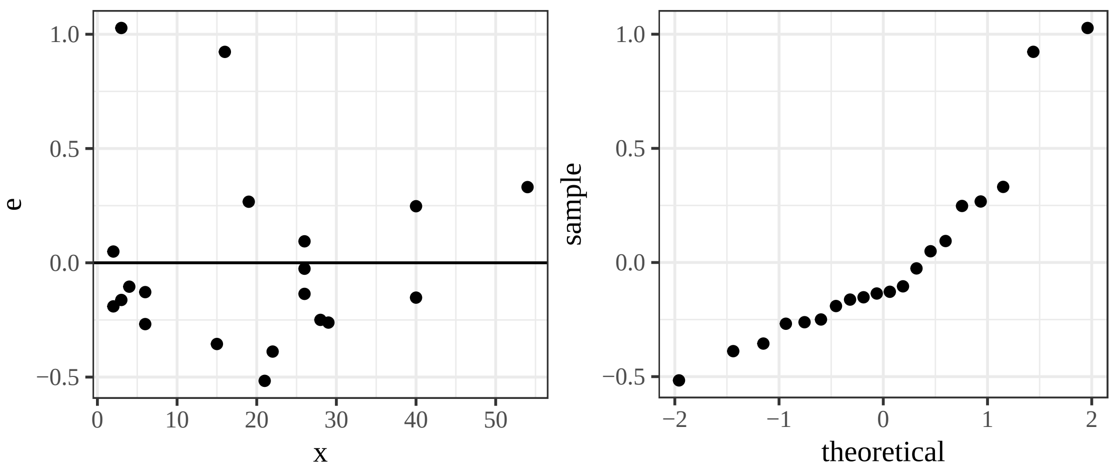
$$\hat{y} = b_0 + b_1 x_1$$

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_4 x_4$$

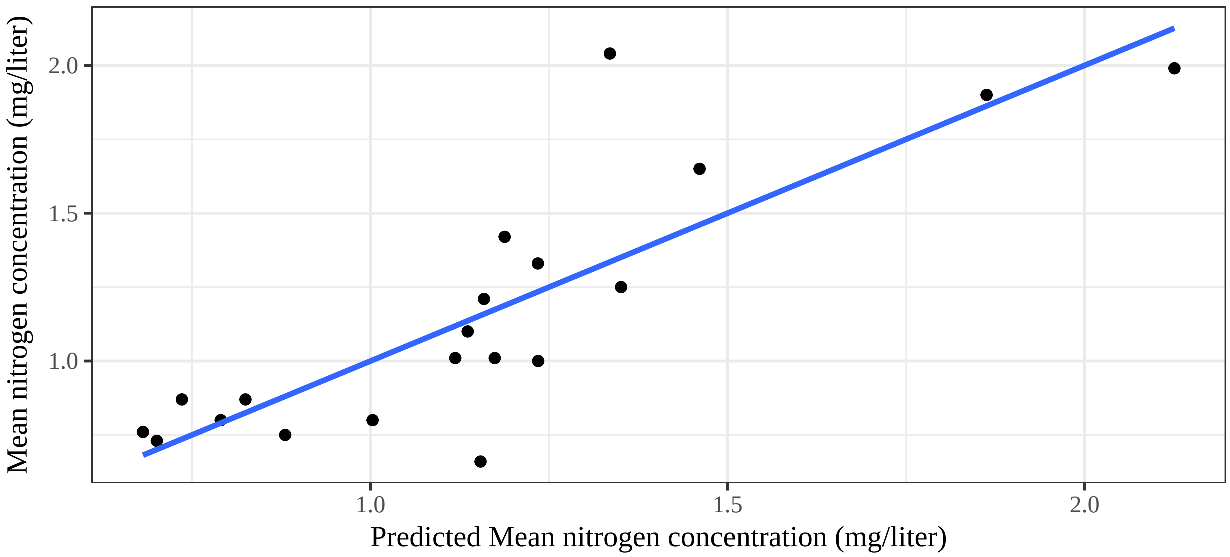
and evaluate fit quality.

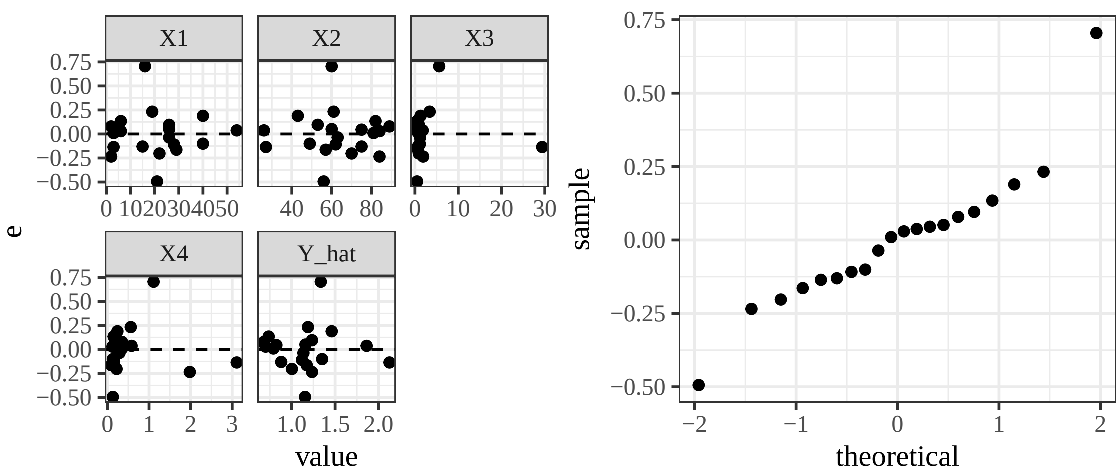
```
Call:
lm(formula = Y ~ X1, data = rivers)

Residuals:
    Min      1Q  Median      3Q     Max 
-0.5165 -0.2527 -0.1321  0.1325  1.0274 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 0.926929   0.154478   6.000 1.13e-05 ***
X1          0.011885   0.006401   1.857   0.0798 .  
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 

Residual standard error: 0.411 on 18 degrees of freedom
Multiple R-squared:  0.1608,    Adjusted R-squared:  0.1141 
F-statistic: 3.448 on 1 and 18 DF,  p-value: 0.07977 
```


Mean nitrogen concentration (mg/liter)
2.0
1.5
1.0
0
10
20
30
40
50
Percent agriculture


1.0
0.5
0.0
−0.5
e
0
10
20
30
40
50
x
sample
−2
−1
0
1
2
theoretical

```
Call:
lm(formula = Y ~ X1 + X2 + X3 + X4, data = rivers)

Residuals:
     Min       1Q   Median       3Q      Max 
-0.49404 -0.13180  0.01951  0.08287  0.70480 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)  
(Intercept)  1.722214   1.234082   1.396   0.1832  
X1           0.005809   0.015034   0.386   0.7046  
X2          -0.012968   0.013931  -0.931   0.3667  
X3          -0.007227   0.033830  -0.214   0.8337  
X4           0.305028   0.163817   1.862   0.0823 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 

Residual standard error: 0.2649 on 15 degrees of freedom
Multiple R-squared:  0.7094,    Adjusted R-squared:  0.6319 
F-statistic: 9.154 on 4 and 15 DF,  p-value: 0.0005963
```





There are some more residual plots we can look at for multiple regression that are helpful:

1.

2.

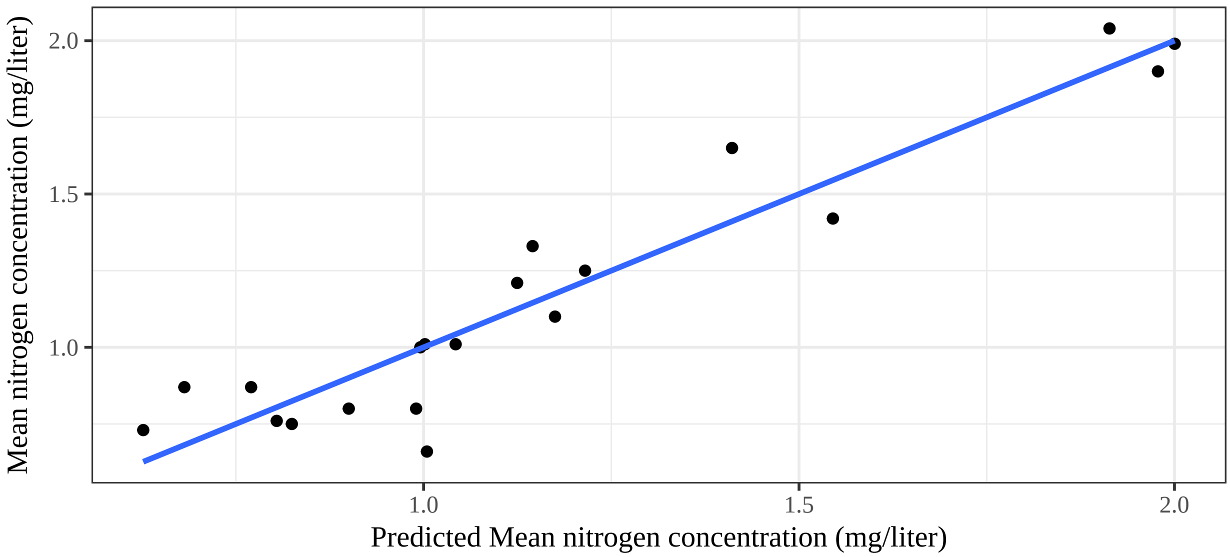
3.

4.

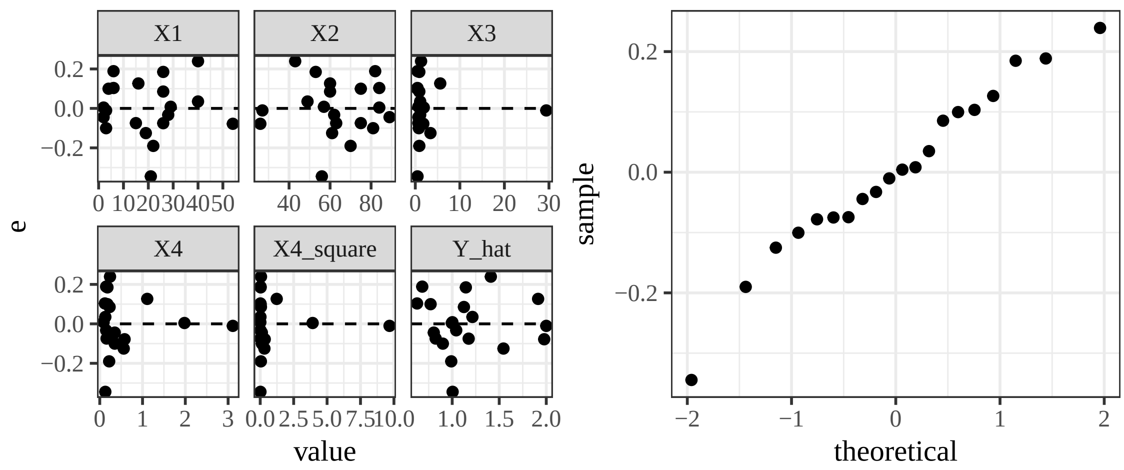
5.

Bonus model:

```
Call:
lm(formula = Y ~ X1 + X2 + X3 + X4 + I(X4^2), data = rivers)

Residuals:
     Min       1Q   Median       3Q      Max
-0.34446 -0.07579 -0.00299  0.10060  0.23920

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.294245   0.765169   1.691 0.112880
X1           0.004900   0.009266   0.529 0.605206
X2          -0.010462   0.008599  -1.217 0.243847
X3           0.073779   0.026304   2.805 0.014045 *
X4           1.271589   0.216387   5.876 4.03e-05 ***
I(X4^2)     -0.532452   0.105436  -5.050 0.000177 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1632 on 14 degrees of freedom
Multiple R-squared:  0.897, Adjusted R-squared:  0.8602
F-statistic: 24.39 on 5 and 14 DF,  p-value: 1.9e-06
```



Mean nitrogen concentration (mg/liter)
Predicted Mean nitrogen concentration (mg/liter)



X1
X2
X3
X4
X4_square
Y_hat
e
value
sample
theoretical

4.2.3 Overfitting

Equation simplicity (*parsimony*) is important for