Linear Regression

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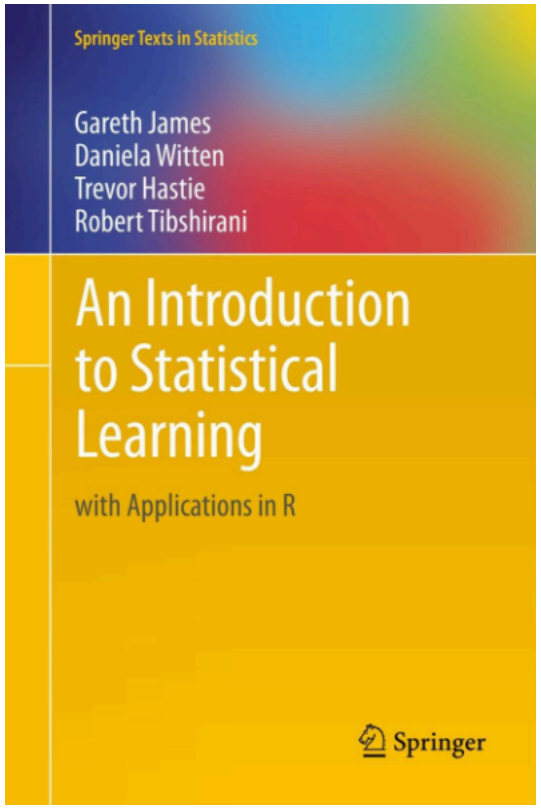
REFERENCE

STATS 202: Data Mining (Stanford)



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Ch3. Linear Regression
Ch4. Classification

Simple linear regression

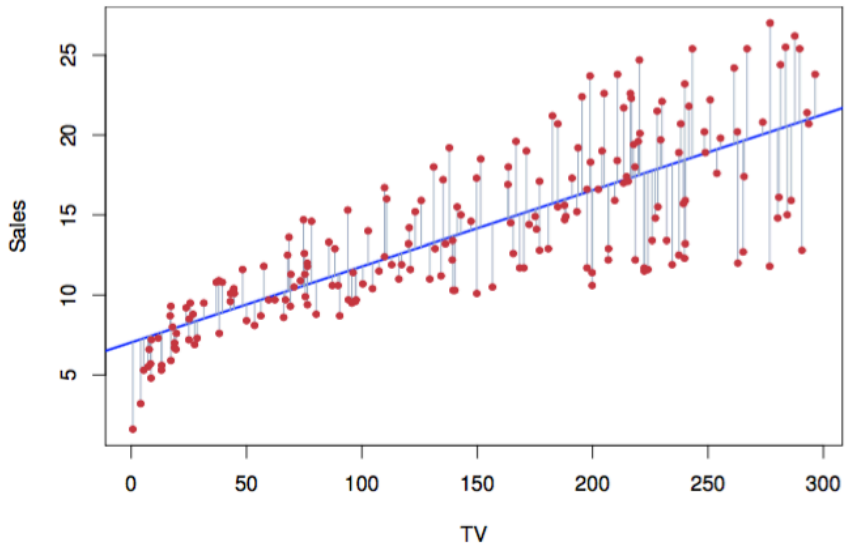


Figure 3.1

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

$$\varepsilon_i \sim \mathcal{N}(0, \sigma) \quad \text{i.i.d.}$$

The estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are chosen to minimize the residual sum of squares (RSS):

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

$$= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2.$$

Estimates $\hat{\beta}_0$ and $\hat{\beta}_1$

A little calculus shows that the minimizers of the RSS are:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^{n}(x_i - \overline{x})^2},$$

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}.$$

Assesing the accuracy of $\hat{\beta}_0$ and $\hat{\beta}_1$

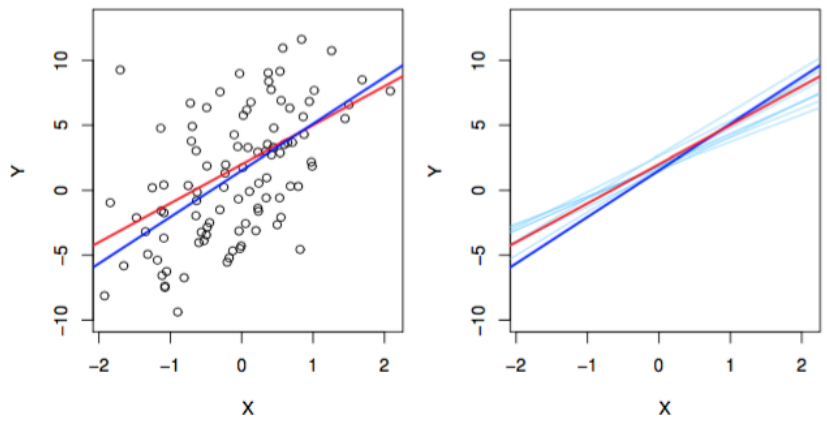


Figure 3.3

The Standard Errors for the parameters are:

$$\mathrm{SE}(\hat{\beta}_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\overline{x}^2}{\sum_{i=1}^{n}(x_i - \overline{x})^2} \right]$$

$$\mathrm{SE}(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \overline{x})^2}.$$

The 95% confidence intervals:

$$\hat{\beta}_0 \pm 2 \cdot \mathrm{SE}(\hat{\beta}_0)$$

$$\hat{\beta}_1 \pm 2 \cdot \mathrm{SE}(\hat{\beta}_1)$$

Hypothesis test

H_0: There is no relationship between X and Y.

H_a: There is some relationship between X and Y.

$$H_0: \beta_1 = 0.$$
$$H_a: \beta_1 \neq 0.$$

Test statistic: $t = \frac{\hat{\beta}_1 - 0}{\mathsf{SE}(\hat{\beta}_1)}$.

Under the null hypothesis, this has a t-distribution with $n - 2$ degrees of freedom.

	Coefficient	Std. error	t-statistic	p-value
`Intercept`	7.0325	0.4578	15.36	< 0.0001
`TV`	0.0475	0.0027	17.67	< 0.0001

TABLE 3.1. *For the* `Advertising` *data, coefficients of the least squares model for the regression of number of units sold on TV advertising budget. An increase of* \$1,000 *in the TV advertising budget is associated with an increase in sales by around 50 units (Recall that the* `sales` *variable is in thousands of units, and the* `TV` *variable is in thousands of dollars).*

Interpreting the hypothesis test

- If we reject the null hypothesis, can we conclude that there is significant evidence of a linear relationship?
  - No. A quadratic relationship may be a better fit, for example.
- If we don't reject the null hypothesis, can we assume there is no relationship between X and Y?
  - No. This test is only powerful against certain monotone alternatives. There could be more complex non-linear relationships.

Multiple linear regression

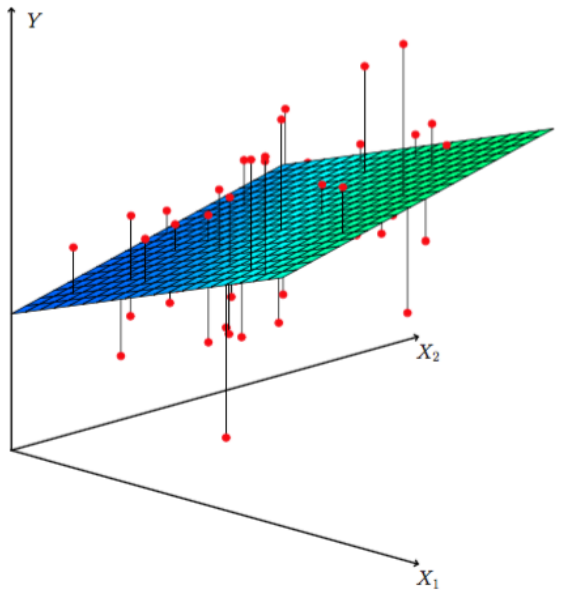


Figure 3.4

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$$

$$\varepsilon \sim \mathcal{N}(0, \sigma) \quad \text{i.i.d.}$$

or, in matrix notation:

$$E\mathbf{y} = \mathbf{X}\beta,$$

where $\mathbf{y} = (y_1, \ldots, y_n)^T$, $\beta = (\beta_0, \ldots, \beta_p)^T$ and $\mathbf{X}$ is our usual data matrix with an extra column of ones on the left to account for the intercept.

Multiple linear regression answers several questions

- Is at least one of the variables X_i useful for predicting the outcome Y?
- Which subset of the predictors is most important?
- How good is a linear model for these data?
- Given a set of predictor values, what is a likely value for Y, and how accurate is this prediction?

The estimates $\hat{\beta}$

Our goal again is to minimize the RSS:

$$\begin{aligned}\text{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i,1} - \cdots - \hat{\beta}_p x_{i,p})^2.\end{aligned}$$

One can show that this is minimized by the vector $\hat{\beta}$:

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}.$$

Which variables are important?

Consider the hypothesis:

$$H_0 : \beta_{p-q+1} = \beta_{p-q+2} = \cdots = \beta_p = 0.$$

Let RSS_0 be the residual sum of squares for the model which excludes these variables. The F-statistic is defined by:

$$F = \frac{(\mathsf{RSS}_0 - \mathsf{RSS})/q}{\mathsf{RSS}/(n-p-1)}.$$

Under the null hypothesis, this has an F-distribution.

Example: If $q = p$, we test whether any of the variables is important.

$$\mathsf{RSS}_0 = \sum_{i=1}^{n} (y_i - \overline{y})^2$$

Which variables are important?

A multiple linear regression in R has the following output:

```
Residuals:
    Min      1Q  Median      3Q     Max
-15.594  -2.730  -0.518   1.777  26.199

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.646e+01  5.103e+00   7.144 3.28e-12 ***
crim        -1.080e-01  3.286e-02  -3.287 0.001087 **
zn           4.642e-02  1.373e-02   3.382 0.000778 ***
indus        2.056e-02  6.150e-02   0.334 0.738288
chas         2.687e+00  8.616e-01   3.118 0.001925 **
nox         -1.777e+01  3.820e+00  -4.651 4.25e-06 ***
rm           3.810e+00  4.179e-01   9.116  < 2e-16 ***
age          6.922e-04  1.321e-02   0.052 0.958229
dis         -1.476e+00  1.995e-01  -7.398 6.01e-13 ***
rad          3.060e-01  6.635e-02   4.613 5.07e-06 ***
tax         -1.233e-02  3.761e-03  -3.280 0.001112 **
ptratio     -9.527e-01  1.308e-01  -7.283 1.31e-12 ***
black        9.312e-03  2.686e-03   3.467 0.000573 ***
lstat       -5.248e-01  5.072e-02 -10.347  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.745 on 492 degrees of freedom
Multiple R-Squared: 0.7406,     Adjusted R-squared: 0.7338
F-statistic: 108.1 on 13 and 492 DF,  p-value: < 2.2e-16
```

Which variables are important?

The t-statistic associated to the ith predictor is the square root of the F-statistic for the null hypothesis which sets only $\beta_i = 0$.

A low p-value indicates that the predictor is important.

Warning: If there are many predictors, even under the null hypothesis, some of the t-tests will have low p-values just by chance.

How many variables are important?

When we select a subset of the predictors, we have 2^p choices.

A way to simplify the choice is to greedily add variables (or to remove them from a baseline model). This creates a sequence of models, from which we can select the best.

- **Forward selection:** Starting from a *null model* (the intercept), include variables one at a time, minimizing the RSS at each step.
- **Backward selection:** Starting from the *full model*, eliminate variables one at a time, choosing the one with the largest p-value at each step.
- **Mixed selection:** Starting from a *null model*, include variables one at a time, minimizing the RSS at each step. If the p-value for some variable goes beyond a threshold, eliminate that variable.

Choosing one model in the range produced is a form of *tuning*.

How many variables are important?

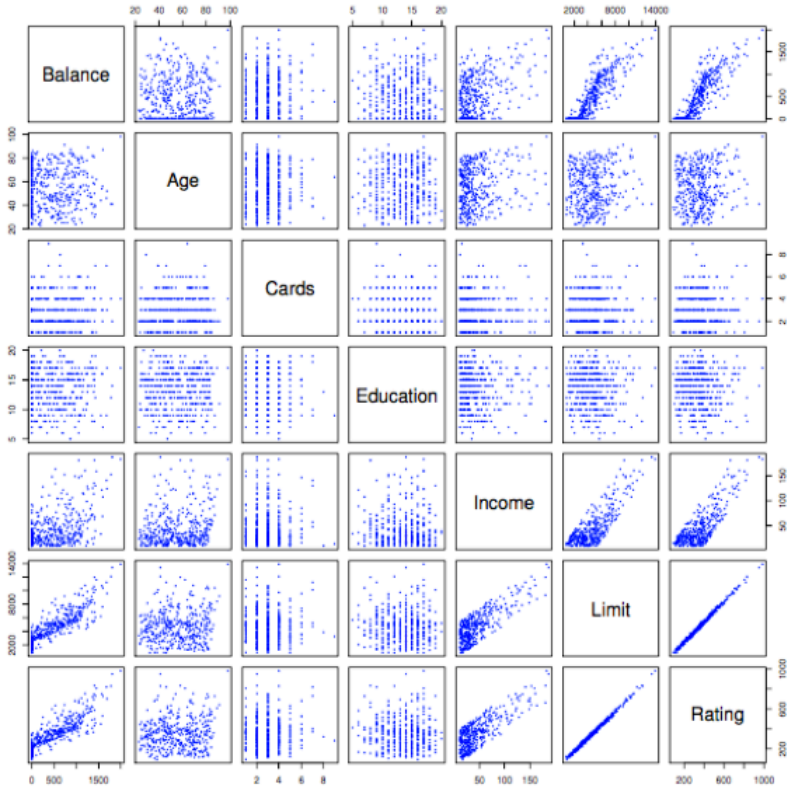
The output of a stepwise selection method is a range of models:

- $\{\}$
- $\{\texttt{tv}\}$
- $\{\texttt{tv}, \texttt{newspaper}\}$
- $\{\texttt{tv}, \texttt{newspaper}, \texttt{radio}\}$
- $\{\texttt{tv}, \texttt{newspaper}, \texttt{radio}, \texttt{facebook}\}$
- $\{\texttt{tv}, \texttt{newspaper}, \texttt{radio}, \texttt{facebook}, \texttt{twitter}\}$

6 choices are better than $2^6 = 64$. We use different *tuning methods* to decide which model to use; e.g. cross-validation, AIC, BIC.

Dealing with categorical or qualitative predictors

Example: Credit dataset



In addition, there are 4 qualitative variables:

- `gender`: male, female.
- `student`: student or not.
- `status`: married, single, divorced.
- `ethnicity`: African American, Asian, Caucasian.

Dealing with categorical or qualitative predictors

For each qualitative predictor, e.g. `status`:

- Choose a baseline category, e.g. single
- For every other category, define a new predictor:
  - X_{married} is 1 if the person is married and 0 otherwise.
  - X_{divorced} is 1 if the person is divorced and 0 otherwise.

The model will be:

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_7 X_7 + \beta_{\text{married}} X_{\text{married}} + \beta_{\text{divorced}} X_{\text{divorced}} + \varepsilon.$$

β_{married} is the relative effect on `balance` for being married compared to the baseline category.

Dealing with categorical or qualitative predictors

- The model fit $\hat{f}$ and predictions $\hat{f}(x_0)$ are independent of the choice of the baseline category.
- However, the interpretation of parameters and associated hypothesis tests depend on the baseline category.
  - **Solution:** To check whether `status` is important, use an F-test for the hypothesis $\beta_{\text{married}} = \beta_{\text{divorced}} = 0$. This does not depend on the coding of the baseline category.

How uncertain are the predictions?

The function `predict` in R output predictions from a linear model; eg. $x_0 = (5, 10, 15)$:

```
> predict(lm.fit,data.frame(lstat=(c(5,10,15))),
      interval="confidence")
    fit    lwr    upr
1 29.80 29.01 30.60
2 25.05 24.47 25.63
3 20.30 19.73 20.87
```

"Confidence intervals" reflect the uncertainty on $\hat{\beta}$; ie. confidence interval for $f(x_0)$.

```
> predict(lm.fit,data.frame(lstat=(c(5,10,15))),
      interval="prediction")
    fit     lwr    upr
1 29.80 17.566 42.04
2 25.05 12.828 37.28
3 20.30  8.078 32.53
```

"Prediction intervals" reflect uncertainty on $\hat{\beta}$ and the irreducible error ε as well; i.e. confidence interval for y_0.

Recap

So far, we have:

- Defined Multiple Linear Regression
- Discussed how to test the relevance of variables.
- Described one approach to choose a subset of variables.
- Explained how to code qualitative variables.
- Discussed confidence intervals surrounding preditions.
- Now, how do we evaluate model fit? Is the linear model any good? What can go wrong?

How good is the fit?

To assess the fit, we focus on the residuals.

- $R^2 = \text{Corr}(Y, \hat{Y})$, always increases as we add more variables.
- The residual standard error (RSE) does not always improve with more predictors:

$$\text{RSE} = \sqrt{\frac{1}{n-p-1}\text{RSS}}.$$

- **Visualizing the residuals** can reveal phenomena that are not accounted for by the model.

Potential issues in linear regression

1. Interactions between predictors
2. Non-linear relationships
3. Correlation of error terms
4. Non-constant variance of error (heteroskedasticity).
5. Outliers
6. High leverage points
7. Collinearity

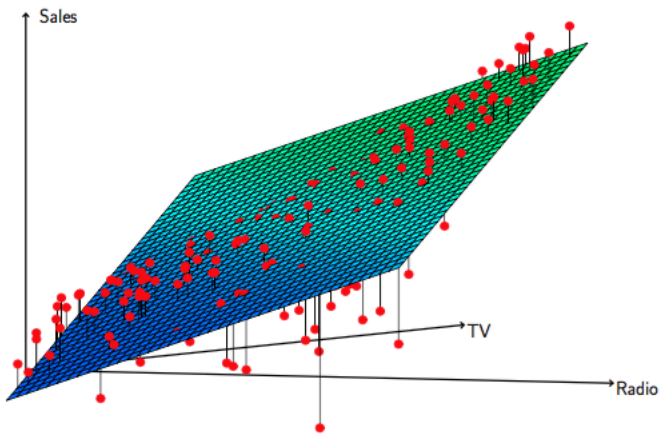
Interactions between predictors

Linear regression has an *additive* assumption:

$$\texttt{sales} = \beta_0 + \beta_1 \times \texttt{tv} + \beta_2 \times \texttt{radio} + \varepsilon$$

i.e. An increase of \$100 dollars in TV ads causes a fixed increase in sales, regardless of how much you spend on radio ads.

When we visualize the residuals, we see a pronounced non-linear relationship:



Interactions between predictors

One way to deal with this is to include multiplicative variables in the model:

$$\texttt{sales} = \beta_0 + \beta_1 \times \texttt{tv} + \beta_2 \times \texttt{radio} + \beta_3 \times (\texttt{tv} \cdot \texttt{radio}) + \varepsilon$$

The **interaction variable** is high when both `tv` and `radio` are high.

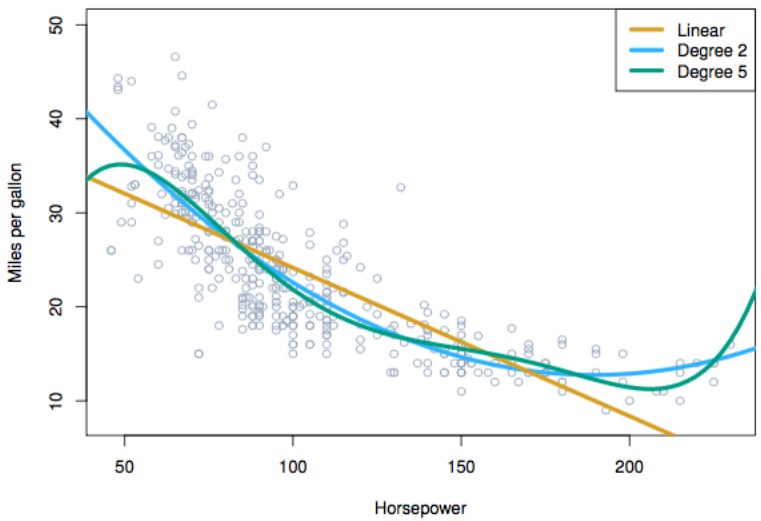
Interactions between predictors

R makes it easy to include interaction variables in the model:

```
> lm.fit=lm(Sales~.+Income:Advertising+Price:Age,data=Carseats)
> summary(lm.fit)

Call:
lm(formula = Sales ~ . + Income:Advertising + Price:Age, data =
    Carseats)

Residuals:
    Min      1Q  Median      3Q     Max
-2.921  -0.750   0.018   0.675   3.341

Coefficients:
                     Estimate  Std. Error t value Pr(>|t|)
(Intercept)          6.575565    1.008747    6.52  2.2e-10 ***
CompPrice            0.092937    0.004118   22.57  < 2e-16 ***
Income               0.010894    0.002604    4.18  3.6e-05 ***
Advertising          0.070246    0.022609    3.11  0.00203 **
Population           0.000159    0.000368    0.43  0.66533
Price               -0.100806    0.007440  -13.55  < 2e-16 ***
ShelveLocGood        4.848676    0.152838   31.72  < 2e-16 ***
ShelveLocMedium      1.953262    0.125768   15.53  < 2e-16 ***
Age                 -0.057947    0.015951   -3.63  0.00032 ***
Education           -0.020852    0.019613   -1.06  0.28836
UrbanYes             0.140160    0.112402    1.25  0.21317
USYes               -0.157557    0.148923   -1.06  0.29073
Income:Advertising   0.000751    0.000278    2.70  0.00729 **
Price:Age            0.000107    0.000133    0.80  0.42381
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Non-linearities

Example: Auto dataset.



A scatterplot between a predictor and the response may reveal a non-linear relationship.

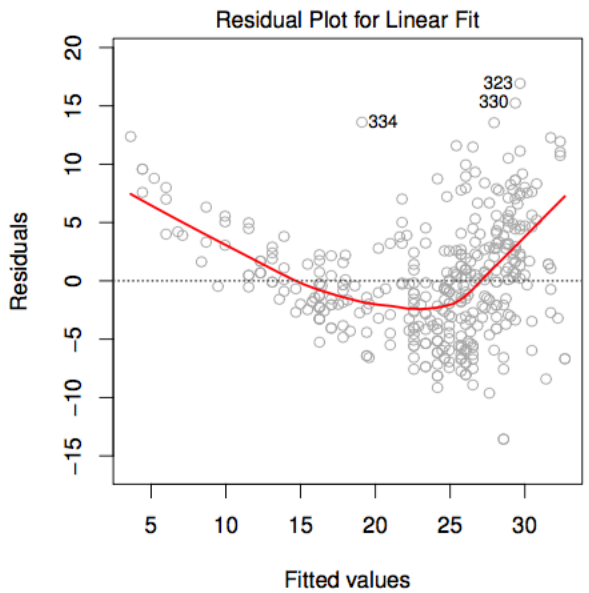
Solution: include polynomial terms in the model.

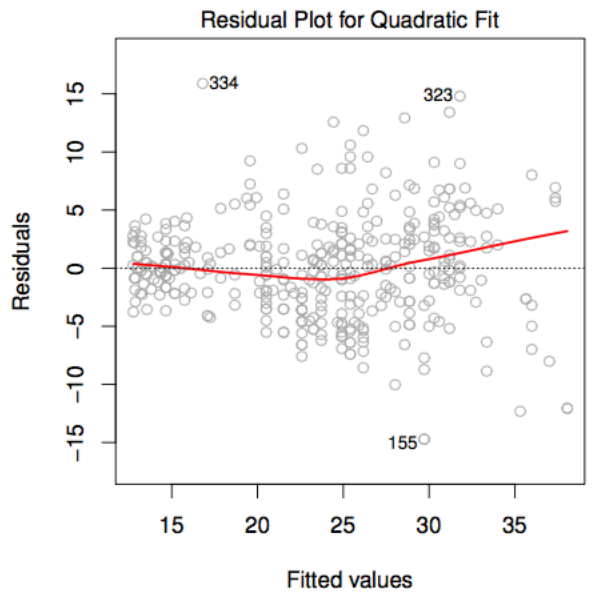
$$\texttt{MPG} = \beta_0 + \beta_1 \times \texttt{horsepower} + \varepsilon$$
$$+ \beta_2 \times \texttt{horsepower}^2 + \varepsilon$$
$$+ \beta_3 \times \texttt{horsepower}^3 + \varepsilon$$
$$+ \ldots + \varepsilon$$

Non-linearities

In 2 or 3 dimensions, this is easy to visualize. What do we do when we have many predictors?

Plot the residuals against the *fitted values* and look for a pattern:





Correlation of error terms

We assumed that the errors for each sample are independent:

$$y_i = f(x_i) + \varepsilon_i \quad ; \quad \varepsilon_i \sim \mathcal{N}(0, \sigma) \text{ i.i.d.}$$

What if this assumption breaks down?

The main effect is that this invalidates any assertions about Standard Errors, confidence intervals, and hypothesis tests:

Example: Suppose that by accident, we double the data (we use each sample twice). Then, the standard errors would be artificially smaller by a factor of $\sqrt{2}$.

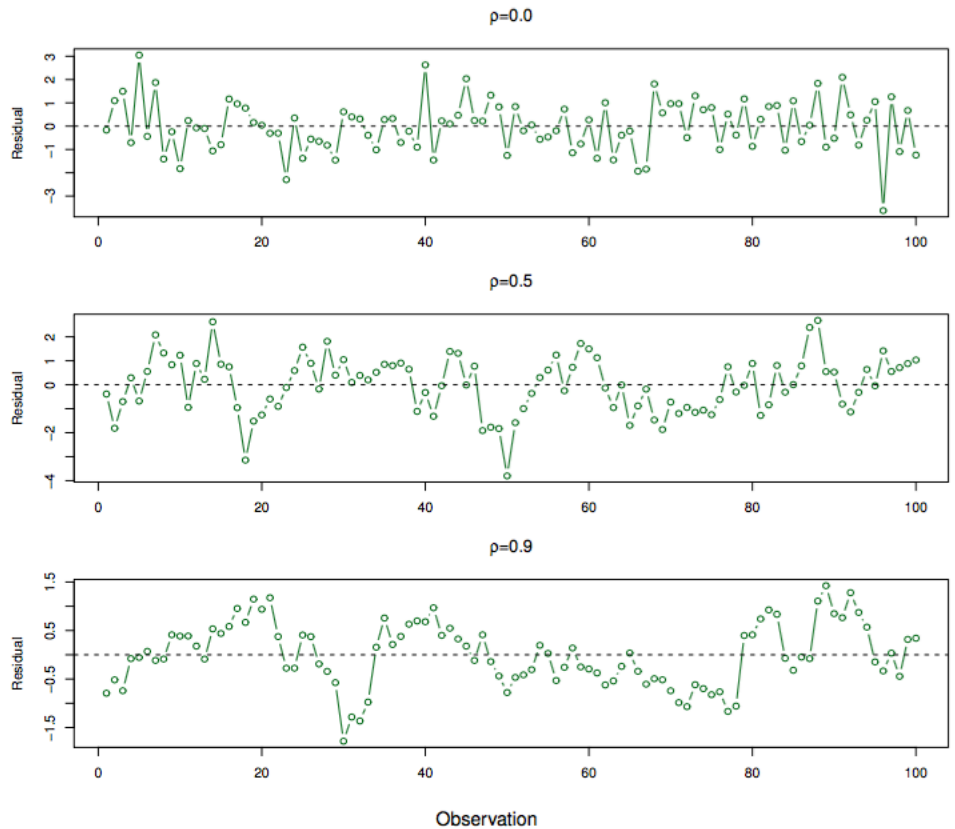
Correlation of error terms

When could this happen in real life:

- **Time series:** Each sample corresponds to a different point in time. The errors for samples that are close in time are correlated.
- **Spatial data:** Each sample corresponds to a different location in space.
- Study on predicting height from weight at birth. Suppose some of the subjects in the study are in the same family, their shared environment could make them deviate from $f(x)$ in similar ways.

Correlation of error terms

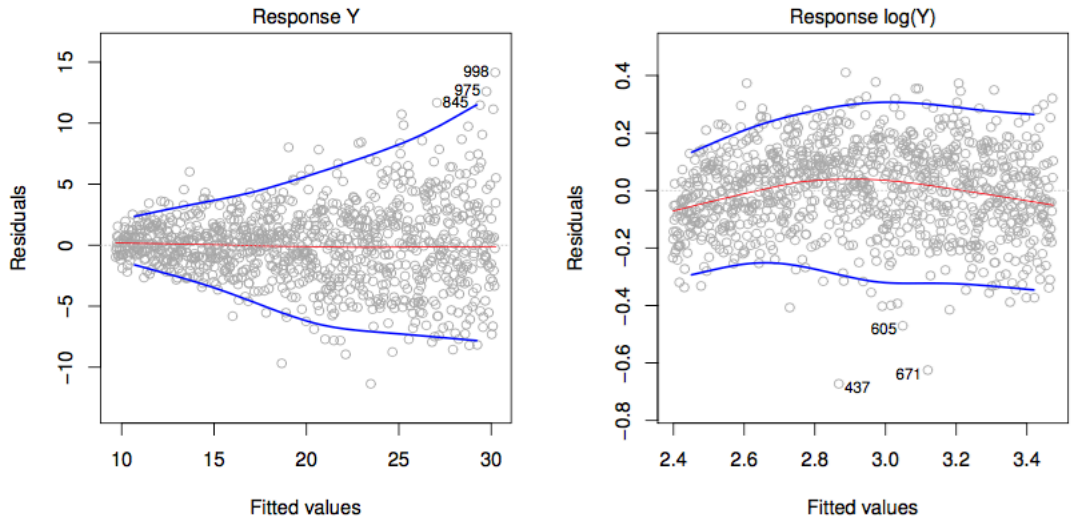
Simulations of time series with increasing correlations between ε_i.



Non-constant variance of error (heteroskedasticity)

The variance of the error depends on the input.

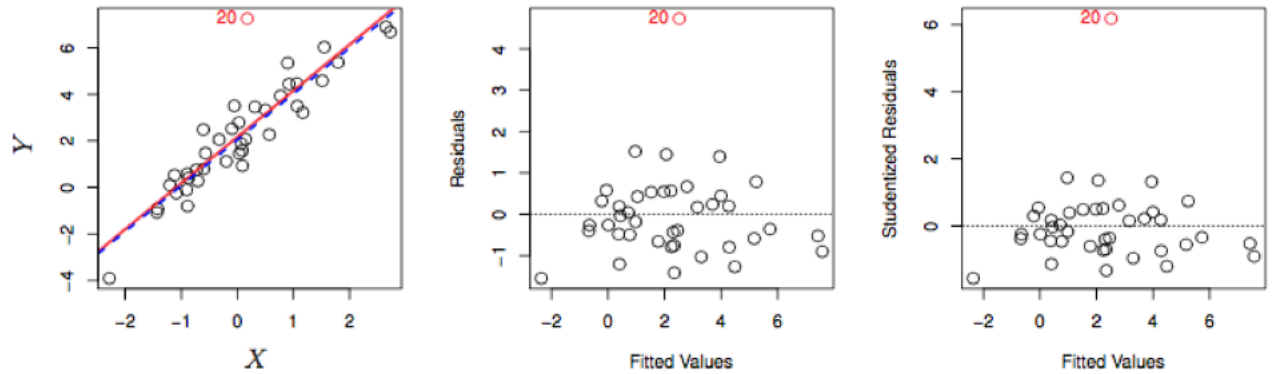
To diagnose this, we can plot residuals vs. fitted values:



Solution: If the trend in variance is relatively simple, we can transform the response using a logarithm, for example.

Outliers

Outliers are points with very high errors.



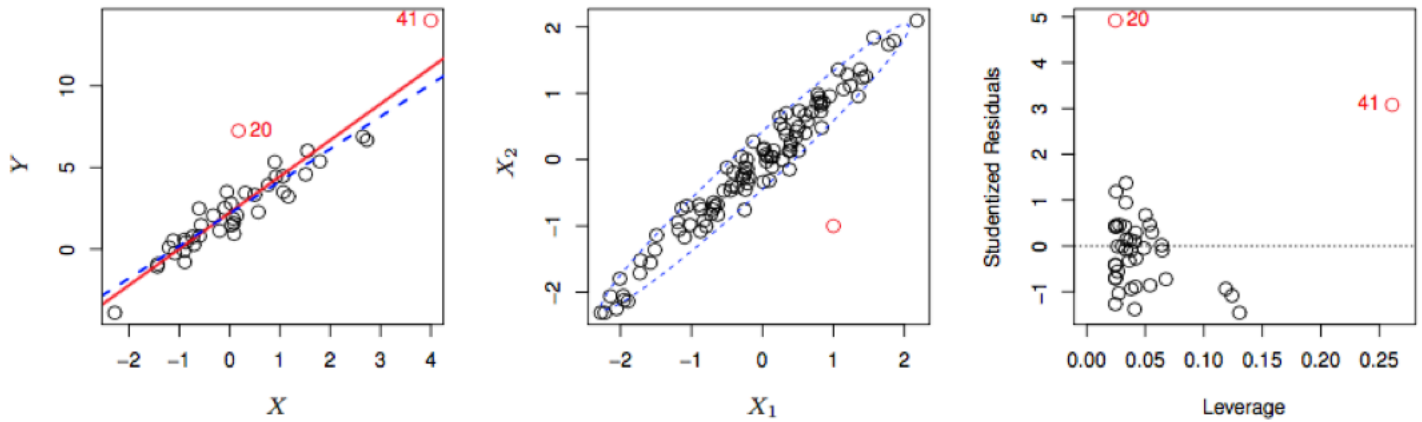
While they may or may not affect the fit, they might affect our assessment of model quality.

Possible solutions:

- If we believe an outlier is due to an error in data collection, we can remove it.
- An outlier might be evidence of a missing predictor, or the need to specify a more complex model.

High leverage points

High leverage points are observations with unusual input values.
They can have an outsized effect on the fit $\hat{\beta}$!



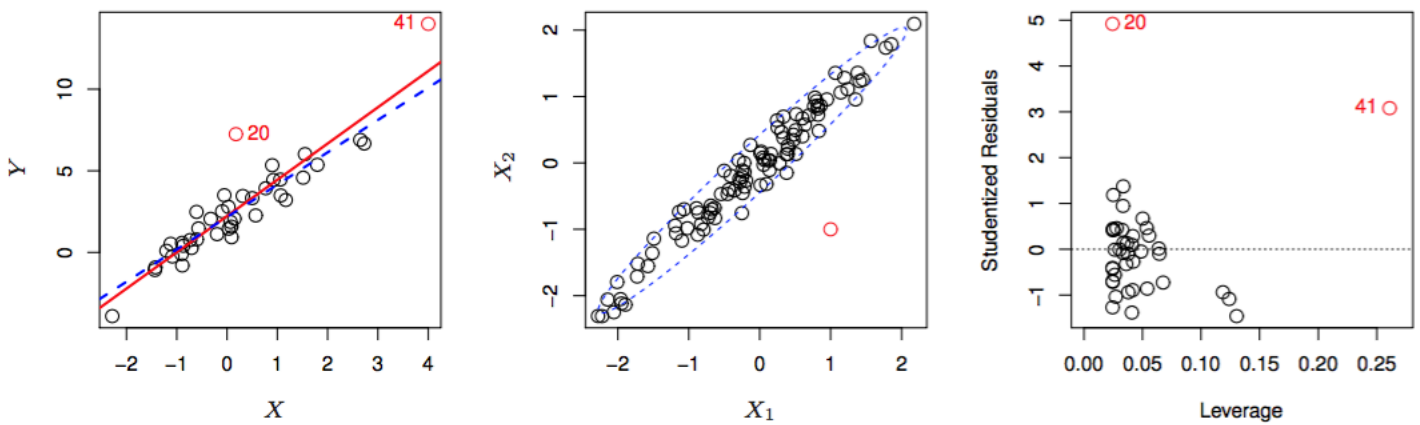
Quantified with the **leverage statistic** or **self influence**:

$$h_{ii} = \frac{\partial \hat{y}_i}{\partial y_i} = \underbrace{(\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T)}_{\text{Hat matrix}}{}_{i,i} \in [1/n, 1].$$

Hat matrix satisfies $\hat{y} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T y = \mathbf{H}y$

Studentized residuals

- The residual $\hat{\epsilon}_i = y_i - \hat{y}_i$ is an estimate for the noise $\epsilon_i = y_i - f(x_i)$.
- The standard error of $\hat{\epsilon}_i$ is $\sigma\sqrt{1 - h_{ii}}$.
- A **studentized residual** is $\hat{\epsilon}_i$ divided by its standard error.
- It follows a Student-t distribution with $n - p - 2$ degrees of freedom.

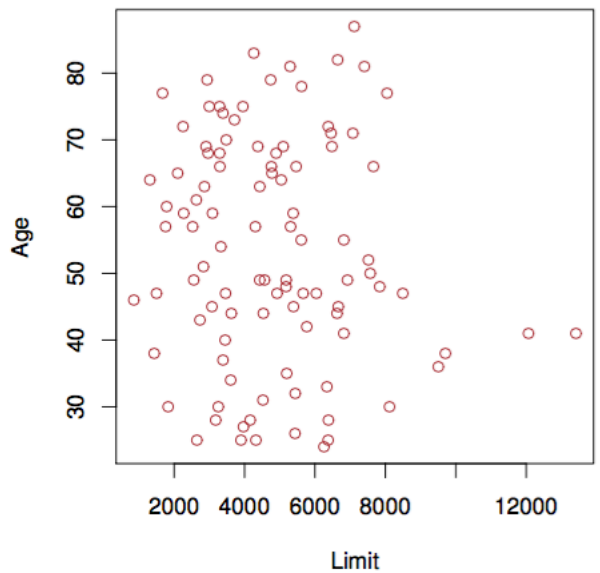


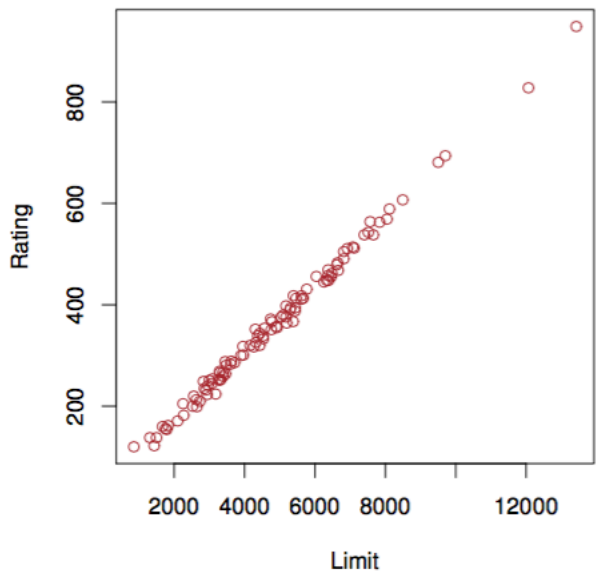
Collinearity

Two predictors are collinear if they are highly correlated:

$$\texttt{limit} \approx a \times \texttt{rating} + b$$

i.e. if one variable is approximately a linear function of the other.
In that case they contain approximately the same information.



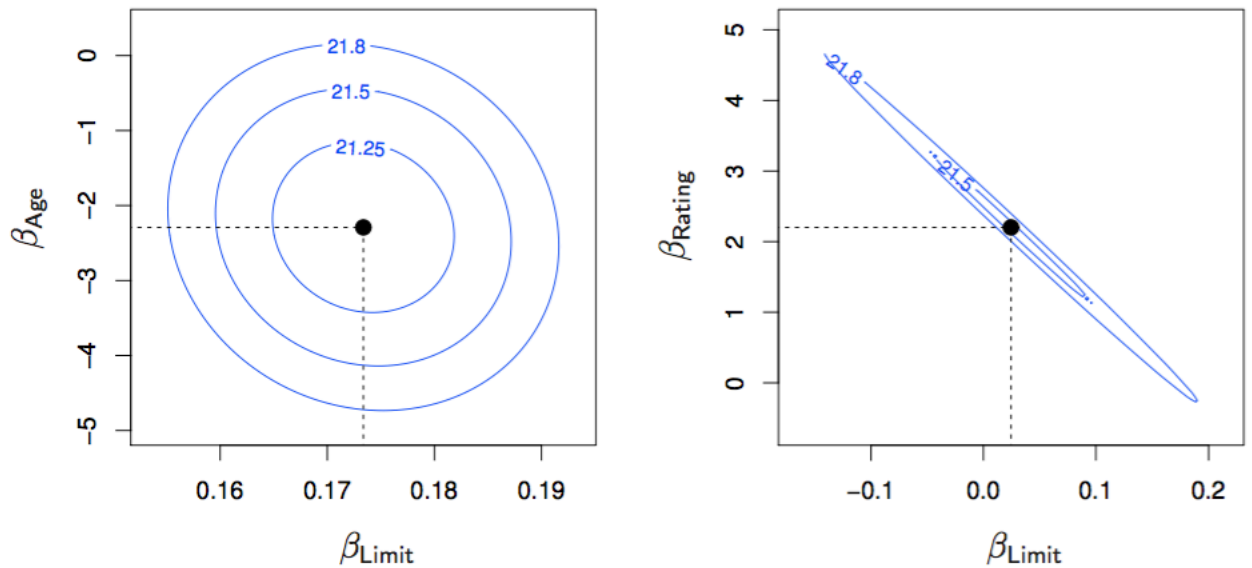


Collinearity

Problem: Coefficient estimates become less certain and more variable (as training data changes). Consider the extreme case of using two identical predictors `limit`:

$$\begin{aligned}\texttt{balance} &= \beta_0 + \beta_1 \times \texttt{limit} + \beta_2 \times \texttt{limit} \\ &= \beta_0 + (\beta_1 + 100) \times \texttt{limit} + (\beta_2 - 100) \times \texttt{limit}\end{aligned}$$

The fit $(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2)$ is just as good as $(\hat{\beta}_0, \hat{\beta}_1 + 100, \hat{\beta}_2 - 100)$.



Collinearity

If 2 variables are collinear, we can easily diagnose this using their correlation.

A group of q variables is **multilinear** if one variable is approximately a linear function of the other variables. Pairwise correlations may not reveal multilinear variables.

The Variance Inflation Factor (VIF) measures how linearly predictable a variable is from the other variables:

$$VIF(\hat{\beta}_j) = \frac{1}{1 - R^2_{X_j|X_{-j}}},$$

where $R^2_{X_j|X_{-j}}$ is the R^2 statistic for Multiple Linear regression of the predictor X_j onto the remaining predictors.

Assignments

9. This question involves the use of multiple linear regression on the `Auto` data set.

   (a) Produce a scatterplot matrix which includes all of the variables in the data set.

   (b) Compute the matrix of correlations between the variables using the function `cor()`. You will need to exclude the `name` variable, which is qualitative.

   (c) Use the `lm()` function to perform a multiple linear regression with `mpg` as the response and all other variables except `name` as the predictors. Use the `summary()` function to print the results. Comment on the output. For instance:

      i. Is there a relationship between the predictors and the response?

      ii. Which predictors appear to have a statistically significant relationship to the response?

      iii. What does the coefficient for the `year` variable suggest?

(d) Use the `plot()` function to produce diagnostic plots of the linear regression fit. Comment on any problems you see with the fit. Do the residual plots suggest any unusually large outliers? Does the leverage plot identify any observations with unusually high leverage?

(e) Use the `*` and `:` symbols to fit linear regression models with interaction effects. Do any interactions appear to be statistically significant?

(f) Try a few different transformations of the variables, such as $\log(X)$, $\sqrt{X}$, X^2. Comment on your findings.

10. This question should be answered using the `Carseats` data set.

(a) Fit a multiple regression model to predict `Sales` using `Price`, `Urban`, and `US`.

(b) Provide an interpretation of each coefficient in the model. Be careful—some of the variables in the model are qualitative!

(c) Write out the model in equation form, being careful to handle the qualitative variables properly.

(d) For which of the predictors can you reject the null hypothesis $H_0 : \beta_j = 0$?

(e) On the basis of your response to the previous question, fit a smaller model that only uses the predictors for which there is evidence of association with the outcome.

(f) How well do the models in (a) and (e) fit the data?

(g) Using the model from (e), obtain 95 % confidence intervals for the coefficient(s).

(h) Is there evidence of outliers or high leverage observations in the model from (e)?

15. This problem involves the `Boston` data set, which we saw in the lab for this chapter. We will now try to predict per capita crime rate using the other variables in this data set. In other words, per capita crime rate is the response, and the other variables are the predictors.

    (a) For each predictor, fit a simple linear regression model to predict the response. Describe your results. In which of the models is there a statistically significant association between the predictor and the response? Create some plots to back up your assertions.

    (b) Fit a multiple regression model to predict the response using all of the predictors. Describe your results. For which predictors can we reject the null hypothesis $H_0 : \beta_j = 0$?

(c) How do your results from (a) compare to your results from (b)? Create a plot displaying the univariate regression coefficients from (a) on the x-axis, and the multiple regression coefficients from (b) on the y-axis. That is, each predictor is displayed as a single point in the plot. Its coefficient in a simple linear regression model is shown on the x-axis, and its coefficient estimate in the multiple linear regression model is shown on the y-axis.

(d) Is there evidence of non-linear association between any of the predictors and the response? To answer this question, for each predictor X, fit a model of the form

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon.$$