

Lecture 6: Linear Regression

Reading: Sections 3.1-3

STATS 202: Data mining and analysis

Jonathan Taylor, 10/5

Slide credits: Sergio Bacallado

Simple linear regression

Model:

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

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

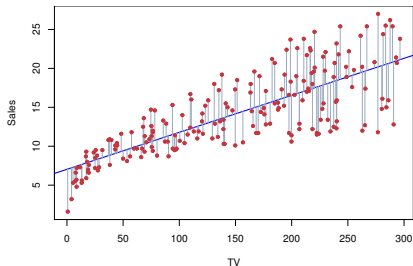


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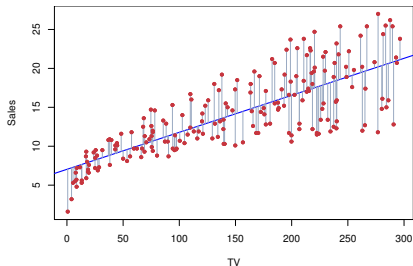


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$$\begin{aligned} \text{RSS} &= \sum_{i=1}^n (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2. \end{aligned}$$

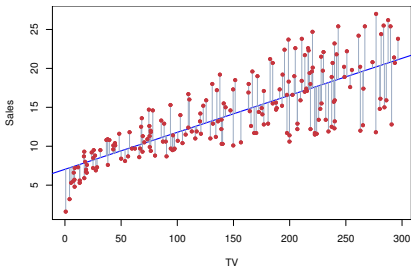


Figure 3.1

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

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

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

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

The **Standard Errors** for the parameters are:

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

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

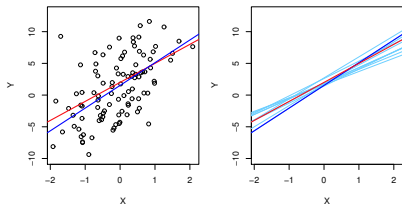


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The 95% confidence intervals:

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

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

Calculations depend on the model above

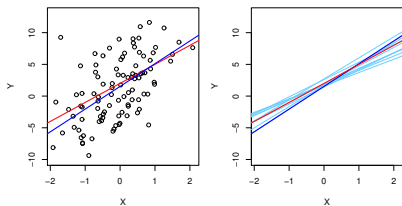


Figure 3.3

Hypothesis test

H_0 : There is no relationship between X and Y .

H_a : There is some relationship between X and Y .

Hypothesis test

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Under the null hypothesis (special case of the model), this has a
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	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).

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 - ▶ **No.** A quadratic relationship may be a better fit, for example. There is evidence of linear association.
- ▶ 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.

拒绝与不拒绝该假设 都存在一定的問題

Multiple linear regression

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

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

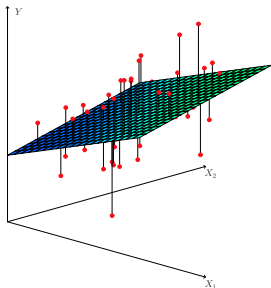


Figure 3.4

Multiple linear regression

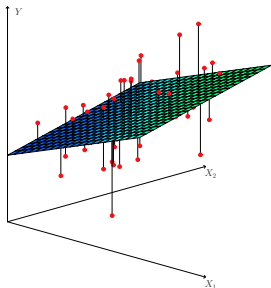


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$$\varepsilon \sim \mathcal{N}(0, \sigma) \quad \text{i.i.d.}$$

or, in matrix notation:

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

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

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- ▶ 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 $\hat{\beta}$

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

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

We also write RSS for the *minimized* sum of squares.

Which variables are important?

Consider the hypothesis:

H_0 : The last q predictors have no relation with Y .

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$$F = \frac{(RSS_0 - RSS)/q}{RSS/(n - p - 1)}.$$

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

$$RSS_0 = \sum_{i=1}^n (y_i - \bar{y})^2$$

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
```

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P-hacking warning: If there are many predictors, even under the null hypothesis, some of the t -tests will have low p -values.

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- ▶ **Backward selection:** Starting from the *full model*, eliminate variables one at a time, choosing the one with the largest p-value at each step.

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- ▶ **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.

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Choosing model this way is a form of *tuning*. P-hacking: hypothesis tests, confidence intervals not valid after selection!

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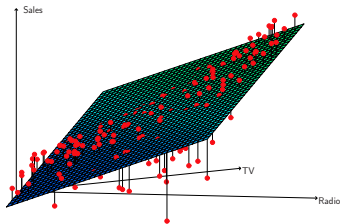
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- ▶ Visualizing the residuals can reveal phenomena that are not accounted for by the model; eg. synergies or interactions:



How good are the predictions?

The function `predict` in R output predictions from a linear model:

```
> 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
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Confidence intervals reflect the uncertainty on $\hat{\beta}$.

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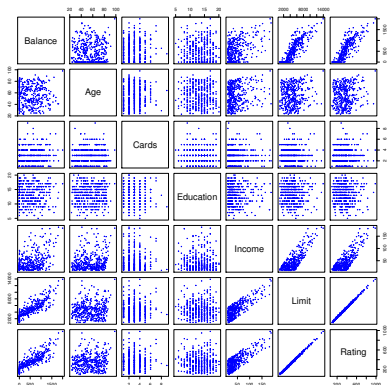
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```
> predict(lm.fit, data.frame(lstat=(c(5,10,15))),  
          interval="prediction")  
      fit   lwr   upr  
1 29.80 17.566 42.04  
2 25.05 12.828 37.28  
3 20.30  8.078 32.53
```

Prediction intervals reflect uncertainty on $\hat{\beta}$ and the irreducible error ε as well.

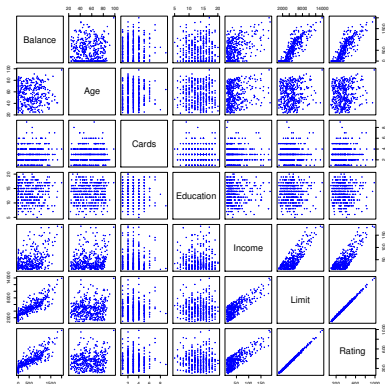
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Example: Credit dataset



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In addition, there are 4 qualitative variables:

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

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The model will be:

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

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- ▶ The model fit and predictions are independent of the choice of the baseline category.
- ▶ However, hypothesis tests derived from these variables are affected by the choice.
 - ▶ **Solution:** To check whether ethnicity is important, use an F -test for the hypothesis $\beta_{\text{Asian}} = \beta_{\text{Caucasian}} = 0$. This does not depend on the coding.
- ▶ Other ways to encode qualitative predictors produce the same fit \hat{f} , but the coefficients have different interpretations.

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

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- ▶ **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. Colinearity

Interactions between predictors

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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.

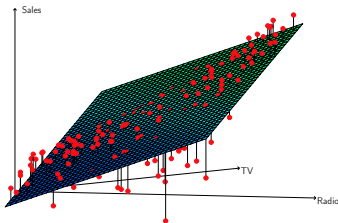
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i.e. An increase of \$100 dollars in TV ads causes a fixed increase in sales, regardless of how much you spend on radio ads.

If we visualize the residuals, it is clear that this is false:



Interactions between predictors

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

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

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)

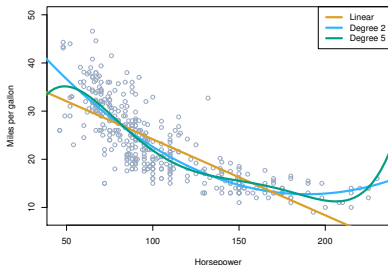
Call:
lm(formula = Sales ~ . + Income:Advertising + Price:Age, data =
    Carseats)

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

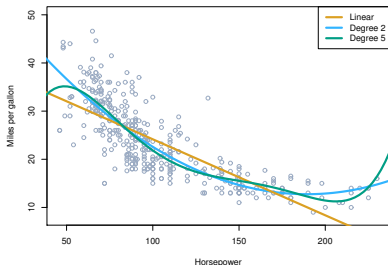
Example: Auto dataset.



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

Non-linearities

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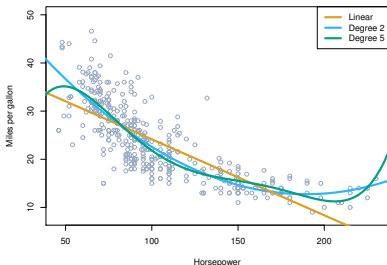
A scatterplot between a predictor and the response may reveal a non-linear relationship.

Solution: include polynomial terms in the model.

$$\text{MPG} = \beta_0 + \beta_1 \times \text{horsepower} + \varepsilon$$

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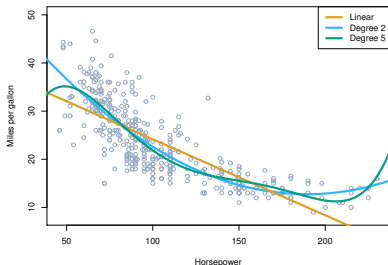
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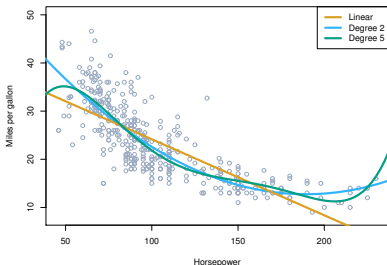
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$$\begin{aligned} \text{MPG} = & \beta_0 + \beta_1 \times \text{horsepower} \\ & + \beta_2 \times \text{horsepower}^2 \\ & + \beta_3 \times \text{horsepower}^3 + \varepsilon \end{aligned}$$

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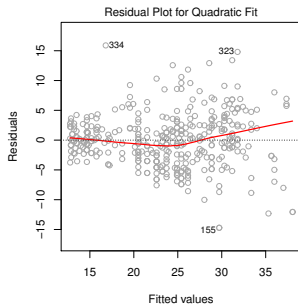
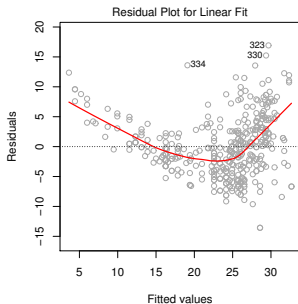
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Plot the residuals against the *response* and look for a pattern:



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 breaks down?

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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 $\sqrt{2}$.

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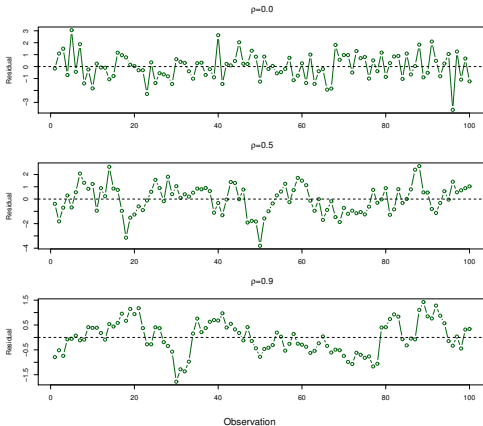
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- ▶ **Time series:** Each sample corresponds to a different point in time. The errors for samples that are close in time are correlated.
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- ▶ Study on predicting height from weight at birth. Suppose 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 .



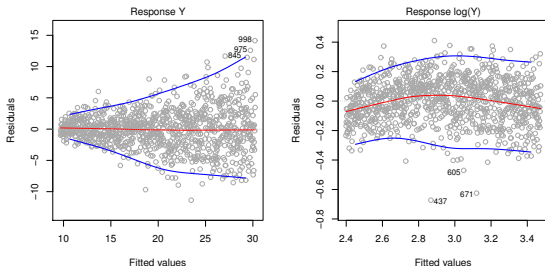
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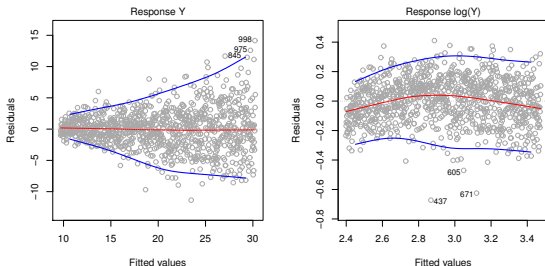
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Solution: If the trend in variance is relatively simple, we can transform the response using a logarithm, for example.