Lecture 3: Linear Regression

STATS 202: Statistical Learning and Data Science

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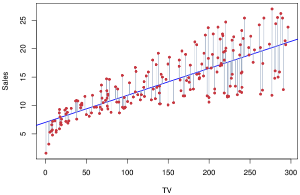
Announcements

- HW1 due this Thursday
- No section this Friday (holiday)
- Accommodation requests for midterms starting
- Sections: please unenroll from Section 03 (Class 23599)

Outline

- Linear regression
  - Coefficients, standard errors, hypothesis testing
- Multiple linear regression
  - Variable selection, stepwise models, categorical variables,
- Regression issues
  - Interactions, non-linear relationships, error correlation, heteroskedasticity



Example of a linear model fit to some data.

Recall:

- Given some input features $X_1, X_2, ..., X_p$
- $Y \in \mathbb{R}$ is the output
- (X, Y) have a joint distribution
- Blue line is the regression fit: an estimate $\hat{f}_n$ of the line we want

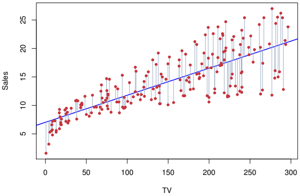
$$f_0 = \mathbb{E}_0[Y | X_1, X_2, ..., X_p] \qquad (1)$$

In linear regression, we assume

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad (2)$$

$$\epsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2) \quad (3)$$

$$\mathbb{E}[y|x] = \beta_0 + \beta_1 x \quad (4)$$



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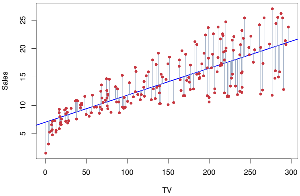


Example of a linear model fit to some data.

We can get coefficient estimates $(\hat{\beta}_0, \hat{\beta}_1)$ by minimizing some objective function, e.g. the residual sum of squares (RSS):

$$\begin{aligned} RSS &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 && (5) \\ &= \sum_{i=1}^{n} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2 && (6) \end{aligned}$$

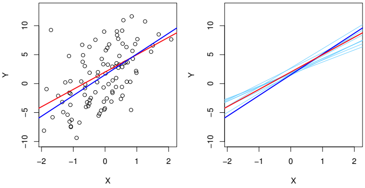
Some calculus shows that the minimizers of the RSS are:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \quad (7)$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \quad (8)$$

where $\bar{y}$ and $\bar{x}$ are the sample averages of y_i and x_i, respectively.

Accuracy of coefficient estimates



True function f_0 and estimate $\hat{f}_n$.

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- How do we evaluate the certainty of $(\hat{\beta}_0, \hat{\beta}_1)$?

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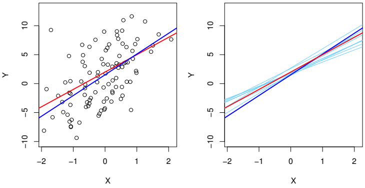

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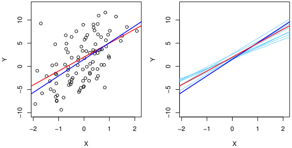
- Different samples will result in different estimates $(\hat{\beta}_0, \hat{\beta}_1)$
- How do we evaluate the certainty of $(\hat{\beta}_0, \hat{\beta}_1)$?
- **Recall**: When estimating mean μ_0 of variable X, we can compute its standard error $\mathrm{SE}(\hat{\mu}_n)$ as

$$\mathrm{SE}(\hat{\mu}_n) = \sqrt{\frac{\sigma_0^2}{n}} \qquad (9)$$

- We can take a similar approach with our coefficients
  - i.e. estimate standard errors

Estimating $\mathrm{SE}(\hat{\beta}_j)$



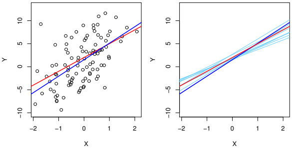
True function f_0 and estimates $\hat{f}_n$.

$$\mathrm{SE}(\hat{\beta}_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x}_n)^2} \right]$$
$$\mathrm{SE}(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \tag{10}$$

where $\sigma^2 = \mathrm{Var}(\epsilon)$.

- Assumes ϵ_i are uncorrelated with common variance σ^2

Estimating $SE(\hat{\beta}_j)$



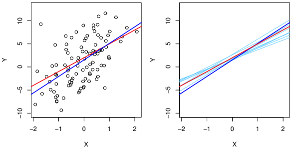
True function f_0 and estimates $\hat{f}_n$.

- While, we don't know σ_0, we can estimate it

$$\hat{SE}(\hat{\beta}_0)^2 = \hat{\sigma}^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x_n})^2} \right]$$
$$\hat{SE}(\hat{\beta}_1)^2 = \frac{\hat{\sigma}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \tag{11}$$

where $\hat{\sigma} = \sqrt{RSS/(n-2)}$.

Estimating $\mathrm{SE}(\hat{\beta}_j)$



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

$$\hat{\mathrm{SE}}(\hat{\beta}_1)^2 = \frac{\hat{\sigma}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \tag{11}$$

where $\hat{\sigma} = \sqrt{RSS/(n-2)}$.
95% CI's can then be calculated:

$$\hat{\beta}_0 \quad \pm \quad t_{\alpha/2} \cdot \hat{\mathrm{SE}}(\hat{\beta}_0) \tag{12}$$

$$\hat{\beta}_1 \quad \pm \quad t_{\alpha/2} \cdot \hat{\mathrm{SE}}(\hat{\beta}_1) \tag{13}$$

Hypothesis testing

When we want to evaluate some kind of relationship, we can test it statistically, e.g.

$$
\begin{aligned}
H_0 &: \text{There is no relationship between } X \text{ and } Y && (14) \\
H_a &: \text{There is a relationship between } X \text{ and } Y && (15)
\end{aligned}
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Note: Hypothesis tests are typically set up such that H_a is the outcome that we care about

- e.g. In non-inferiority tests, H_0 is typically specified such that there **is** a deficiency in the treatment being evaluated.

Hypothesis testing

For linear models, we typically test e.g.

$$H_0 \quad : \quad \beta_1 = 0 \tag{16}$$
$$H_a \quad : \quad \beta_1 \neq 0 \tag{17}$$

- If $\beta_1 = 0$, then our model simplifies to $\mathbb{E}[y|x] = \beta_0$, meaning X is not associated to Y.

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- If $\beta_1 = 0$, then our model simplifies to $\mathbb{E}[y|x] = \beta_0$, meaning X is not associated to Y.
- To be sure $\beta_1 \neq 0$, we want $\hat{\beta}_1$ to be far from 0 and for $\hat{\text{SE}}(\hat{\beta}_1)$
- Will typically calculate a statistic to help us evaluate this
  - e.g. A t-statistic

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- Follows a t-distribution with $n - 2$ degrees of freedom.
- Can be used to calculate a p-value
  - i.e. the probability of observing our statistic (or a larger one) under the null hypothesis
  - If the probability is low enough, then we reject H_0

An applied example

	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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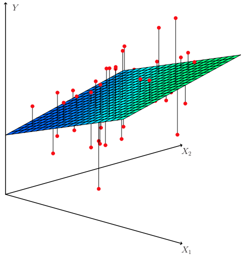
1. If we reject the null hypothesis, can we assume there is a linear relationship?
   - No. A quadratic relationship may be a better fit, for example.
2. If we don't reject the null hypothesis, can we assume there is no relationship between X and Y?
   - No. This test is only powerful against certain monotone alternatives (with enough data). There could be more complex non-linear relationships (or you could need more data).

Multiple linear regression

Extension of linear regression to handle multiple predictors

In multiple linear regression, we assume



$$
\begin{aligned}
Y &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \epsilon \\
\epsilon_i &\overset{iid}{\sim} \mathcal{N}(0, \sigma^2) \\
\mathbb{E}[Y|\mathbf{X}] &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots
\end{aligned}
\tag{21}
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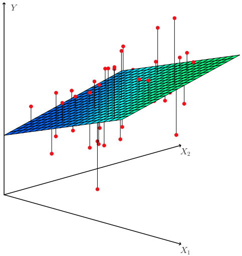

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$$

In matrix notation:

$$\mathbb{E}[Y|\mathbf{X}] = \mathbf{X}\beta \tag{22}$$

where

$$\mathbf{X} = (1, X_1, X_2, ..., X_p) \tag{23}$$

$$\boldsymbol{\beta} = (\beta_0, \beta_1, ..., \beta_p)^\top \tag{24}$$

Questions to consider

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- Is at least one of the variables X_j 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?

Estimating β

Our goal is the same: minimize the RSS

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{25}$$

$$= \sum_{i=1}^{n} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_{i,1} + ... + \hat{\beta}_p x_{i,p}))^2 \tag{26}$$

Can be shown that RSS is miminized with:

$$\boldsymbol{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \tag{27}$$

where the vectors are now matrices, e.g.

$$\mathbf{X} = \begin{bmatrix} 1 & X_{1,1} & \cdots & X_{1,p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n,1} & \cdots & X_{n,p} \end{bmatrix} \tag{28}$$

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Note: only exists when $\mathbf{X}^\top \mathbf{X}$ is invertible (requires $n \geq p$).

Which variables are important?

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

$$F = \frac{(RSS_0 - RSS)/q}{RSS/(n-p-1)} \tag{31}$$

Under the null hypothesis, statistic follows F-distribution.

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Example: If $q = p$, testing if $\beta_j = 0 \ \forall \ j$.

$$RSS_0 = \sum_{i=1}^{n} (y_i - \bar{y})^2 \tag{32}$$

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Some notes:

- The t-statistic associated to the j^{th} predictor is (equivalent to) the square root of the F-statistic for the null hypothesis which sets only $\beta_j = 0$.

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- A low p-value for the j^{th} predictor 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. Ways of accounting for this include e.g.
  - controlling the family-wise error rate (FWER)
  - controlling the false discovery rate (FDR)

Which variables are important?

Example of multiple linear regression output (in R):

```
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
```

How many variables are important?

In selecting a subset of the predictors, we have 2^p choices.

One way to simplify the choice is to define a range of models with an increasing number of variables, then select the best. AKA stepwise regression.

The approach:

1. Construct a sequence of p models with increasing number of variables.
2. Select the best model among them.

How many variables are important?

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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 a model in the range produced is a form of tuning. Will cover this more in Chapter 6.

How many variables are important?

Example output of a stepwise selection method:

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

6 choices are better than $2^6 = 64$.

We can use different objectives to decide on optimal model, e.g. cross-validation, AIC, BIC, etc.

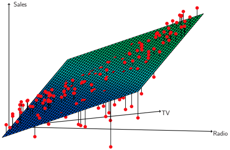
How good is the fit?

To assess fit, we focus on the residuals.

- The RSS always decreases as we add more variables.
- The residual standard error (RSE) corrects this:

$$RSE = \sqrt{\frac{1}{n-p-1} RSS} \tag{33}$$

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



How good is the predictions?

We can get confidence intervals for our predictions:

```
> 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
```

The confidence intervals reflect the uncertainty from $\hat{\beta}$.

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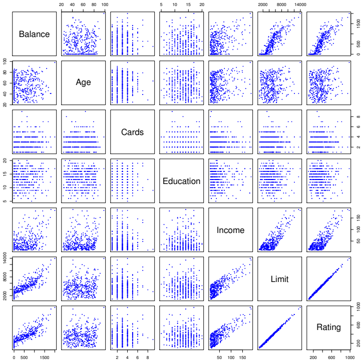
The confidence intervals reflect the uncertainty from $\hat{\beta}$.

```
> 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 from **both** $\hat{\beta}$ and ϵ (i.e. the irreducible error).

Dealing with categorical/qualitative predictors

Example: credit dataset



Example of a linear model fit to some data.

Additionally:

4 qualitative variables

- `gender`: male, female
- `student`: yes, no
- `status`: married, single, divorced
- `ethnicity`: African American, Asian, Caucasian

Dealing with categorical/qualitative predictors

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

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- For every other category, define a new predictor (aka dummy indicator):
  - X_{Asian} is 1 if the person is Asian and 0 otherwise.
  - $X_{Caucasian}$ is 1 if the person is Caucasian and 0 otherwise.

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  - X_{Asian} is 1 if the person is Asian and 0 otherwise.
  - $X_{Caucasian}$ is 1 if the person is Caucasian and 0 otherwise.
- The model will be:

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_{Asian} X_{Asian} + \beta_{Caucasian} X_{Caucasian} + \epsilon \tag{34}$$

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

Dealing with categorical/qualitative predictors

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_{Asian} X_{Asian} + \beta_{Caucasian} X_{Caucasian} + \epsilon \quad (35)$$

- The model fit and predictions are independent of the choice of the baseline category.
- Other ways to encode qualitative predictors produce the same fit $\hat{f}_n$, but the coefficients have different interpretations.
- Hypothesis tests derived from these dummy indicator are affected by the choice.

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- Other ways to encode qualitative predictors produce the same fit $\hat{f}_n$, but the coefficients have different interpretations.
- Hypothesis tests derived from these dummy indicator are affected by the choice.
  - **Solution**: To check whether ethnicity is important, use an F-test for the hypothesis $\beta_{Asian} = \beta_{Caucasian} = 0$.

Recap

So far, we have:

- Defined Multiple Linear Regression
- Discussed how to estimate model parameters
- Discussed how to test the importance of variables
- Described one approach to choose a subset of variables
- Explained how to code dummy indicators

What are some potential issues?

Potential issues in linear regression

- Interactions between predictors
- Non-linear relationships
- Correlation of error terms
- Non-constant variance of error (heteroskedasticity)
- Outliers
- High leverage points
- Collinearity
- Mis-specification

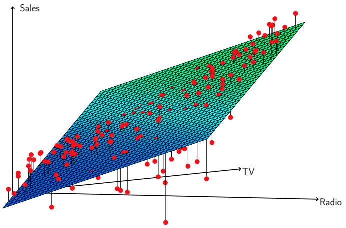
Interactions between predictors

Linear regression has an *additive* assumption, e.g.:

$$sales = \beta_0 + \beta_1 \cdot \mathtt{tv} + \beta_2 \cdot \mathtt{radio} + \epsilon \tag{36}$$

e.g. An increase of \$ 100 dollars in TV ads correlates to a fixed increase in sales, independent 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:

- Include multiplicative variables (aka interaction variables) in the model

$$sales = \beta_0 + \beta_1 \cdot tv + \beta_2 \cdot radio + \beta_3 \cdot (tv \times radio) + \epsilon \quad (37)$$

- Makes the effect of TV ads dependent on the radio ads (and vice versa)
- The *interaction variable* is high when both tv and radio are high

Interactions between predictors

Two ways of including interaction variables (in R):

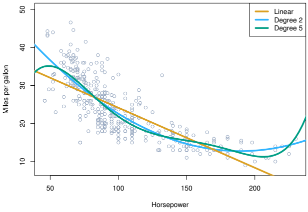
- Create a new variable that is the product of the two
- Specify the interaction in the model formula

```
> 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
```



Scatterplots between X and Y may reveal non-linear relationships

- **Solution**: Include polynomial terms in the model

$$\begin{aligned} MPG = & \beta_0 + \beta_1 \cdot horsepower \\ & + \beta_2 \cdot horsepower^2 \\ & + \beta_3 \cdot horsepower^3 + \ldots + \epsilon \end{aligned} \tag{38}$$

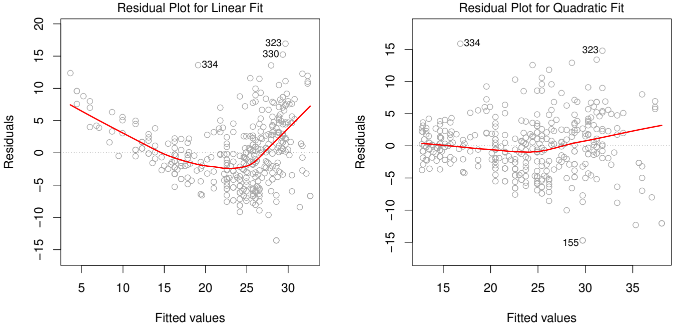
Non-linear relationships

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

Non-linear relationships

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

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:

$$y_i = f(x_i) + \epsilon_i : \epsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2) \tag{39}$$

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When it doesn't hold:

- Invalidates any assertions about Standard Errors, confidence intervals, and hypothesis tests

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

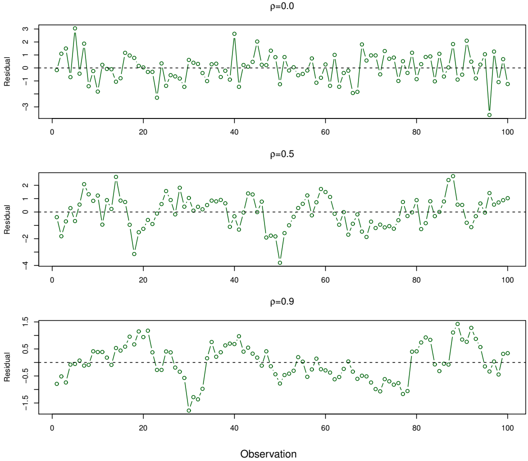
Correlation of error terms

Examples of when this happens:

- *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.
- *Clustered data*: 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

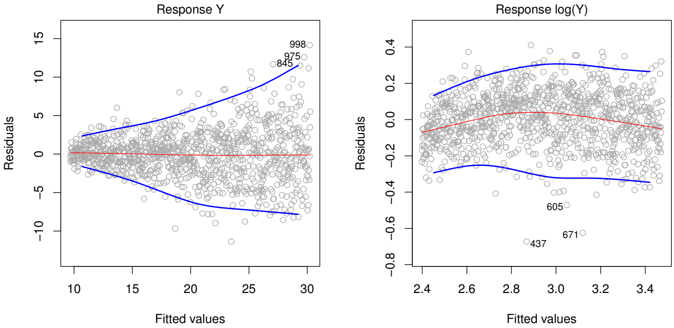
Simulations of time series with increasing correlations on ϵ_i.



Non-constant variance of error (heteroskedasticity)

The variance of the error depends on the input value.

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



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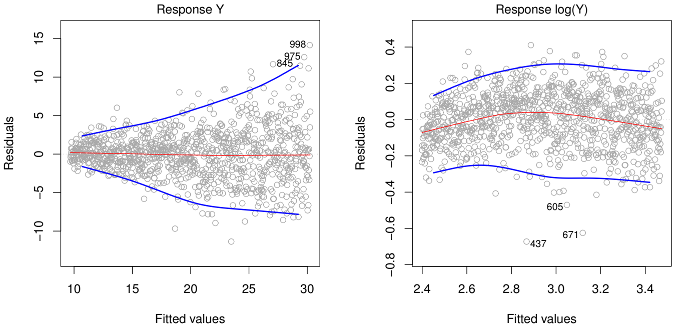

Solution: If the trend in variance is relatively simple, we can transform the response using a logarithm, for example.

References

[1] ISL. Chapters 3.

[2] ESL. Chapters 3.