Day 4: Linear Regression

ME314: Introduction to Data Science and Machine Learning

LSE Methods Summer Programme 2019

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Day 4 Outline

Simple linear regression

- Estimation of the parameters
- Confidence intervals
- Hypothesis testing
- Assessing overall accuracy of the model
- Multiple Linear Regression
- Interpretation
- Model fit

Qualitative predictors

- Qualitative predictors in regression models
- Interactions
- Non-linear effects

Simple linear regression

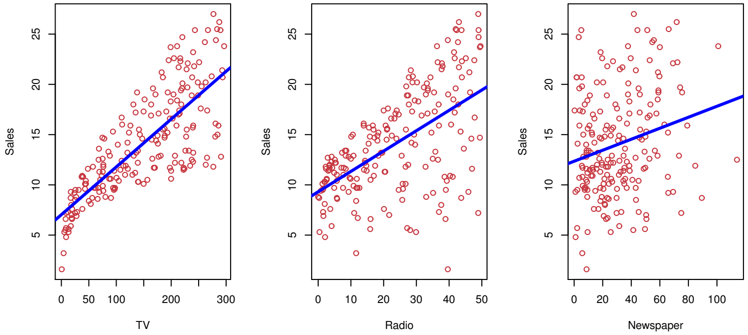
- Linear regression is a simple approach to supervised learning. It assumes that the dependence of Y on $X_1, X_2, \ldots, X_p$ is linear.
- True regression functions are never linear!
- Although it may seem overly simplistic, linear regression is extremely useful both conceptually and practically.

Linear regression for the advertising data

Consider the advertising data. Questions we might ask:

- Is there a relationship between advertising budget and sales?
- How strong is the relationship between advertising budget and sales?
- Which media contribute to sales?
- How accurately can we predict future sales?
- Is the relationship linear?
- Is there synergy among the advertising media?

Advertising data



Simple linear regression using a single predictor X

- We assume a model

$$Y = \beta_0 + \beta_1 X + \epsilon,$$

  where β_0 and β_1 are two unknown constants that represent the intercept and slope, also known as coefficients or parameters, and ϵ is the error term.

- Given some estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ for the model coefficients, we predict future sales using

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x,$$

  where $\hat{y}$ indicates a prediction of Y on the basis of $X = x$. The hat symbol denotes an estimated value.

Estimation of the parameters by least squares

- Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction for Y based on the ith value of X. Then $e_i = y_i - \hat{y}_i$ represents the ith residual.
- We define the residual sum of squares (RSS) as

$$\mathrm{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2,$$

or equivalently as

$$\mathrm{RSS} = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \cdots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2.$$

Estimation of the parameters by least squares

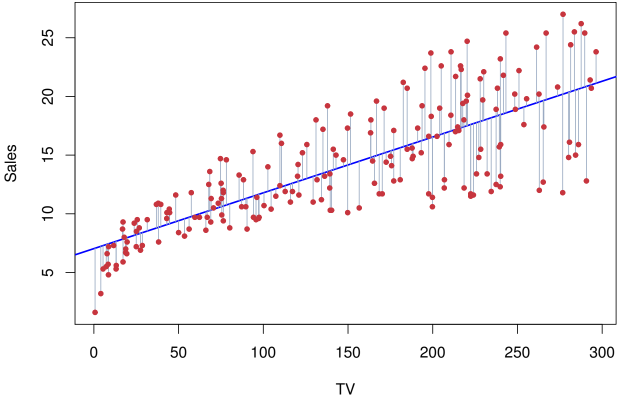
- The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. The minimizing values can be shown to be

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

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x},$$

where $\bar{y} \equiv \frac{1}{n}\sum_{i=1}^{n} y_i$ and $\bar{x} \equiv \frac{1}{n}\sum_{i=1}^{n} x_i$ are the sample means.

Example: advertising data



The least squares fit for the regression of sales on TV. The fit is found by minimizing the sum of squared residuals. In this case a linear fit captures the essence of the relationship, although it is somewhat deficient in the left of the plot.

Assessing the Accuracy of the Coefficient Estimates

- The standard error of an estimator reflects how it varies under repeated sampling. We have

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

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

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

- These standard errors can be used to compute confidence intervals. A 95% confidence interval is defined as a range of values such that with 95% probability, the range will contain the true unknown value of the parameter. It has the form

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

Confidence Intervals

That is, there is approximately a 95% chance that the interval

$$\left[\hat{\beta}_1 - 2 \times \mathrm{SE}(\hat{\beta}_1), \hat{\beta}_1 + 2 \times \mathrm{SE}(\hat{\beta}_1)\right]$$

will contain the true value of β_1 (under a scenario where we got repeated samples like the present sample).

Hypothesis testing

- Standard errors can also be used to perform hypothesis tests on the coefficients. The most common hypothesis test involves testing the null hypothesis of

  H_0: There is no relationship between X and Y versus the alternative hypothesis.

  H_A: There is some relationship between X and Y.

- Mathematically, this corresponds to testing versus

$$H_0 : \beta_1 = 0$$

versus

$$H_A : \beta_1 \neq 0,$$

since if $\beta_1 = 0$ then the model reduces to $Y = \beta_0 + \epsilon$, and X is not associated with Y.

Hypothesis testing

- To test the null hypothesis, we compute a t-statistic, given by

$$t = \frac{\hat{\beta}_1 - 0}{\mathrm{SE}(\hat{\beta}_1)},$$

- This will have a t-distribution with $n - 2$ degrees of freedom, assuming $\beta_1 = 0$.
- Using statistical software, it is easy to compute the probability of observing any value equal to $\mid t \mid$ or larger. We call this probability the p-value.

Assessing the Overall Accuracy of the Model

- We compute the Residual Standard Error

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2},$$

  where the residual sum-of-squares is $RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$.

- R-squared or fraction of variance explained is

$$R^2 = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}}$$

  where TSS $= \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the total sum of squares.

- It can be shown that in this simple linear regression setting that $R^2 = r^2$, where r is the correlation between X and Y:

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}.$$

Results for the advertising data

```
advertising <- read.csv("http://www-bcf.usc.edu/~gareth/ISL/Adve
names(advertising)

## [1] "X..DOCTYPE.html.PUBLIC....W3C..DTD.XHTML.1.0.Transitiona

simple.regression <-
    lm(advertising$sales ~ advertising$TV)

## Error in model.frame.default(formula =
advertising$sales ~ advertising$TV, :  invalid type (NULL)
for variable 'advertising$sales'
```

Results for the advertising data

```
summary(simple.regression)

## Error in summary(simple.regression):  object
'simple.regression' not found
```

Multiple Linear Regression

- Here our model is

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon,$$

- We interpret β_j as the average effect on Y of a one unit increase in X_j, holding all other predictors fixed. In the advertising example, the model becomes

$$\text{sales} = \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \beta_p \times \text{newspaper} + \epsilon.$$

Interpreting regression coefficients

- The ideal scenario is when the predictors are uncorrelated – a balanced design:
  - Each coefficient can be estimated and tested separately.
  - Interpretations such as "a unit change in X_j is associated with a β_j change in Y, while all the other variables stay fixed", are possible.
- Correlations amongst predictors cause problems:
  - The variance of all coefficients tends to increase, sometimes dramatically
  - Interpretations become hazardous – when X_j changes, everything else changes.
- Claims of causality should be avoided for observational data.

The woes of (interpreting) regression coefficients

"Data Analysis and Regression" Mosteller and Tukey 1977

- a regression coefficient β_j estimates the expected change in Y per unit change in X_j, with all other predictors held fixed. But predictors usually change together!
- Example: Y total amount of change in your pocket; $X_1 =$ number of coins; $X_2 =$ number of pennies, nickels and dimes. By itself, regression coefficient of Y on X_2 will be > 0. But how about with X_1 in model?
- $Y =$ number of tackles by a rugby player in a season; W and H are his weight and height. Fitted regression model is $\hat{Y} = \beta_0 + .50W - .10H$. How do we interpret $\hat{\beta}_2 < 0$?

Two quotes by famous Statisticians

- "Essentially, all models are wrong, but some are useful" George Box
- "The only way to find out what will happen when a complex system is disturbed is to disturb the system, not merely to observe it passively" Fred Mosteller and John Tukey, paraphrasing George Box

Estimation and Prediction for Multiple Regression

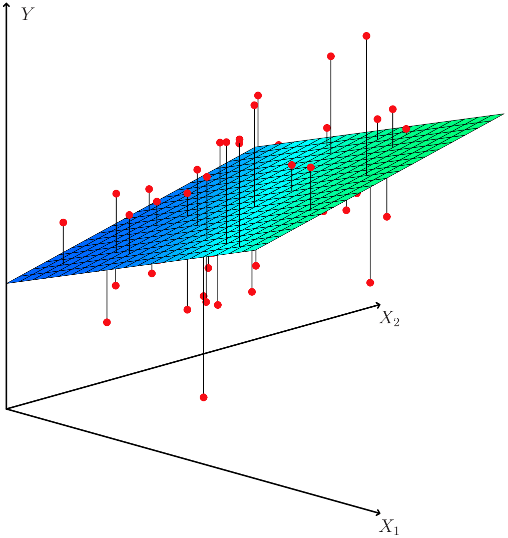
- Given estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$, we can make predictions using the formula

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_p x_p.$$

- We estimate $\beta_0, \beta_1, \ldots, \beta_p$ as the values that minimize the sum of squared residuals

$$\mathrm{RSS} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2.$$

This is done using standard statistical software. The values $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$ that minimize RSS are the multiple least squares regression coefficient estimates.



Y
X_2
X_1

Results for the advertising data

```
multiple.regression <-
    lm(advertising$sales ~ advertising$TV +
           advertising$radio + advertising$newspaper)
```

```
## Error in model.frame.default(formula =
advertising$sales ~ advertising$TV + :  invalid type
(NULL) for variable 'advertising$sales'
```

```
cor(advertising[,-1])
```

```
## <0 x 0 matrix>
```

Results for the advertising data

```
summary(multiple.regression)

## Error in summary(multiple.regression):  object
'multiple.regression' not found
```

Some important questions

1. Is at least one of the predictors $X_1, X_2, \ldots, X_p$ useful in predicting the response?
2. Do all the predictors help to explain Y, or is only a subset of the predictors useful?
3. How well does the model fit the data?
4. Given a set of predictor values, what response value should we predict, and how accurate is our prediction?

Is at least one predictor useful?

- For the first question, we can use the F-statistic

$$F = \frac{(TSS - RSS)/p}{RSS/(n-p-1)} \sim F_{p,n-p-1}$$

Deciding on the important variables

- The most direct approach is called all subsets or best subsets regression: we compute the least squares fit for all possible subsets and then choose between them based on some criterion that balances training error with model size.
- However we often can't examine all possible models, since there are 2^p of them; for example when $p = 40$ there are over a billion models!
- Instead we need an automated approach that searches through a subset of them. We discuss two commonly use approaches next.

Forward selection

- Begin with the null model - a model that contains an intercept but no predictors.
- Fit p simple linear regressions and add to the null model the variable that results in the lowest RSS.
- Add to that model the variable that results in the lowest RSS amongst all two-variable models.
- Continue until some stopping rule is satisfied, for example when all remaining variables have a p-value above some threshold.

Backward selection

- Start with all variables in the model.
- Remove the variable with the largest p-value – that is, the variable that is the least statistically significant.
- The new (p - 1) - variable model is fit, and the variable with the largest p-value is removed.
- Continue until a stopping rule is reached. For instance, we may stop when all remaining variables have a significant p-value defined by some significance threshold.

Model selection - continued

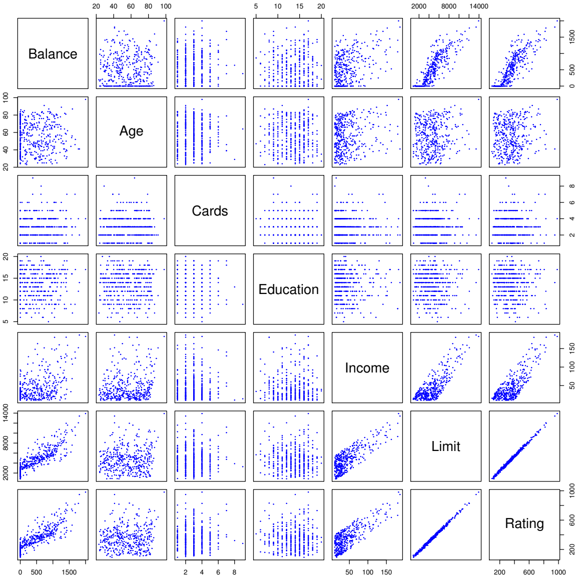
- Later we discuss more systematic criteria for choosing an "optimal" member in the path of models produced by forward or backward stepwise selection.
- These include Mallow's C_p, Akaike information criterion (AIC), Bayesian information criterion (BIC), adjusted R^2 and Cross-validation (CV).

Qualitative predictors

Other Considerations in the Regression Model

Qualitative Predictors

- Some predictors are not quantitative but are qualitative, taking a discrete set of values.
- These are also called categorical predictors or factor variables.
- See for example the scatterplot matrix of the credit card data in the next slide.
- In addition to the 7 quantitative variables shown, there are four qualitative variables: `gender`, `student` (student status), `status` (marital status), and `ethnicity` (Caucasian, African American (AA) or Asian).



Balance
Age
Cards
Education
Income
Limit
Rating

Qualitative Predictors – continued

- Example: investigate differences in credit card balance between males and females, ignoring the other variables. We create a new variable

$$x_i = \begin{cases} 1 & \text{if } i\text{th person is female} \\ 0 & \text{if } i\text{th person is male} \end{cases}$$

- Resulting model:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person is female} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person is male} \end{cases}$$

- Interpretation?

Credit card data

```
credit <- read.csv("http://www-bcf.usc.edu/~gareth/ISL/Credit.cs
names(credit)

## [1] "X..DOCTYPE.html.PUBLIC....W3C..DTD.XHTML.1.0.Transitiona

gender.regression <- lm(credit$Balance ~ credit$Gender)

## Error in model.frame.default(formula = credit$Balance ~
credit$Gender, :  invalid type (NULL) for variable
'credit$Balance'
```

Results for gender model

```
summary(gender.regression)

## Error in summary(gender.regression):  object
'gender.regression' not found
```

Qualitative predictors with more than two levels

- With more than two levels, we create additional dummy variables. For example, for the `ethnicity` variable we create two dummy variables. The first could be

$$x_{i1} = \begin{cases} 1 & \text{if } i\text{th person is Asian} \\ 0 & \text{if } i\text{th person is not Asian,} \end{cases}$$

- and the second could be

$$x_{i2} = \begin{cases} 1 & \text{if } i\text{th person is Caucasian} \\ 0 & \text{if } i\text{th person is not Caucasian.} \end{cases}$$

Qualitative predictors with more than two levels

- Then both of these variables can be used in the regression equation, in order to obtain the model

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person is Asian} \\ \beta_0 + \beta_2 + \epsilon_i & \text{if } i\text{th person is Caucasian} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person is AA} \end{cases}$$

- There will always be one fewer dummy variable than the number of levels. The level with no dummy variable – African American in this example – is known as the baseline.

Credit card data

```
ethnicity.regression <- lm(credit$Balance ~ credit$Ethnicity)

## Error in model.frame.default(formula = credit$Balance ~
credit$Ethnicity, :  invalid type (NULL) for variable
'credit$Balance'

summary(ethnicity.regression)

## Error in summary(ethnicity.regression):  object
'ethnicity.regression' not found
```

Extensions of the Linear Model

Removing the additive assumption: interactions and nonlinearity
Interactions:

- In our previous analysis of the `Advertising` data, we assumed that the effect on `sales` of increasing one advertising medium is independent of the amount spent on the other media.
- For example, the linear model

$$\widehat{sales} = \beta_0 + \beta_1 \times TV + \beta_2 \times radio + \beta_3 \times newspaper$$

  states that the average effect on `sales` of a one-unit increase in `TV` is always β_1, regardless of the amount spent on `radio`.

Interactions – continued

- But suppose that spending money on radio advertising actually increases the effectiveness of TV advertising, so that the slope term for TV should increase as `radio` increases.
- In this situation, given a fixed budget of \$100,000, spending half on `radio` and half on `TV` may increase sales more than allocating the entire amount to either `TV` or to `radio`.
- In marketing, this is known as a synergy effect, and in statistics it is referred to as an interaction effect.

Modelling interactions – Advertising data

Model takes the form

$$sales = \beta_0 + \beta_1 \times TV + \beta_2 \times radio + \beta_3 \times (radio \times TV) + \epsilon$$

$$= \beta_0 + (\beta_1 + \beta_3 \times radio) \times TV + \beta_2 \times radio + \epsilon$$

Modelling interactions – Advertising data

```
interaction.model <- lm(advertising$sales ~ advertising$TV*adver

## Error in model.frame.default(formula =
advertising$sales ~ advertising$TV * :  invalid type
(NULL) for variable 'advertising$sales'

summary(interaction.model)

## Error in summary(interaction.model):  object
'interaction.model' not found
```

Interpretation

- The results in this estimation suggests that interactions are important (statistically at least – it may be unimportant substantively)
- The p-value for the interaction term $TV \times radio$ is extremely low, indicating that there is strong evidence for $H_A : \beta_3 \neq 0$.
- The R^2 for the interaction model is 96.8%, compared to only 89.7% for the model that predicts *sales* using *TV* and *radio* without an interaction term.

Interpretation – continued

- This means that (96.8 - 89.7)/(100 - 89.7) = 69% of the variability in sales that remains after fitting the additive model has been explained by the interaction term.
- The coefficient estimates in the table suggest that an increase in TV advertising of \$1,000 is associated with increased sales of

$$(\hat{\beta}_1 + \hat{\beta}_3 \times \mathit{radio}) \times 1000 = 19 + 1.1 \times \mathit{radio\ units}.$$

- An increase in radio advertising of \$1,000 will be associated with an increase in sales of

$$(\hat{\beta}_2 + \hat{\beta}_3 \times TV) \times 1000 = 29 + 1.1 \times TV\ \mathit{units}.$$

Hierarchy

- Sometimes it is the case that an interaction term has a very small p-value, but the associated main effects (in this case, *TV* and *radio*) do not.
- The hierarchy principle: If we include an interaction in a model, we should also include the main effects, even if the p-values associated with their coefficients are not significant.

Hierarchy

- The rationale for this principle is that interactions are hard to interpret in a model without main effects – their meaning is changed.
- Specifically, the interaction terms also contain main effects, if the model has no main effect terms.

Interactions between qualitative and quantitative variables

- Consider the *Credit* dataset, and suppose that we wish to predict *balance* using *income* (quantitative) and *student* (qualitative).
- Without an interaction term, the model takes the form

$$\textit{balance}_i \approx \beta_0 + \beta_1 \times \textit{income}_i + \begin{cases} \beta_2 & \text{if } i\text{th person is a student} \\ 0 & \text{if } i\text{th person is not a student} \end{cases}$$

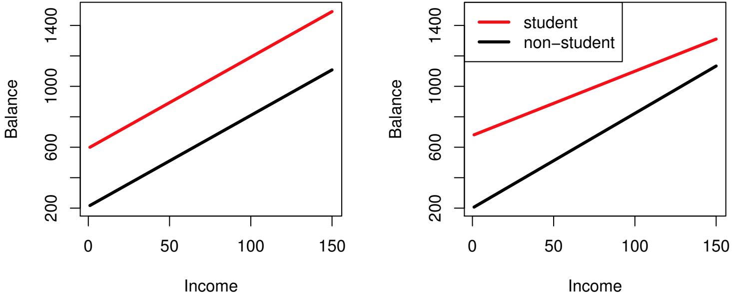
$$= \beta_1 \times \textit{income}_i + \begin{cases} \beta_0 + \beta_2 & \text{if } i\text{th person is a student} \\ \beta_0 & \text{if } i\text{th person is not a student} \end{cases}$$

- With interactions, it takes the form

$$balance_i \approx \beta_0 + \beta_1 \times income_i + \begin{cases} \beta_2 + \beta_3 \times income_i & \text{if } i\text{th person is a student} \\ 0 & \text{if } i\text{th person is not a student} \end{cases}$$

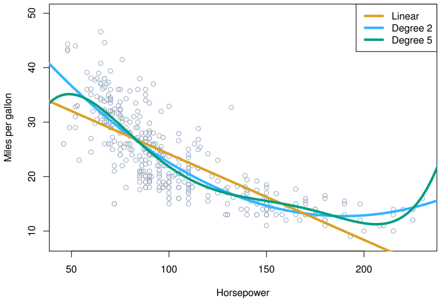
$$= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times income_i & \text{if } i\text{th person is a student} \\ \beta_0 + \beta_1 \times income_i & \text{if } i\text{th person is not a student} \end{cases}$$

Credit data



- For the *Credit* data, the least squares lines are shown for prediction of balance from income for students and non-students.
- Left: no interaction between income and student.
- Right: with an interaction term between income and student.

Non-linear effects of predictors



- Polynomial regression on *Auto* data
- The figure suggests that

$$mpg = \beta_0 + \beta_1 \times horsepower + \beta_2 \times horsepower^2 + \epsilon$$

may provide a better fit.

```r
library(ISLR)

## Error in library(ISLR): there is no package called
'ISLR'

auto.model <- lm(Auto$mpg ~ Auto$horsepower + I(Auto$horsepower^

## Error in eval(predvars, data, env):  object 'Auto' not
found

summary(auto.model)

## Error in summary(auto.model):  object 'auto.model' not
found
```

What we did not cover

- Correlation of the error-terms.
- Non-constant variance of error terms.
- Outliers.
- High leverage points.
- Collinearity.

See text Section 3.3.3

Generalizations of the Linear Model

In much of the rest of this course, we discuss methods that expand the scope of linear models and how they are fit:

- Classification problems: logistic regression, support vector machines
- Non-linearity: kernel smoothing, splines and generalized additive models; nearest neighbor methods.
- Interactions: Tree-based methods, bagging, random forests and boosting (these also capture non-linearities)
- Regularized fitting: Ridge regression and lasso