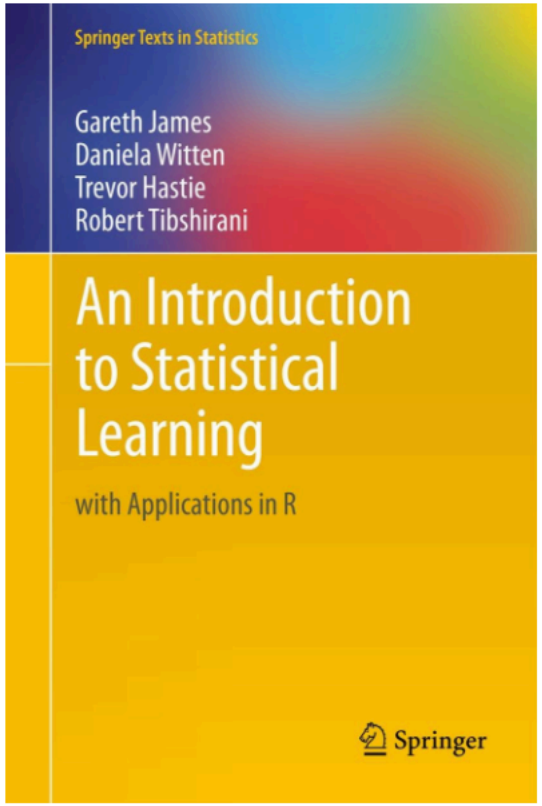

Textbook:

An Introduction to Statistical Learning

Lecture Slides:

Stanford Stats 202: Data Mining and Analysis

Spring 17’ ESC Statistical Data Analysis

REFERENCE

Reading:

An Introduction to Statistical Learning

chapter 3.1 Simple Linear Regression
chapter 3.2 Multiple Linear Regression
chapter 3.3.1 Qualitative Predictors
chapter 3.3.2 Extensions of the Linear Model

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Simple Linear Regression

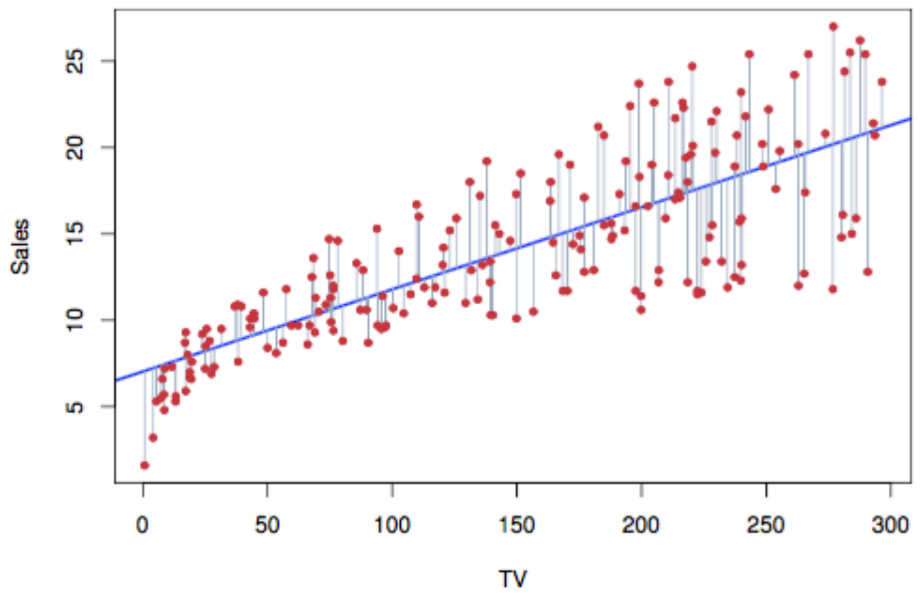


Figure 3.1

- We assume a model using two parameters or coefficients β_0 and β_1 where β_0 represents the intercept and β_1 represents the slope

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

- We assume error ϵ as

$$\epsilon_i \sim iid\ N(0, \sigma^2)$$

- Given some estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, we predict Y using

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

Estimates $\hat{\beta}_0$ and $\hat{\beta}_1$: Least Square Method

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

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

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

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

Accuracy of $\hat{\beta}_0$ and $\hat{\beta}_1$

- Standard error of an estimator can be obtained as

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

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

- Then 95% confidence intervals are

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

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

Hypothesis Test

- An important question: Does a relationship between Y and X exist?
- We can perform hypothesis tests on the coefficients

$$\begin{cases} H_0 : \text{There is no relationship between } X \text{ and } Y \\ H_1 : \text{There is some relationship between } X \text{ and } Y \end{cases}$$

- This can be expressed as

$$\begin{cases} H_0 : \beta_1 = 0 \\ H_1 : \beta_1 \neq 0 \end{cases}$$

- Under H_0, the *t-statistic* can be defined as

$$t = \frac{\hat{\beta}_1}{\sqrt{\sigma^2 / \sum (x_i - \bar{x})^2}} \sim t(n-2)$$

	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

- 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.

Interpretation of Simple Linear Regression

- $\hat{\beta}_0$: Intercept of the regression function

  that is, $E(Y|X = 0)$

- $\hat{\beta}_1$: Slope of the regression function

$$\hat{\beta}_1 = \frac{\partial E(Y \mid X = x)}{\partial x}$$

  that is, the increment of $E(Y|X = x)$ when X increases 1 unit from x

Multiple Linear Regression

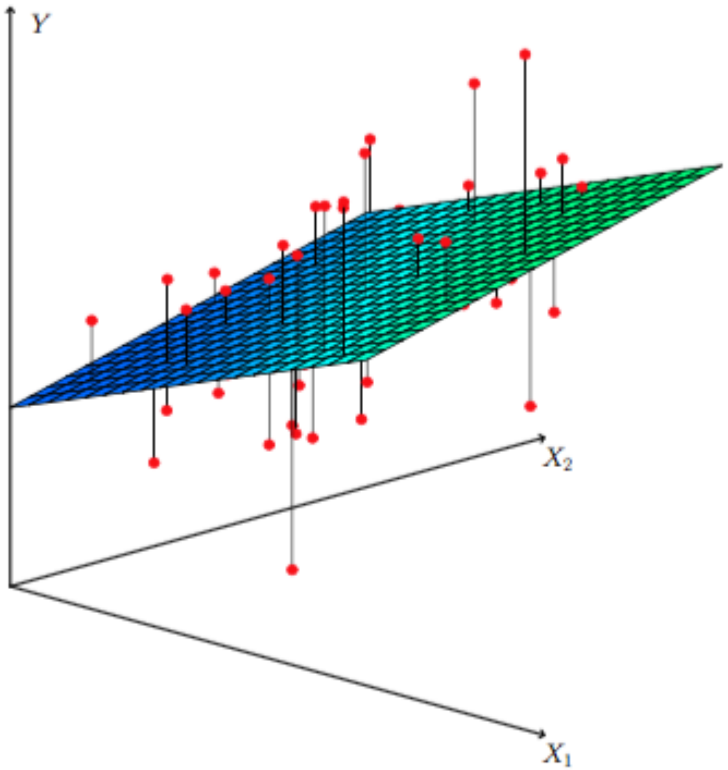


Figure 3.4

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

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

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.

The Estimates $\widehat{\beta}$

- Our goal is to minimize the RSS (training error):

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

- This is minimized by the vector $\hat{\beta}$ (next page):

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

- This only exists when $X^T X$ is invertible. This requires $n \geq p$.

- Same as simple linear regression; we estimate coefficients by minimizing the *RSS*

$$\text{Arg Min RSS} = \sum_{i=1}^{n}(y_i - \hat{y})^2 = (Y - X\beta)^T(Y - X\beta)$$

- Differentiate by β and make it 0 to minimize,

$$\frac{\partial\, RSS}{\partial \beta} = -2X^TY + 2X^TX\beta = 0$$

thus,

$$\hat{\beta} = (X^TX)^{-1}X^TY$$

Testing a Group of Variables

- F-test:

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

RSS_0 is the residual sum of squares for the model in H_0.

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

- Special case: $q = p$. Test whether any of the predictors are related to Y.
- Special case: $q = 1$, exclude a single variable. Test whether this variable is related to Y after linearly correcting for all other variables. Equivalent to t-test in R output.

Interpretation of Multiple Linear Regression

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \cdots + \hat{\beta}_p X_p$$

$\hat{\beta}_j$ represents;

1. $\hat{\beta}_j = \frac{\partial E(Y|X)}{\partial X_j}$: the change of $E(Y)$ per unit increase in X_j while X_k $(k = 0, 1, 2, \ldots p\ , k \neq j)$'s held constant.
2. the additional contribution of X_j on Y, after X_j and Y has been adjusted for X_k $(k = 0, 1, 2, \ldots p\ , k \neq j)$

How many variables are important?

- When choosing a subset of the predictors, we have 2^p choices. We cannot test every possible subset!

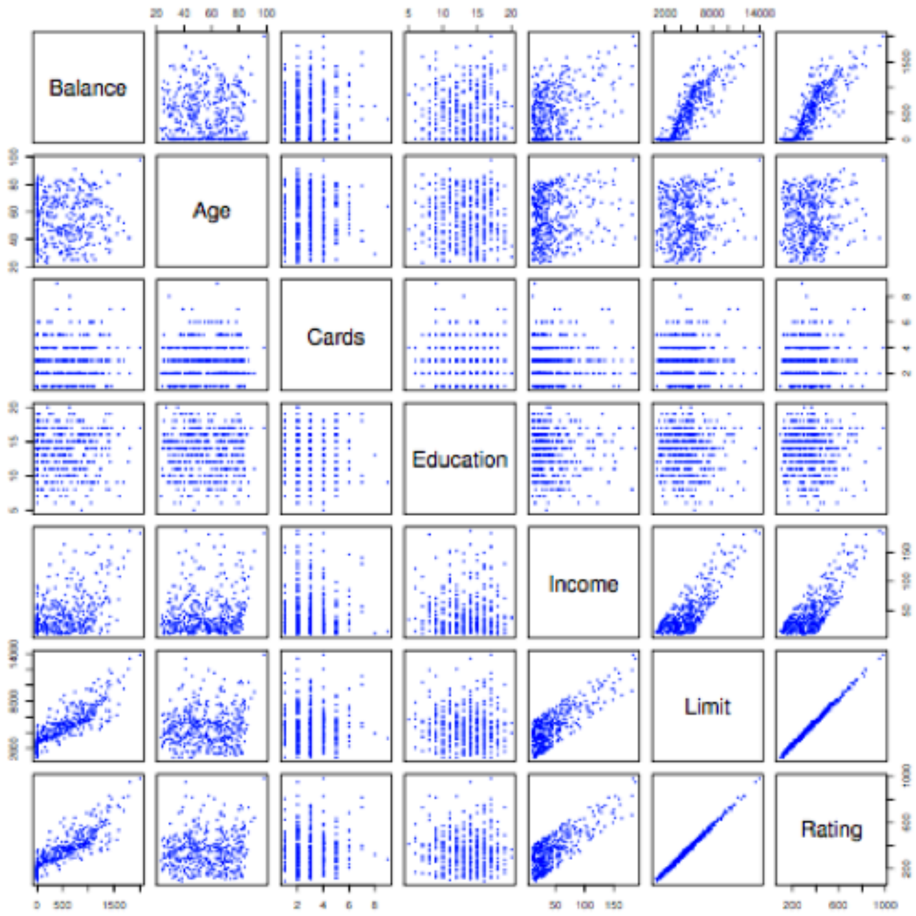
- Instead we will use a **stepwise approach:**
  - Construct a sequence of p models with increasing number of variables.
  - Select the best model among them.

Three Variants of Stepwise Selection

- **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 t-test 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 the variable.

Categorical or Qualitative Predictors

Example: Credit Dataset



- There are 4 qualitative variables:
  - `gender`: male, female
  - `student`: student or not
  - `status`: married, single, divorced
  - `ethnicity`: African, American, Asian, Caucasian

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

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

- $\beta_{married}$ is the relative effect on balance for being married compared to the baseline category.

- 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 $\beta_{married} = \beta_{divorced} = 0$. This does not depend on the coding of the baseline category.

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.

Goodness of the Fit

- To assess the fir, we focus on the residuals.
  - $R^2 = corr(Y, \hat{Y})$, 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.

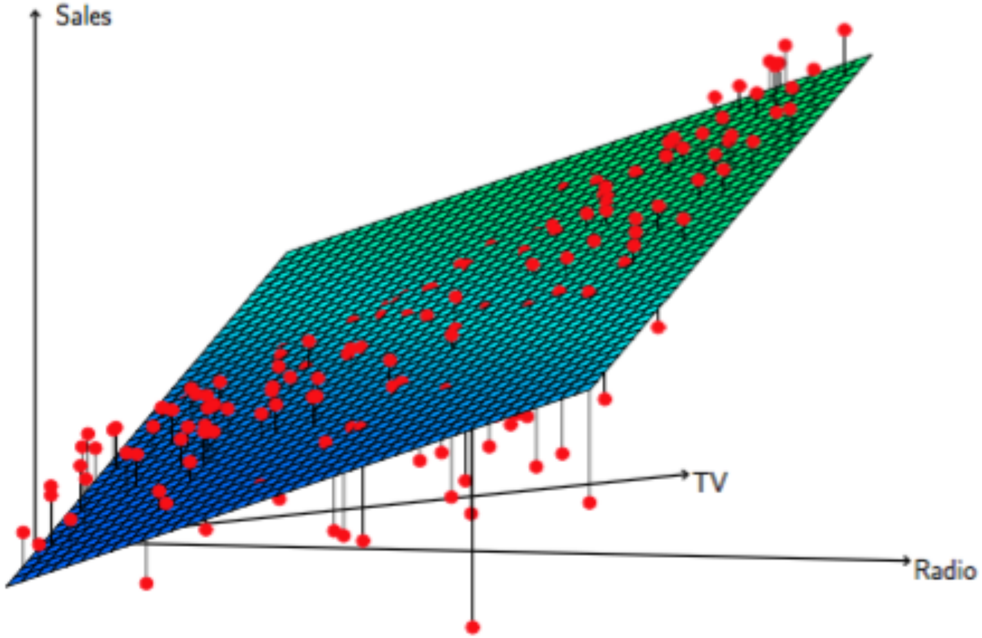
Interactions between Predictors

- 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 sales, regardless of how much you spend on radio ads.

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



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

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

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

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
```

Hierarchy

- Sometimes it is the case that an interaction term has a very small p-value, but the associated main effects 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.
- With significant interaction term, it does not matter whether main effect coefficient is 0 or not. Interaction terms are hard to interpret in a model without main effect - their meaning is changed.
- The interaction terms also contain main effects, if the model has no main effect terms.