SDU Summer School

Deep Learning

Summer 2022

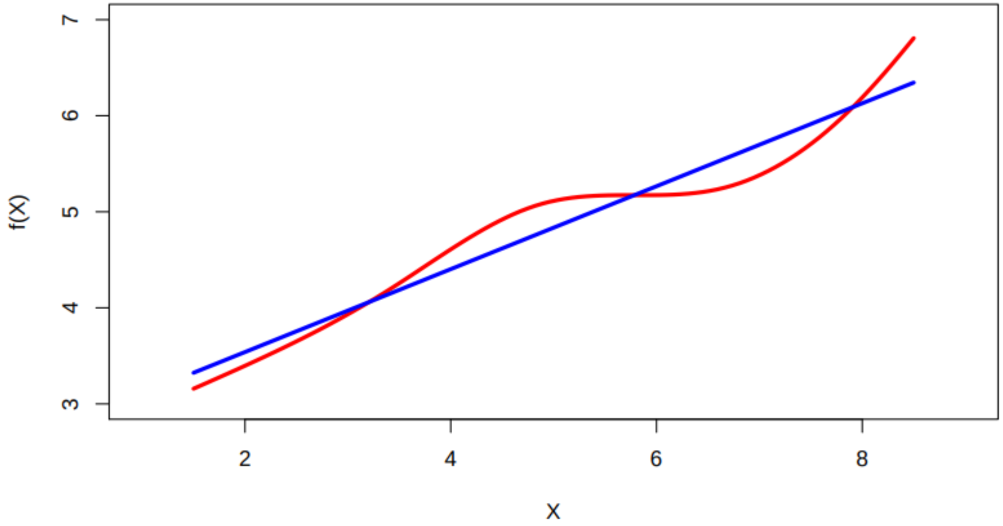
Welcome to the Summer School

Machine Learning Basics

- Simple Linear Regression
- Interpretation
- Multiple Linear Regression

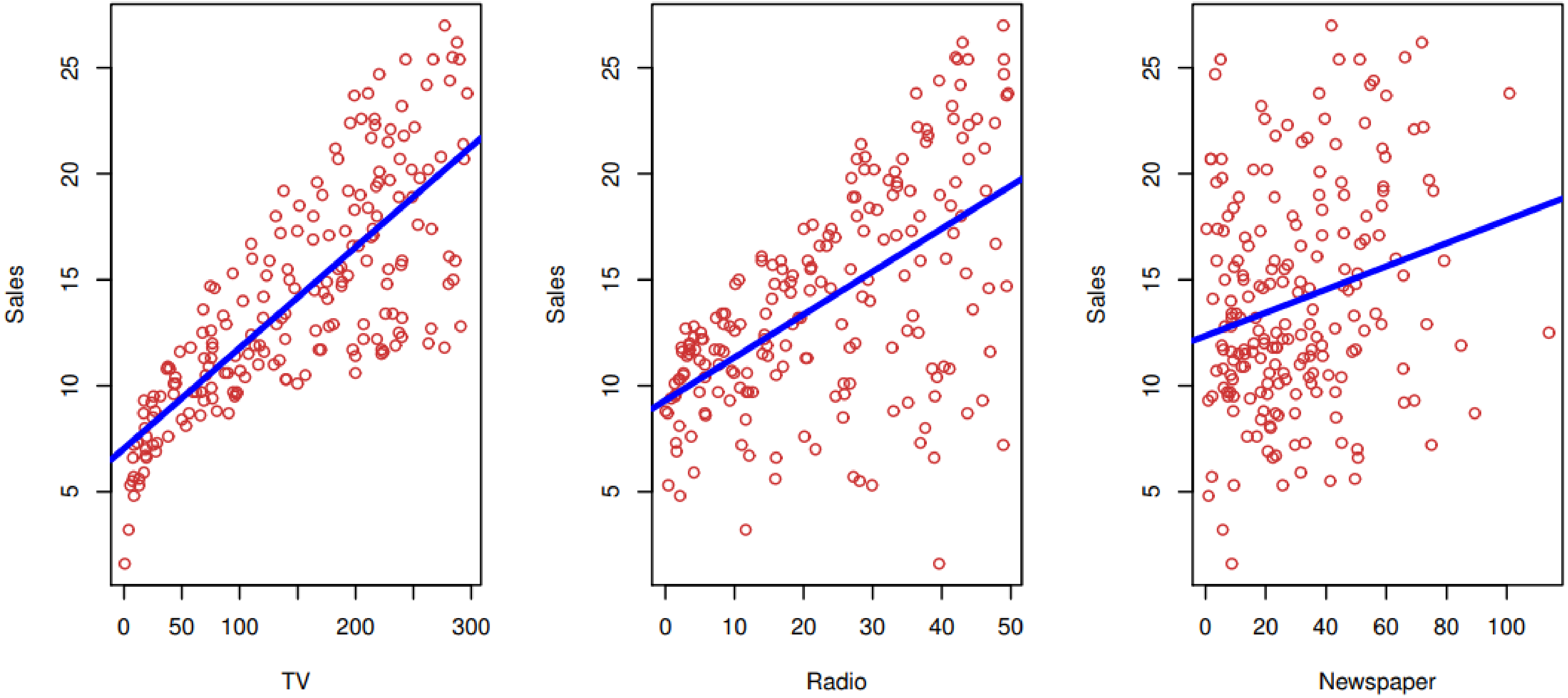
Linear Regression

- 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.

Example: Advertising data



- The Advertising data set consists of the sales of that product in 200 different markets, along with advertising budgets for the product in each of those markets for three different media: TV, radio, and newspaper.

Example: 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?

Simple Linear Regression.

- 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 $\hat{\beta}_1$model coefficients, we **predict** future sales using

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

Estimation of the Parameters by Least Squares

- Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction of Y for the ith observation.
- Then the **residual** is defined as

$$e_i = y_i - \hat{y}_i$$

- We define the **residual sum of squares** as

$$\mathrm{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2 =$$
$$\left(y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1\right)^2 + \left(y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2\right)^2 + \cdots + \left(y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n\right)^2$$

- Our task is to find the $\hat{\beta}_0$ and $\hat{\beta}_1$ minimizing the RSS.

Estimation of the Parameters by Least Squares

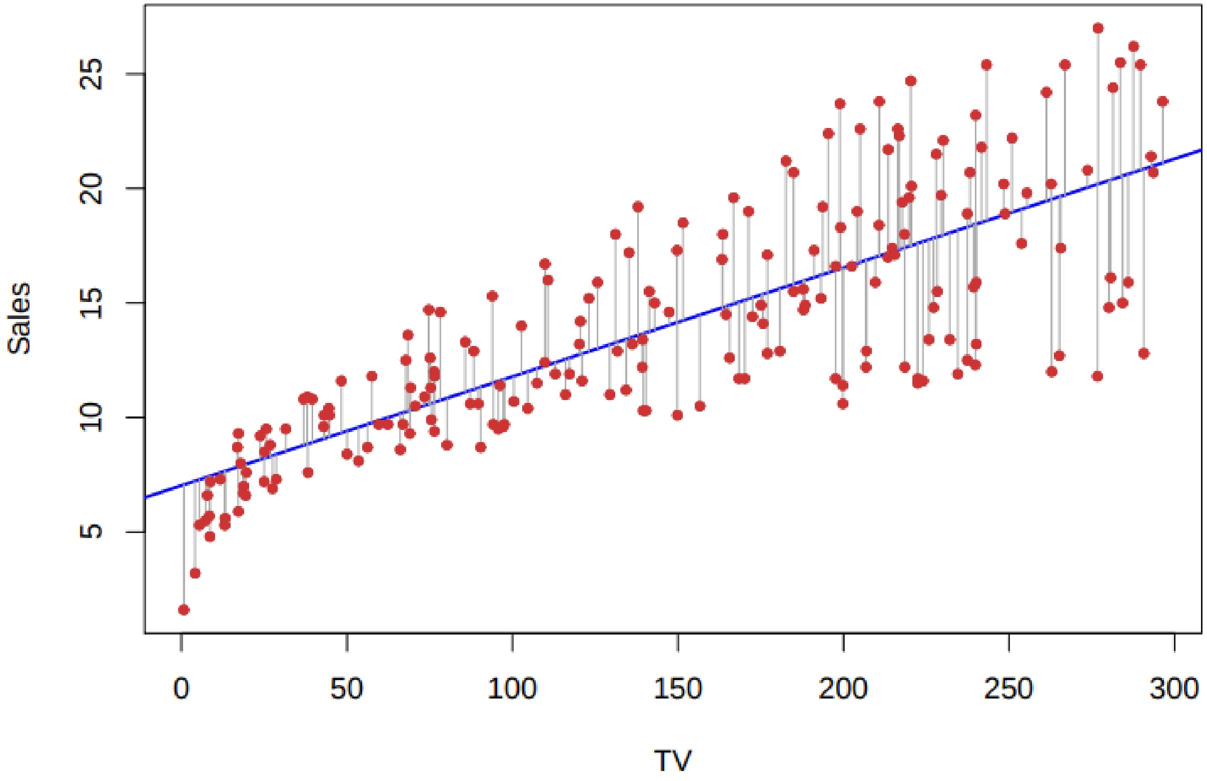
- With simple derivation of the RSS formula, we can show that

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

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

- with the sample means $\bar{y} = \frac{1}{2}\sum_{i=1}^{n} y_i$ and $\bar{x} = \frac{1}{2}\sum_{i=1}^{n} x_i$

Example: Advertising data



- The least squares fit for the regression of sales onto TV.
- In this case a linear fit captures the essence of the relationship, although it is somewhat deficient in the left of the plot.

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Assessing the Accuracy of the Coefficient Estimates

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

- For our example, we have:

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

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

Confidence Intervals

- 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

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

- In other words: there is approximately a 95% chance that the interval

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

will contain the true value of $\hat{\beta}_1$.

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:

$\boldsymbol{H_0}$**:** There is no relationship between X and Y

$$H_0: \beta_1 = 0$$

versus the alternative hypothesis

$\boldsymbol{H_A}$**:** There is some relationship between X and Y

$$H_0: \beta_1 \neq 0$$

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 $|t|$ or larger. We call this probability the **p-value**.

Assessing the Overall Accuracy

- We can compute the **Residual Sum of Squares** (RSS)

$$\mathrm{RSS} = \sum\nolimits_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- With that, we can define the **Residual Standard Error** (RSE)

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}}$$

Assessing the Overall Accuracy

- To assess how much of the variance is explained, we use the **R-squared** measure

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

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

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

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

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Multiple Linear Regression

- We can include several features or predictors into our model

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

- 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

$$\text{sales} = \beta_0 + \beta_1 \cdot \text{TV} + \beta_2 \cdot \text{radio} + \beta_3 \cdot \text{newspaper} + \epsilon$$

In Matrix Form

- We can formulate the entire linear regression also in Matrixform

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{b} + \boldsymbol{e}$$

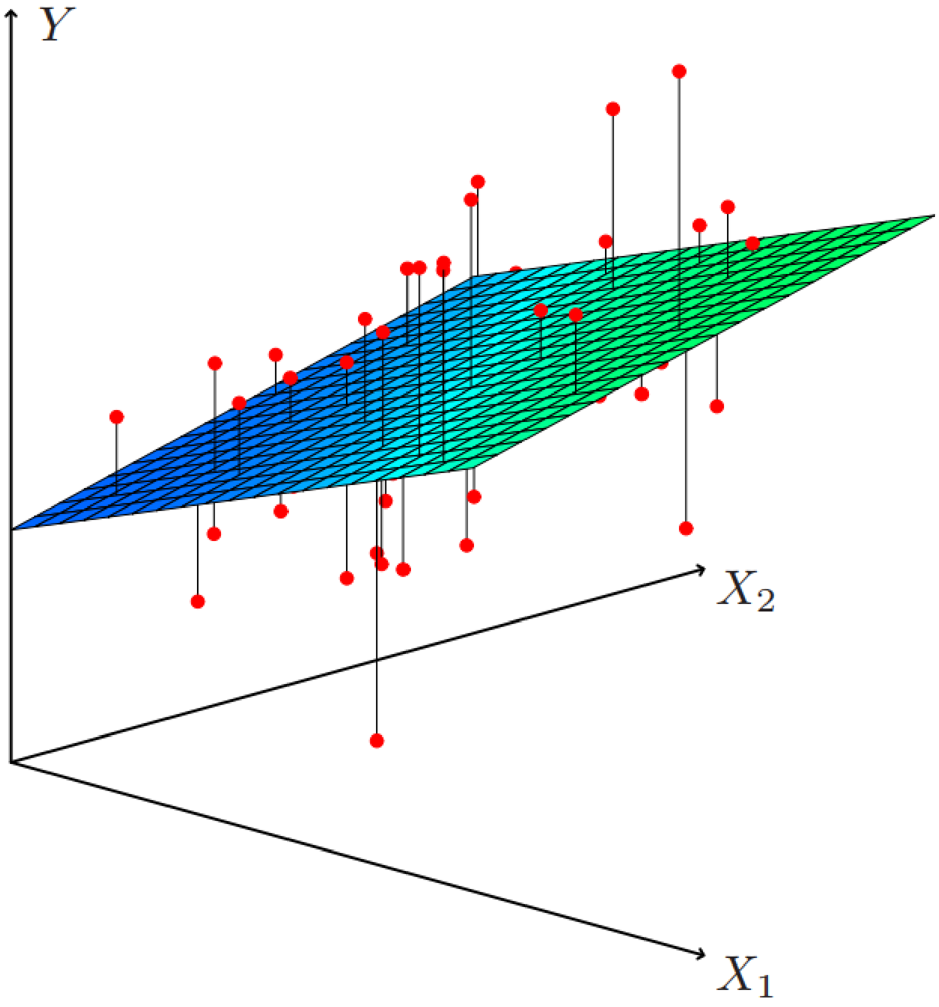
- $\boldsymbol{y} = (y_1, \dots, y_n) \in \mathbb{R}^n$ is the $n \times 1$ response vector
- $\boldsymbol{X} = [1_n, \boldsymbol{X}'] \in \mathbb{R}^{n\times(p+1)}$ is the $n \times (p+1)$ design matrix
  - 1_n is an $n \times 1$ vector of ones
  - $\boldsymbol{X}' = \left[\boldsymbol{X_1}, \boldsymbol{X_2}, \dots, \boldsymbol{X_p}\right] \in \mathbb{R}^{n\times p}$ the $n \times p$ predictor Matrix
- $b = \left(\beta_0, \beta_1, \dots, \beta_p\right) \in \mathbb{R}^{p+1}$ is regression coefficient vector
- $e = (e_1, e_2, \dots, e_3) \in \mathbb{R}^n$ is the $n \times 1$ error vector

Example

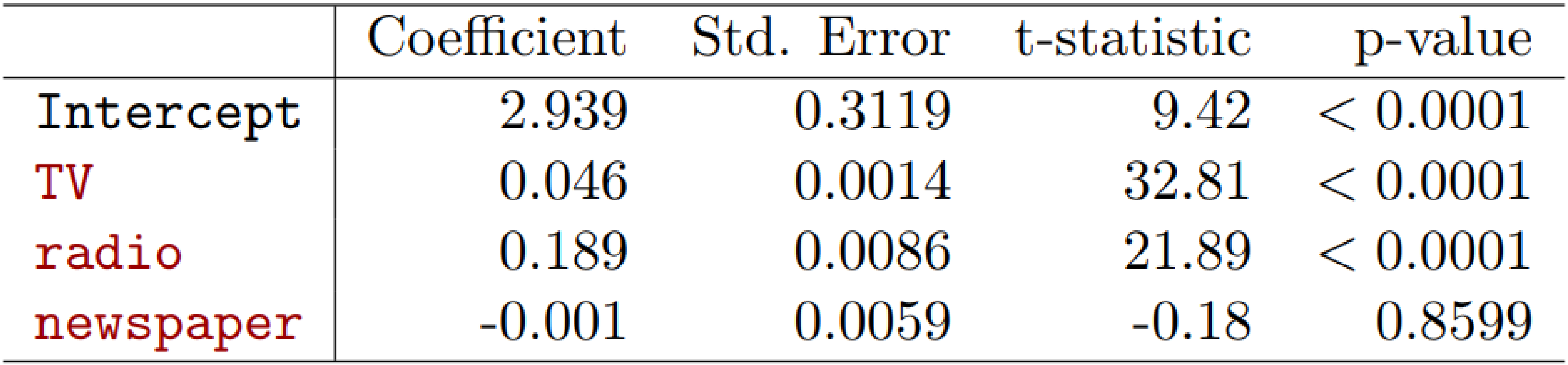
#	TV	Radio	News	Sales
1	230.1	37.8	69.2	**22.1**
2	44.5	39.3	45.1	**10.4**
3	17.2	45.9	69.3	**9.3**
4	151.5	41.3	58.5	**18.5**
5	180.8	10.8	58.4	**12.9**

$$\begin{pmatrix} 22.1 \\ 10.4 \\ 9.3 \\ 18.5 \\ 12.9 \end{pmatrix} = \begin{pmatrix} 1 & 230.1 & 37.8 & 69.2 \\ 1 & 44.5 & 39.3 & 45.1 \\ 1 & 17.2 & 45.9 & 69.3 \\ 1 & 151.5 & 41.3 & 58.5 \\ 1 & 180.8 & 10.8 & 58.4 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} + \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \end{pmatrix}$$

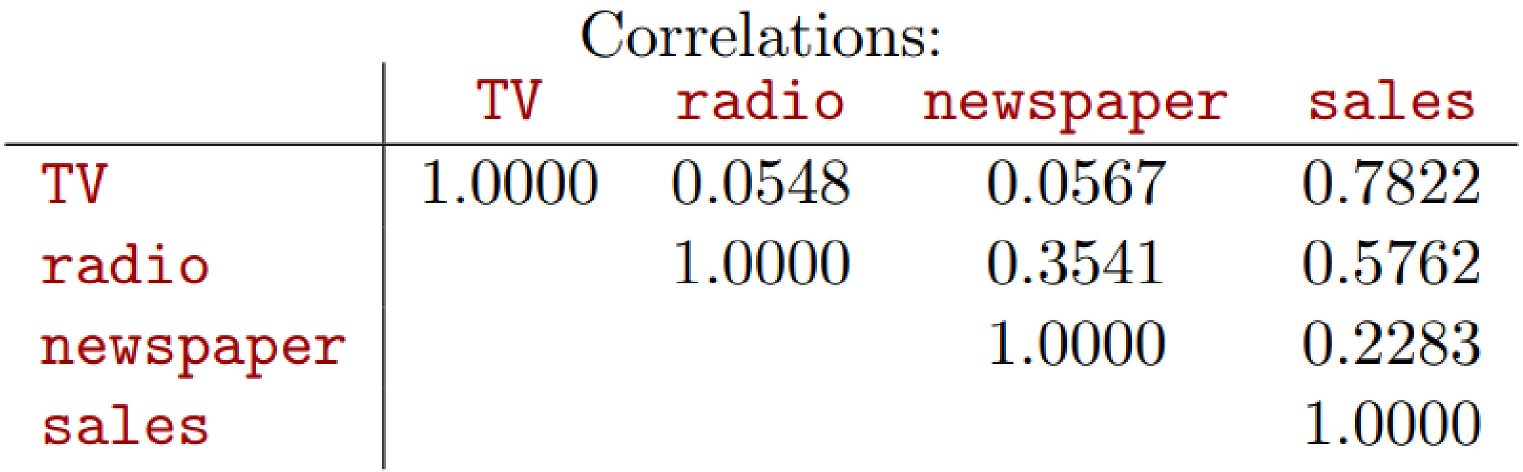
Linear Regression



Results for advertising data



	Coefficient	Std. Error	t-statistic	p-value
Intercept	2.939	0.3119	9.42	< 0.0001
TV	0.046	0.0014	32.81	< 0.0001
radio	0.189	0.0086	21.89	< 0.0001
newspaper	-0.001	0.0059	-0.18	0.8599



Correlations:

	TV	radio	newspaper	sales
TV	1.0000	0.0548	0.0567	0.7822
radio		1.0000	0.3541	0.5762
newspaper			1.0000	0.2283
sales				1.0000

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 = # of coins; X_2 = # 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 football player in a season; W and H are his weight and height. Fitted regression model is $\hat{Y} = b_0 + 0.5 \cdot W - 0.1 \cdot H$. How do we interpret $\beta_2 < 0$?

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

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

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

- It’s similar to a T statistic from a T-Test; The T-test will tell you if a single variable is statistically significant and an F-test will tell you if a group of variables are jointly significant.

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 they 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, like **forward** or **backward** selection.

Generalizations

There exist many different extensions and generalizations to the simple linear regression model:

- **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