Machine Learning and Data Analytics
ME 5013- Fall 2019

Lecture 03

Review:

- Simple Linear Regression

The University of Texas at San Antonio™

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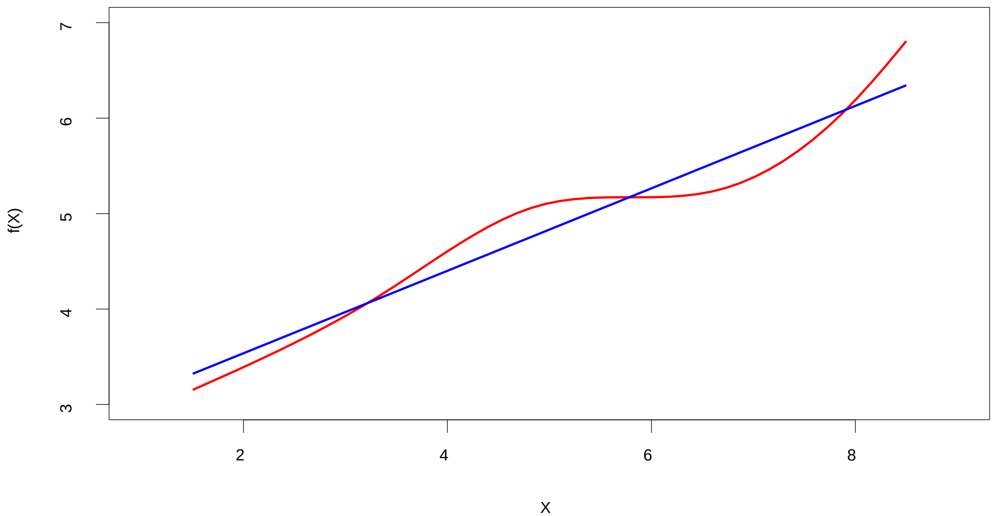
Disclosure: Slides are adopted from Drs. Hastie and Tibshirani on "Statistical Learning" at Stanford university

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.

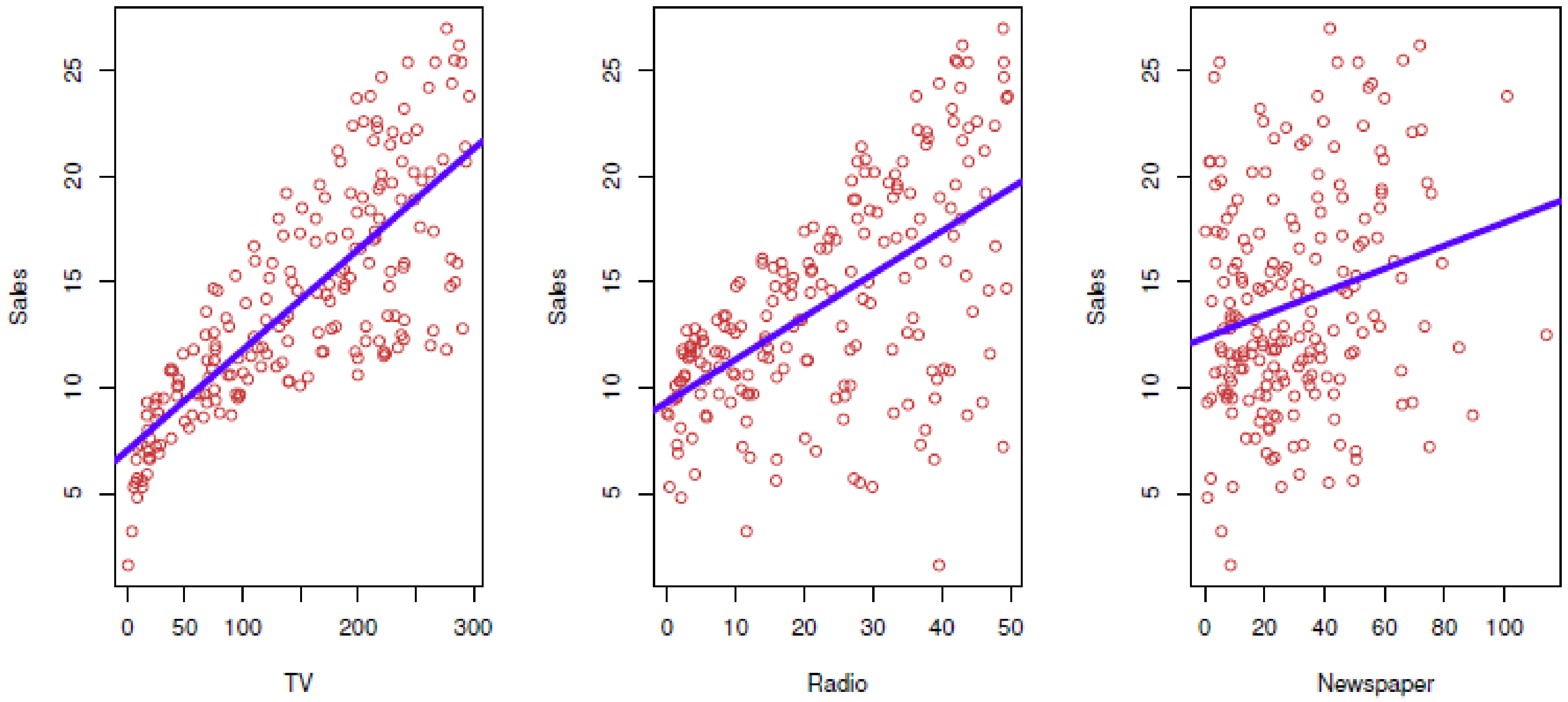
Linear regression for the advertising data

Consider the advertising data shown on the next slide.

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

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

"output" variable
"target" variable
"response" variable

"input" variable
Feature
"Explanatory" variable

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 $\widehat{\beta}_0$ and $\widehat{\beta}_1$ for the model coefficients, we predict future sales using

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

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*

x_i or $x^{(i)}$

- We define the *residual sum of squares* (RSS) as

$$RSS = e_1^2 + e_2^2 + \cdots + e_n^2$$

Cost function

or equivalently as

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

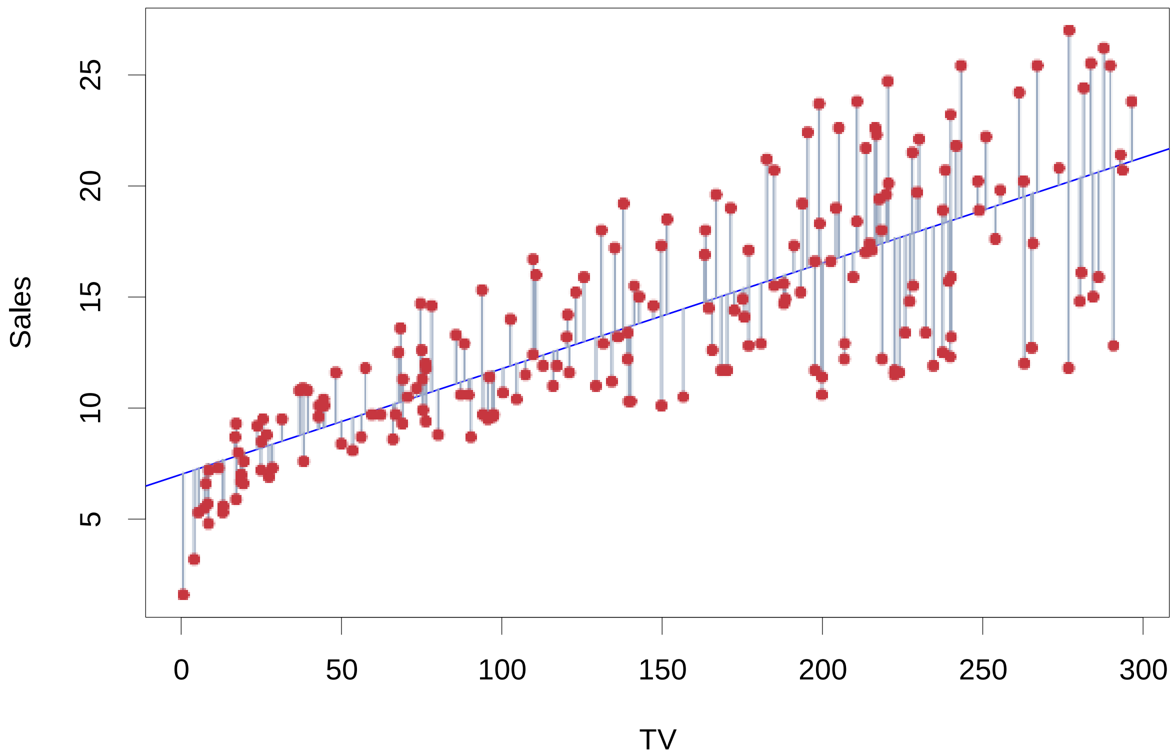
- The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. The minimizing values can be shown to be

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

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

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

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.

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

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

where $\sigma^2 = Var(E)$

- 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

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

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

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

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

For the advertising data, the 95% confidence interval for β_1 is [0.042, 0.053]

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

$$H_0 : \beta_1 = 0$$

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 — continued

- 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*.

Results for the advertising data

	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

- 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:

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

Advertising data results

Quantity	Value
Residual Standard Error	3.26
R^2	0.612
F-statistic	312.1