CS 451/686-02 Data Mining Linear Regression Part A

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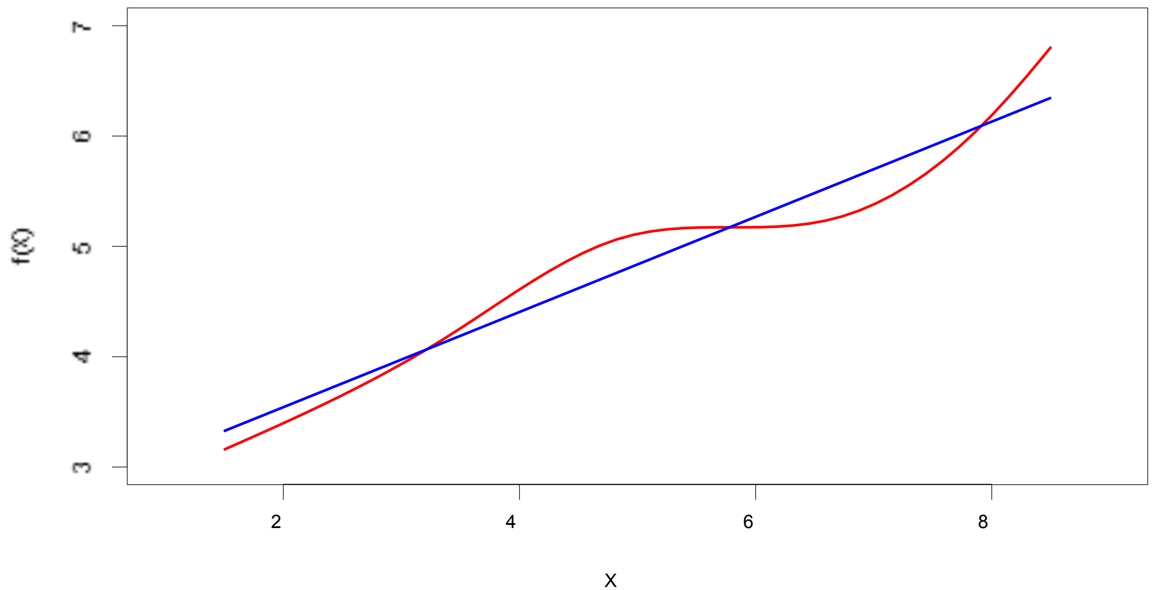
Linear regression

- 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!

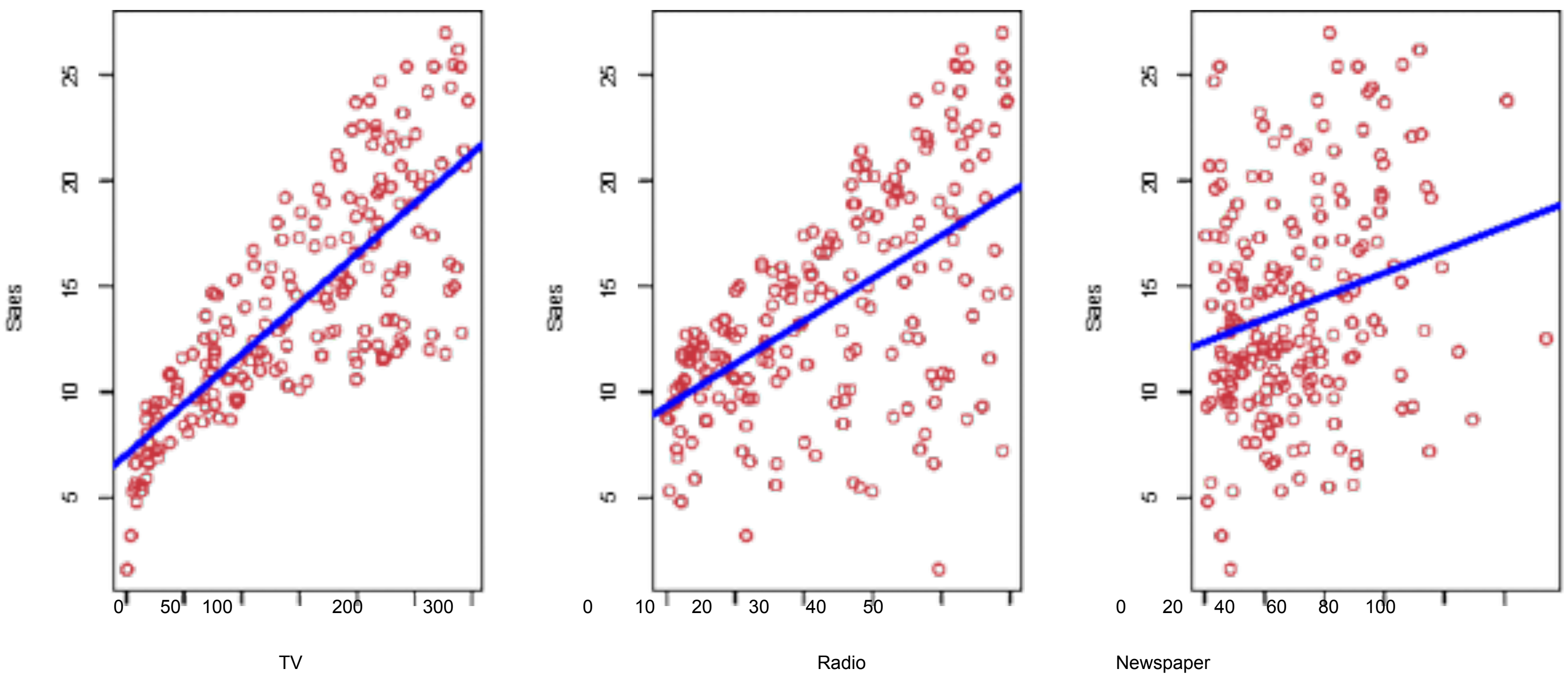


- Although it may seem overly simplistic, linear regression is extremely useful both conceptually and practically.

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

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

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

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

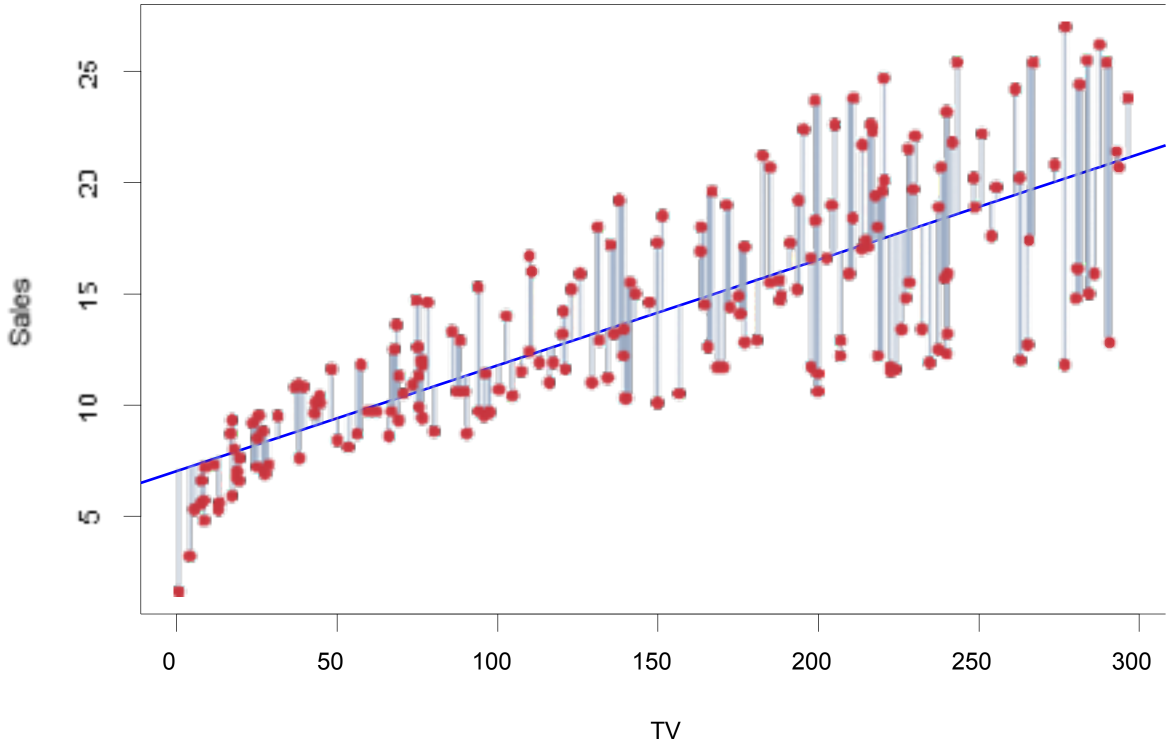
- The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. The minimizing values can be shown to be

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

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

where $\bar{y} \equiv \frac{1}{n}\sum_{i=1}^{n} y_i$ 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 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.

Assessing the Accuracy of the Coefficient Estimates

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

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

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

- 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

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

Confidence intervals — continued

- 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* $Y = \beta_0 + \varepsilon$, *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

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

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

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

Advertising data results

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

Multiple Linear Regression

- Here our model is

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

- 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

$$\text{sales} = \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \beta_3 \times \text{newspaper} + \varepsilon.$$

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