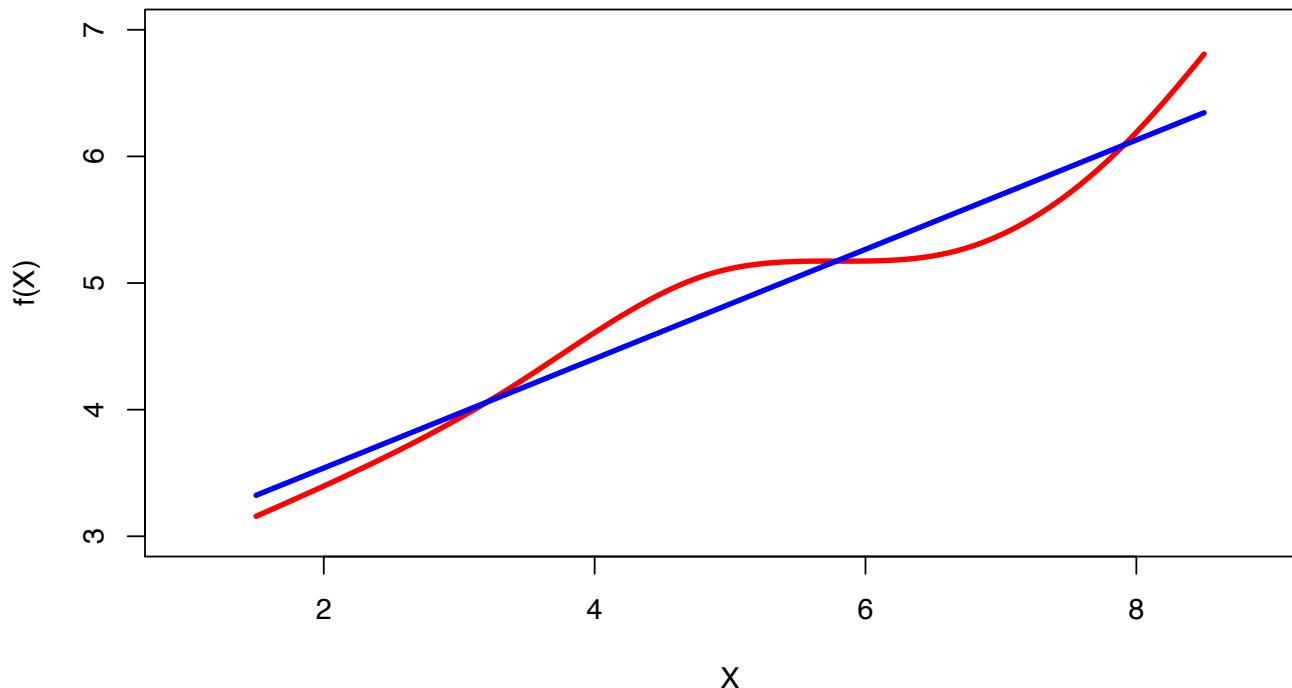


Linear regression

- Linear regression is a simple approach to supervised learning. It assumes that the dependence of Y on X_1, X_2, \dots, 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.

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 i th value of X . Then $e_i = y_i - \hat{y}_i$ represents the i th *residual*
- We define the *residual sum of squares* (RSS) as

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

or equivalently as

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

RSS = Suma residual de cuadrados

Propiedad: la media de los residuos es igual a 0

¡Cuidado! en algunos libros, RSS significa regression sum of squares. En este libro, esto es el VE salvo factor.

Estimation of the parameters by least squares

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- 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.

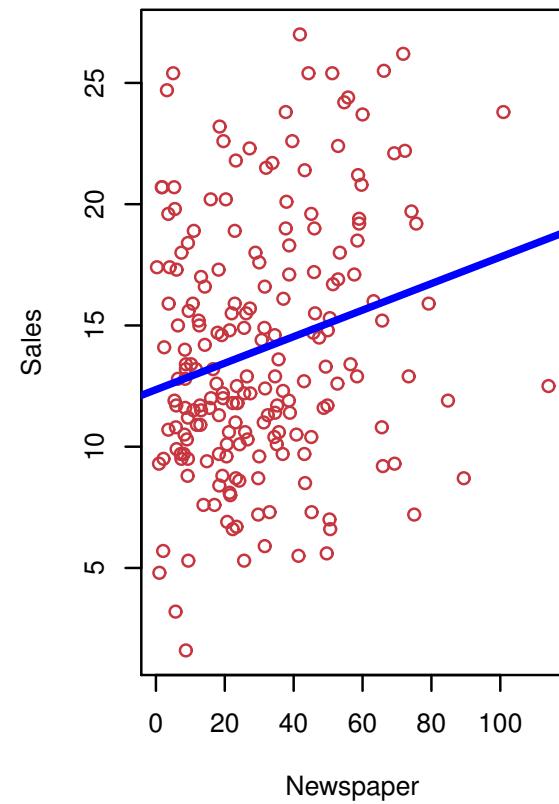
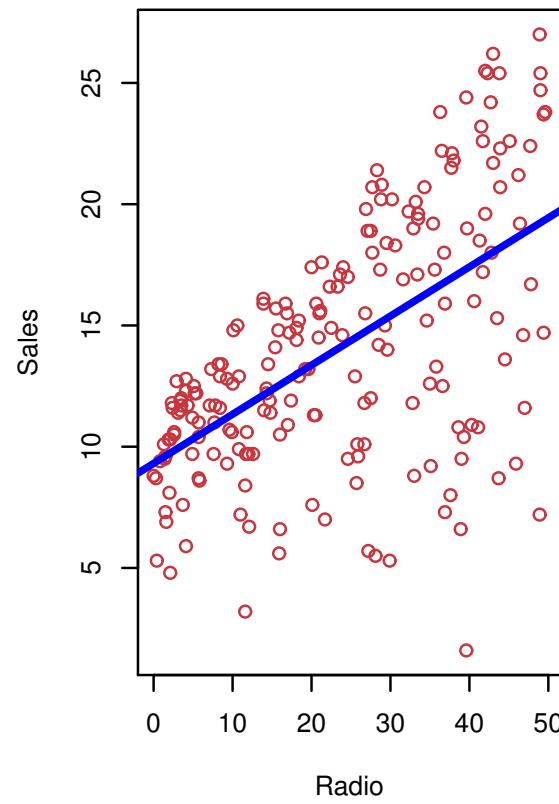
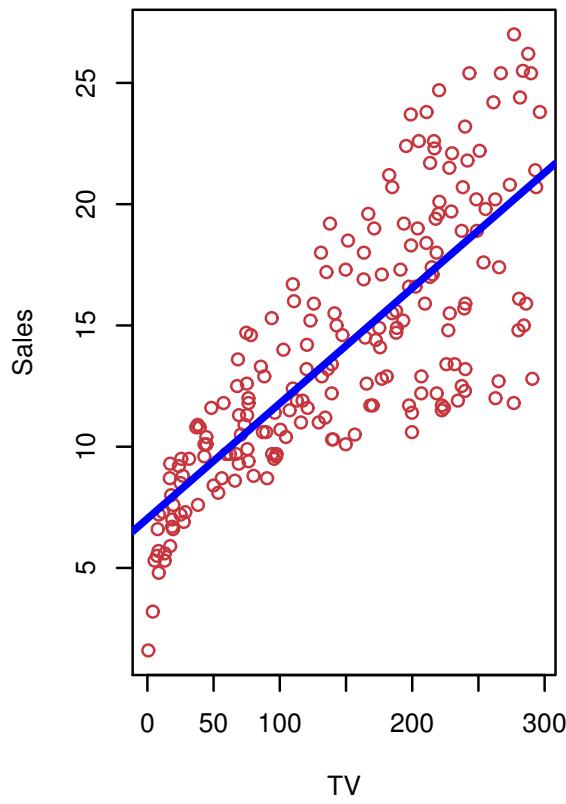
Linear regression for the advertising data

Consider the advertising data shown on the next slide.

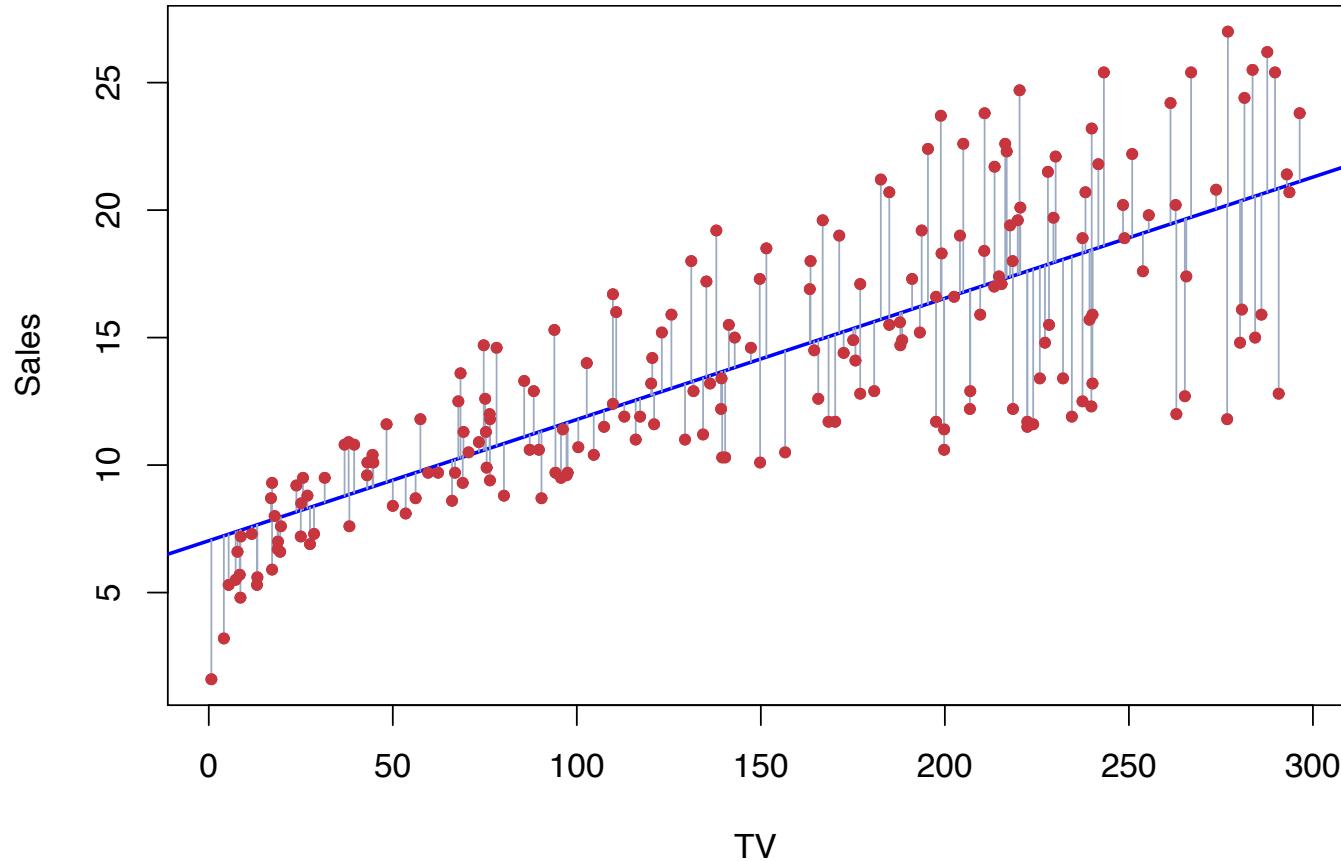
Questions we might ask:

- 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



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.

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 Accuracy of the Coefficient Estimates

Error estándar de los estimadores de los parámetros

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

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

where $\sigma^2 = \text{Var}(\epsilon)$, que se estima con la varianza residual

Estas expresiones se pueden considerar como la varianza de los estimadores. La matriz de varianza-covarianza de los estimadores de los parámetros es:

$$\text{Var}(\hat{\beta}) = \hat{\sigma}^2 (X^t X)^{-1}$$

Assessing the Accuracy of the Coefficient Estimates

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

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

- 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

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

Confidence intervals — continued

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

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

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

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

- 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 of the Model

- We compute the *Residual Standard Error*

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

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

RSE = Error estándar residual
RSS/(n-2) = varianza residual

and

MSE: mean squared error

Assessing the Overall Accuracy of the Model

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

- *R-squared* or fraction of variance explained is

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

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

En este modelo, la variabilidad total de Y (TSS) se descompone en la variabilidad explicada por el modelo (VE) y la residual (RSS). El coeficiente de determinación, R^2 , es la proporción de la variabilidad total explicada por el modelo de regresión:

$$R^2 = \text{VE}/\text{TSS} = (\text{TSS}-\text{RSS})/\text{TSS} = 1 - \text{RSS}/\text{TSS}$$

Assessing the Overall Accuracy of the Model

- We compute the *Residual Standard Error*

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

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- *R-squared* or fraction of variance explained is

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

where $\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2$ 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 :

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

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

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

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.

Estimation and Prediction for Multiple Regression

- Given estimates $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$, 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 $\beta_0, \beta_1, \dots, \beta_p$ as the values that minimize the sum of squared residuals

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

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

- The residual standard error, RSE, provides an absolute measure of lack of fit of the model, but it depends on the units of Y.
- In the multiple lineal model, the RSE is estimated as

$$RSE = \sqrt{RSS/(n-p-1)}$$

- To calculate R^2 , we use the same formula,

$$R^2 = 1 - RSS/TSS$$

Some important questions

1. *Is at least one of the predictors X_1, X_2, \dots, 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

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

Si todos los parámetros son nulos, F debe ser aproximadamente 1.
Si algún parámetro no es nulo, F debería ser mayor que 1.

Quantity	Value
Residual Standard Error	1.69
R^2	0.897
F-statistic	570

Deciding on the important variables

Si hay variables que influyen, ¿cuáles son?

- 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. We discuss two commonly used approaches next.

En clases sucesivas veremos otras metodologías para la selección de variables (variable selection)

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.

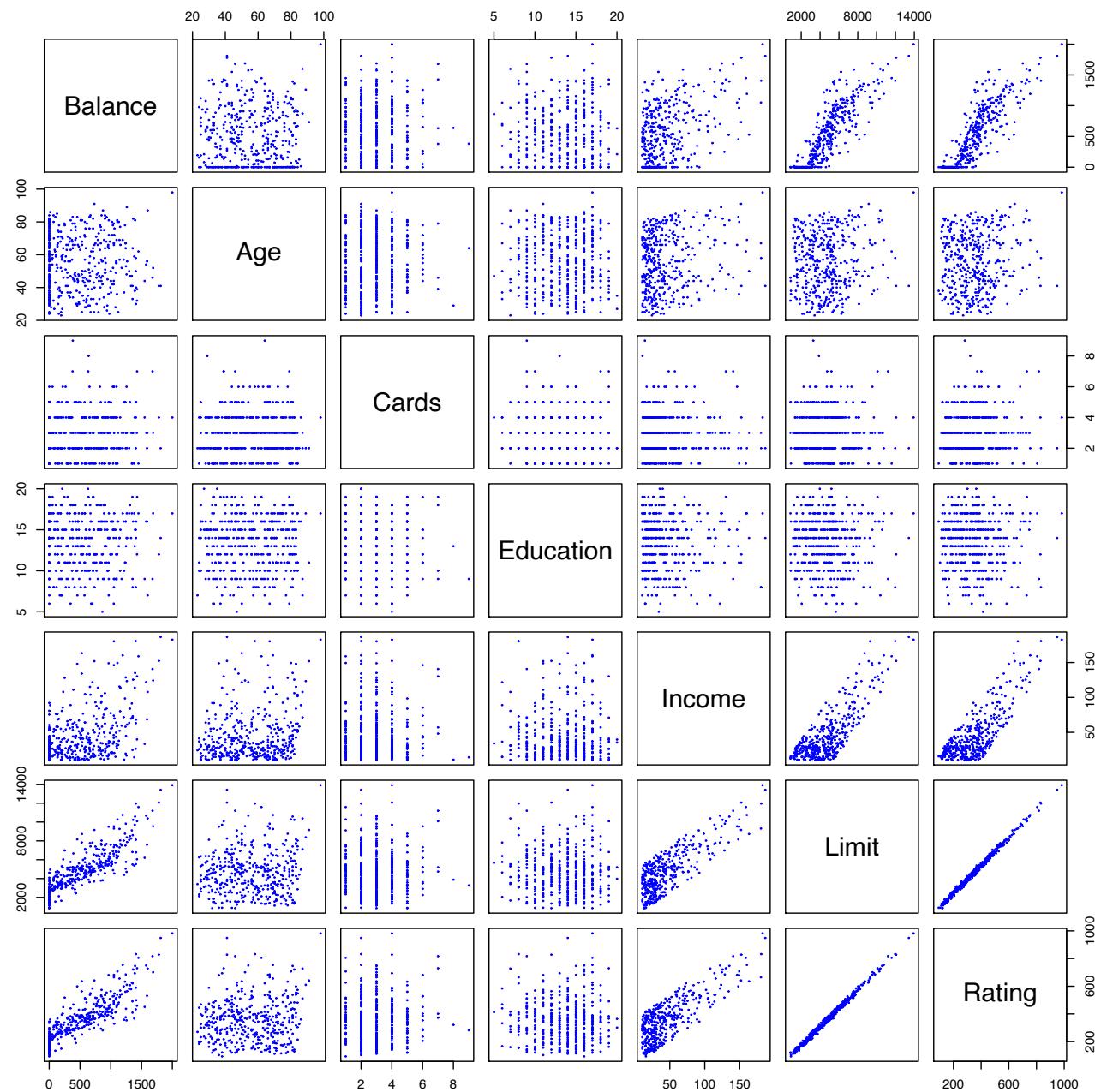
Other Considerations in the Regression Model

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).

Credit Card Data



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:

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

Intrepretation?

Credit card data — continued

Results for gender model:

	Coefficient	Std. Error	t-statistic	p-value
Intercept	509.80	33.13	15.389	< 0.0001
gender [Female]	19.73	46.05	0.429	0.6690

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

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

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

$$\begin{aligned}\text{sales} &= \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \beta_3 \times (\text{radio} \times \text{TV}) + \epsilon \\ &= \beta_0 + (\beta_1 + \beta_3 \times \text{radio}) \times \text{TV} + \beta_2 \times \text{radio} + \epsilon.\end{aligned}$$

Results:

	Coefficient	Std. Error	t-statistic	p-value
Intercept	6.7502	0.248	27.23	< 0.0001
TV	0.0191	0.002	12.70	< 0.0001
radio	0.0289	0.009	3.24	0.0014
TV×radio	0.0011	0.000	20.73	< 0.0001

Interpretation

- The results in this table suggests that interactions are important.
- The p-value for the interaction term **TV**×**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
$$(\hat{\beta}_1 + \hat{\beta}_3 \times \text{radio}) \times 1000 = 19 + 1.1 \times \text{radio} \text{ units.}$$
- An increase in radio advertising of \$1,000 will be associated with an increase in sales of
$$(\hat{\beta}_2 + \hat{\beta}_3 \times \text{TV}) \times 1000 = 29 + 1.1 \times \text{TV} \text{ units.}$$

Interactions between qualitative and quantitative variables

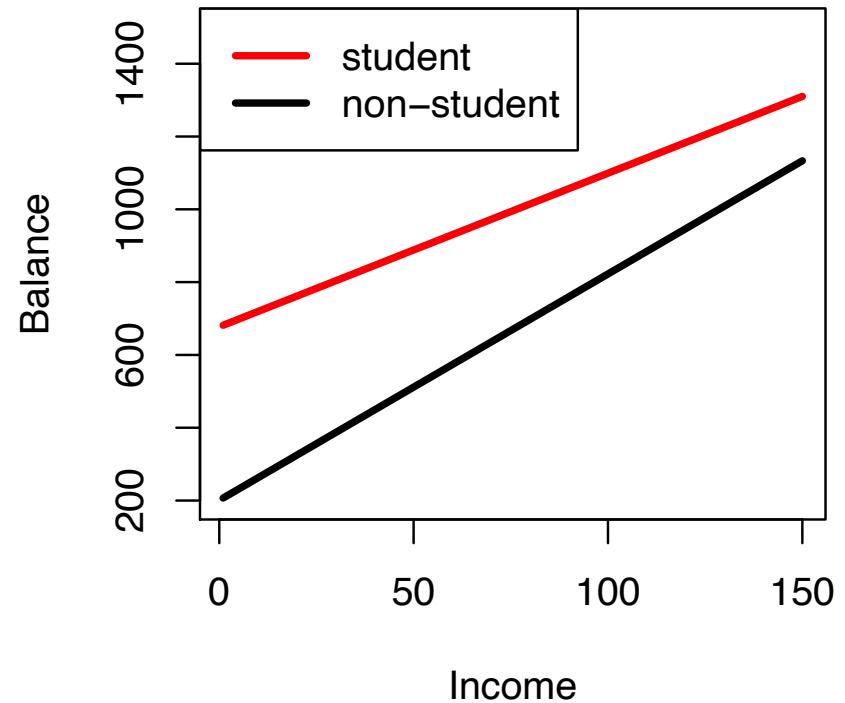
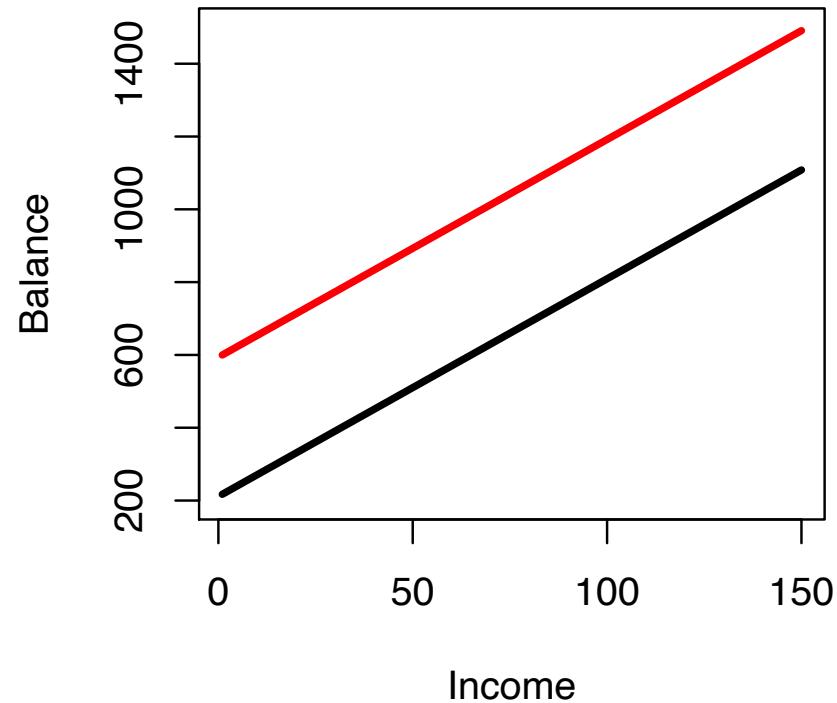
Consider the **Credit** data set, and suppose that we wish to predict **balance** using **income** (quantitative) and **student** (qualitative).

Without an interaction term, the model takes the form

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

With interactions, it takes the form

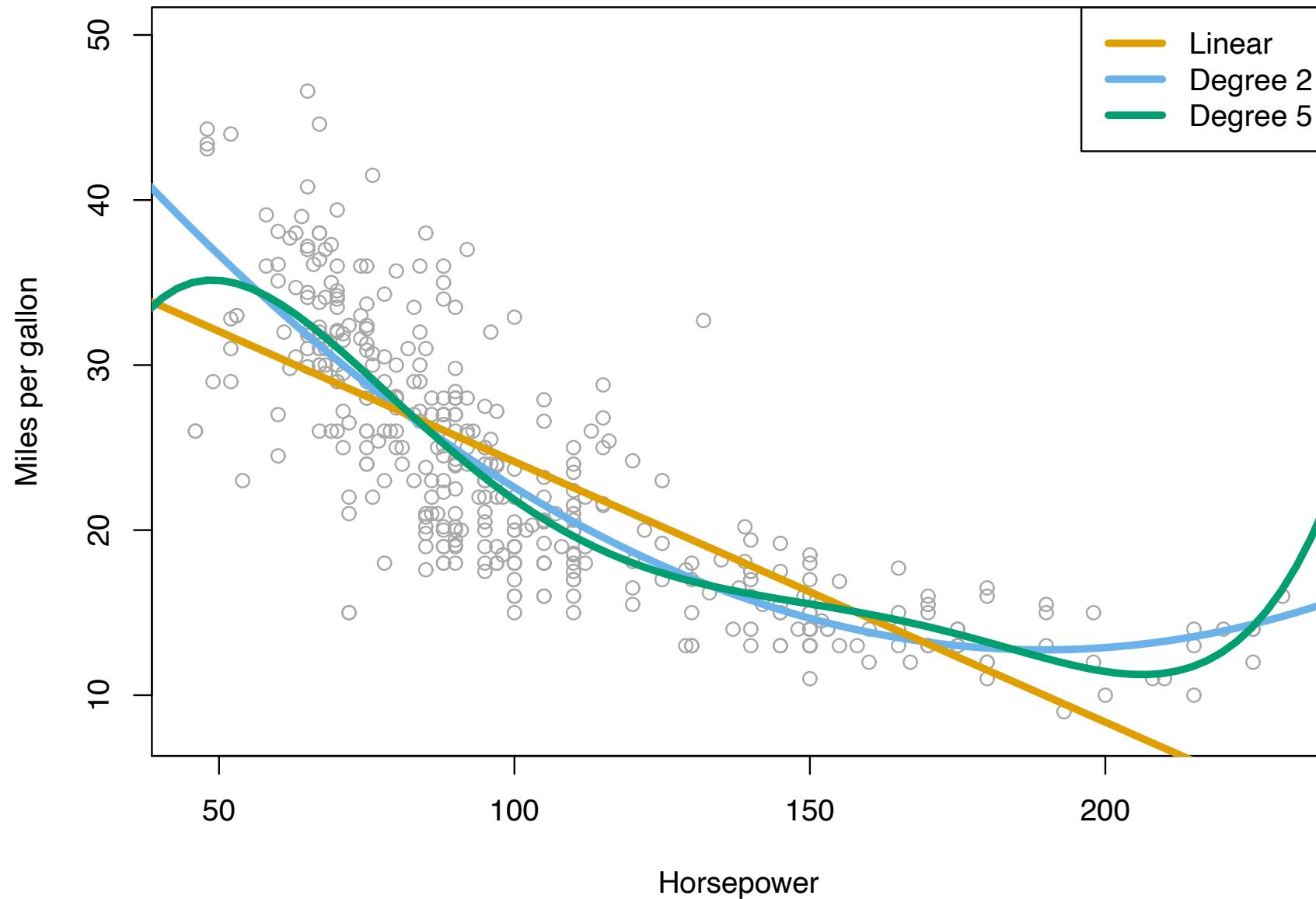
$$\begin{aligned}\text{balance}_i &\approx \beta_0 + \beta_1 \times \text{income}_i + \begin{cases} \beta_2 + \beta_3 \times \text{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\ &= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times \text{income}_i & \text{if student} \\ \beta_0 + \beta_1 \times \text{income}_i & \text{if not student} \end{cases}\end{aligned}$$



Credit data; 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

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

may provide a better fit.

	Coefficient	Std. Error	t-statistic	p-value
Intercept	56.9001	1.8004	31.6	< 0.0001
horsepower	-0.4662	0.0311	-15.0	< 0.0001
horsepower ²	0.0012	0.0001	10.1	< 0.0001

What we did not cover

Outliers

Non-constant variance of error terms

High leverage points

Collinearity (**2 variables->see the correlation matrix**), multicollinearity

See text Section 3.33

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

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