

# Linear Regression

Estimated with Ordinary Least Squares

# Machine Learning can be broadly divided into 3 categories

## 1. **Supervised Learning**

- a. **Regression** - What's a fair price for my apartment?
- b. **Classification** - What number is in the picture?

## 2. **Unsupervised Learning**

- a. **Clustering** - separate articles by topic
- b. **Dimensionality Reduction** - reduce complexity of the data
- c. **Density Estimation** - what's the likelihood of raining today
- d. **Anomaly detection** - detecting hacker attacks

## 3. **Semi-supervised Learning**

- a. **Machine translation with scarce parallel corpuses**

## 4. **Reinforcement Learning**

- a. **Games** - e.g. AlphaGo
- b. **Robotics**

## Today's topic - Linear regression

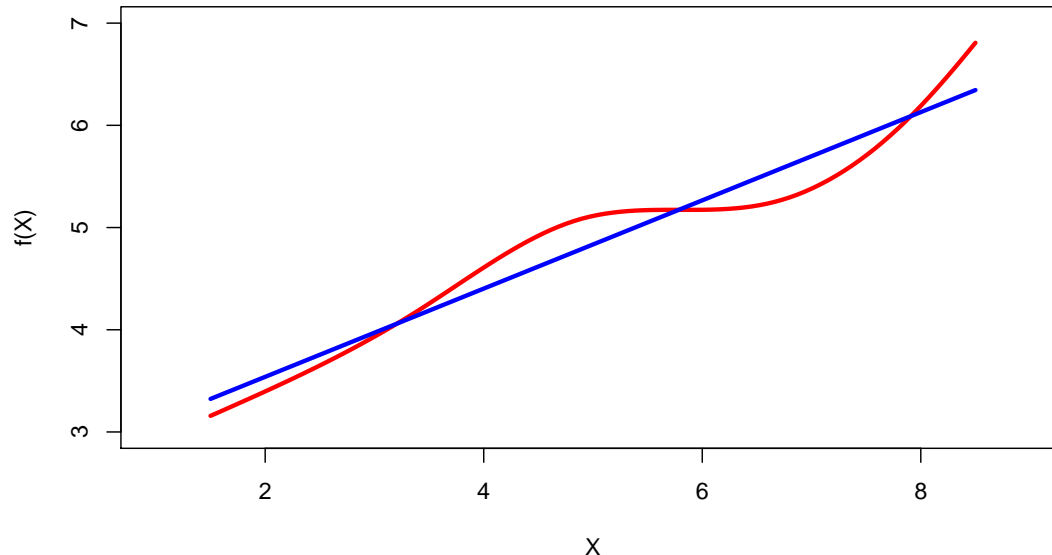
We'll start with supervised learning algorithms, as they are more commonplace.

# 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.

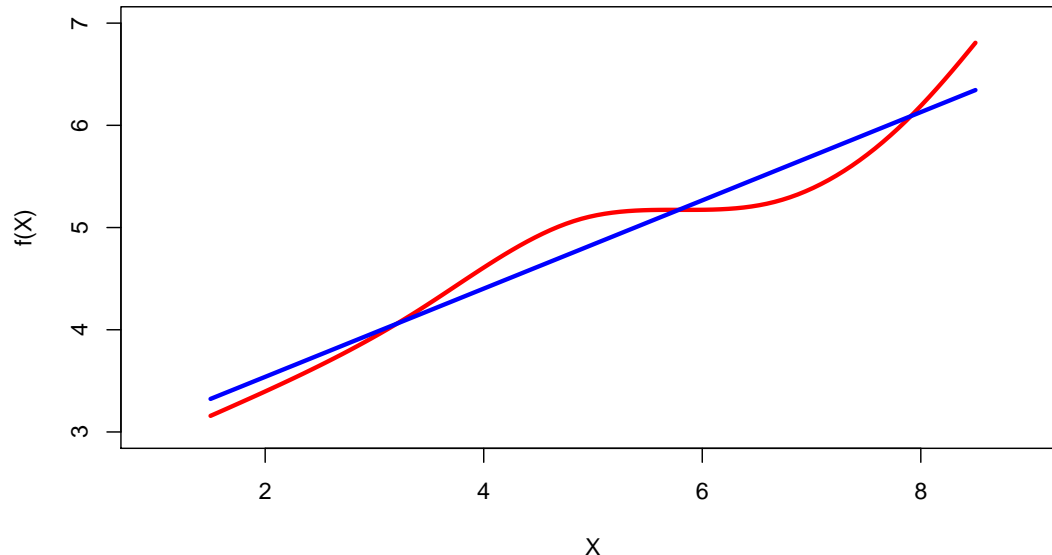
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- although it may seem overly simplistic, linear regression is extremely useful both conceptually and practically.

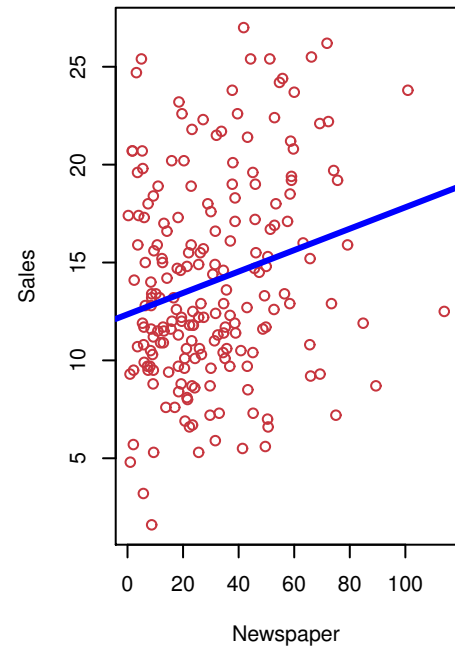
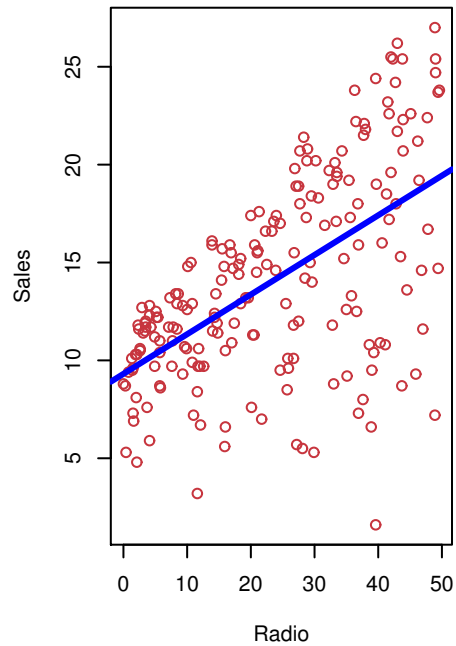
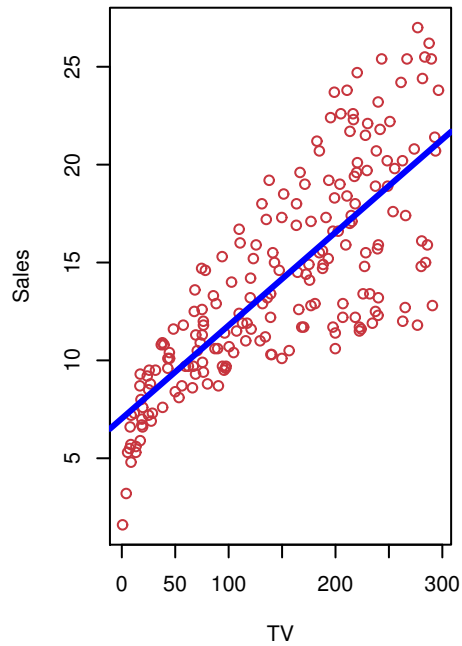
# Linear regression for the advertising data

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

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

where  $\beta_0$  and  $\beta_1$  are two unknown constants that represent the *intercept* and *slope*, also known as *coefficients* or *parameters*, and  $\epsilon$  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*

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

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

or equivalently as

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

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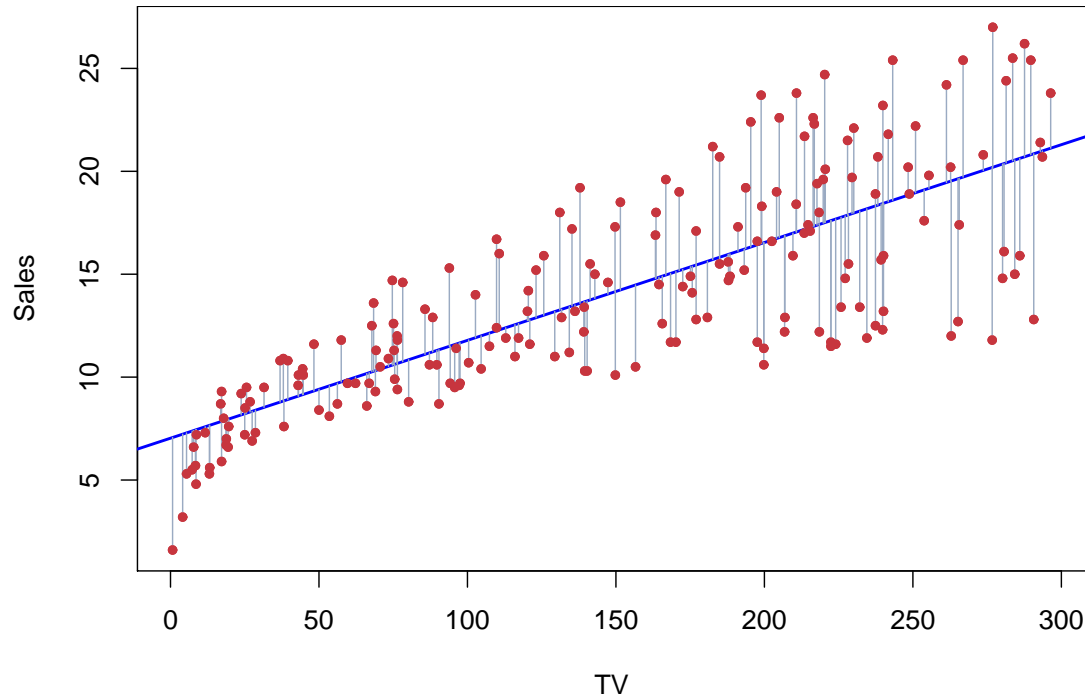
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- The least squares approach chooses  $\hat{\beta}_0$  and  $\hat{\beta}_1$  to minimize the RSS. The minimizing values can be shown to be

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

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.

## 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

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

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

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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

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

will contain the true value of  $\beta_1$  (under a scenario where we got repeated samples like the present sample)



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For the advertising data, the 95% confidence interval for  $\beta_1$  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*

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$H_A$  :      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*.

## 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*

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

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

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- 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

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

- We interpret  $\beta_j$  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  $\beta_j$  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.

# The woes of (interpreting) regression coefficients

*“Data Analysis and Regression” Mosteller and Tukey 1977*

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- 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?

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- $Y =$  number of tackles by a football player in a season;  $W$  and  $H$  are his weight and height. Fitted regression model is  $\hat{Y} = b_0 + .50W - .10H$ . How do we interpret  $\hat{\beta}_2 < 0$ ?

## Two quotes by famous Statisticians

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*“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



# Estimation and Prediction for Multiple Regression

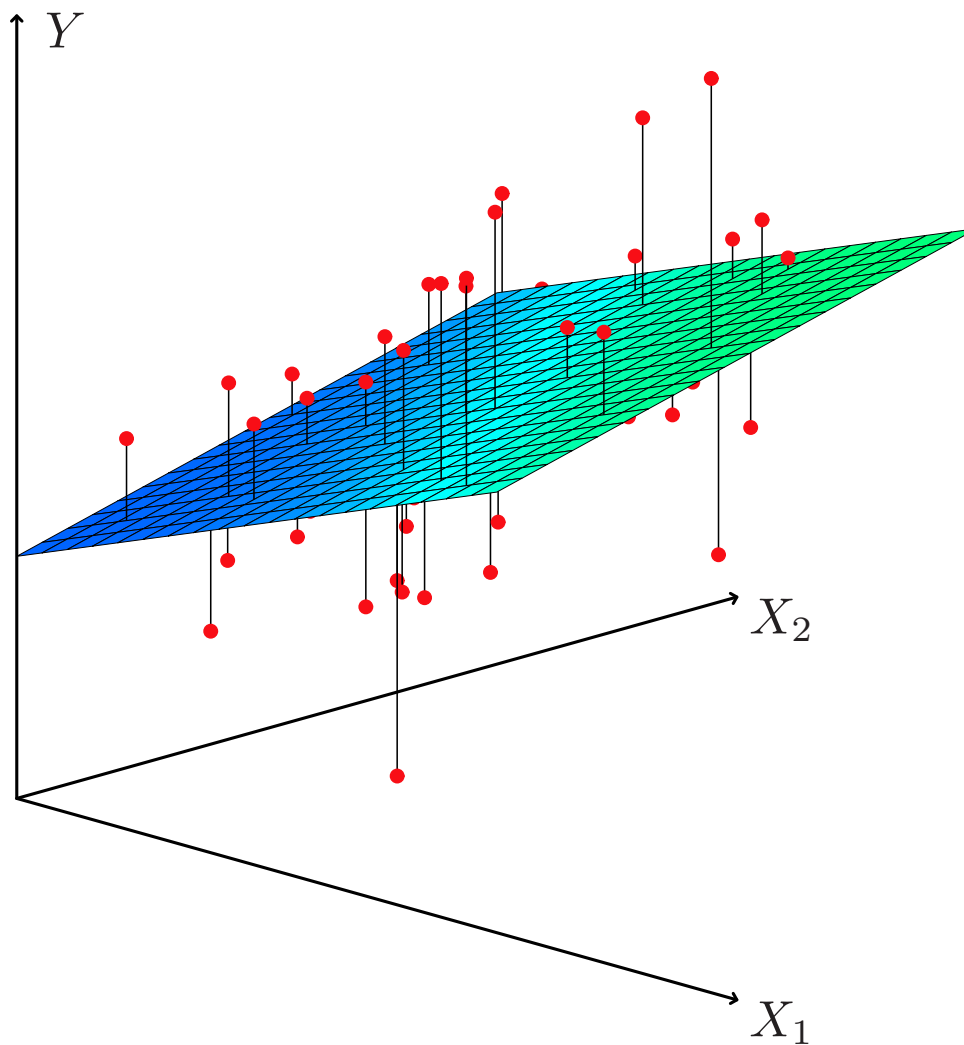
- Given estimates  $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$ , we can make predictions using the formula

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_p x_p.$$

- We estimate  $\beta_0, \beta_1, \dots, \beta_p$  as the values that minimize the sum of squared residuals

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

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.



## 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

# Some important questions

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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

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

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



# 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.

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- 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 use approaches next.

# 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.

## Model selection — continued

- Later we discuss more systematic criteria for choosing an “optimal” member in the path of models produced by forward or backward stepwise selection.
- These include *Mallow's  $C_p$* , *Akaike information criterion (AIC)*, *Bayesian information criterion (BIC)*, *adjusted  $R^2$*  and *Cross-validation (CV)*.

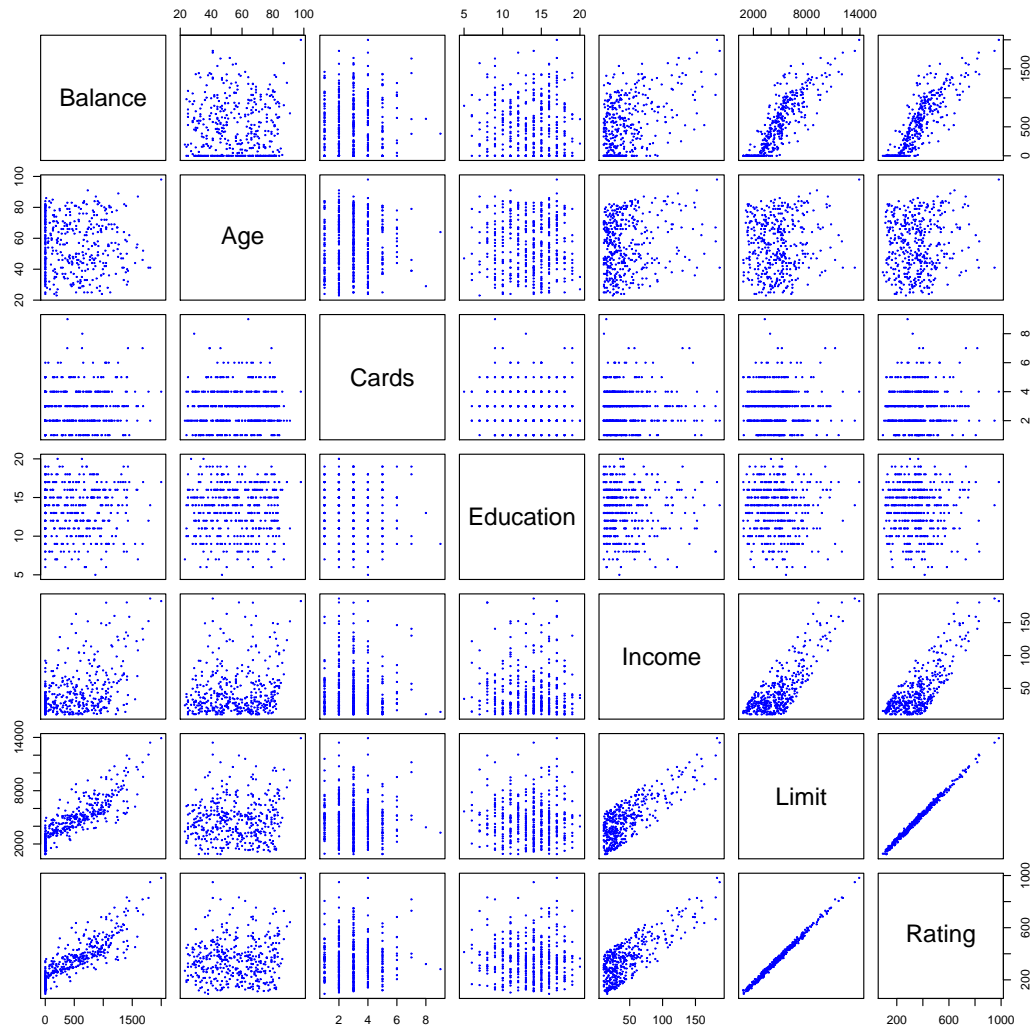
# Other Considerations in the Regression Model

## *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:

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

Intpretation?



## 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

# Qualitative predictors with more than two levels

- With more than two levels, we create additional dummy variables. For example, for the **ethnicity** variable we create two dummy variables. The first could be

$$x_{i1} = \begin{cases} 1 & \text{if } i\text{th person is Asian} \\ 0 & \text{if } i\text{th person is not Asian,} \end{cases}$$

and the second could be

$$x_{i2} = \begin{cases} 1 & \text{if } i\text{th person is Caucasian} \\ 0 & \text{if } i\text{th person is not Caucasian.} \end{cases}$$

## Qualitative predictors with more than two levels — continued.

- Then both of these variables can be used in the regression equation, in order to obtain the model

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person is Asian} \\ \beta_0 + \beta_2 + \epsilon_i & \text{if } i\text{th person is Caucasian} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person is AA.} \end{cases}$$

- There will always be one fewer dummy variable than the number of levels. The level with no dummy variable — African American in this example — is known as the *baseline*.

## Results for ethnicity

	Coefficient	Std. Error	t-statistic	p-value
Intercept	531.00	46.32	11.464	< 0.0001
ethnicity[Asian]	-18.69	65.02	-0.287	0.7740
ethnicity[Caucasian]	-12.50	56.68	-0.221	0.8260

# 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

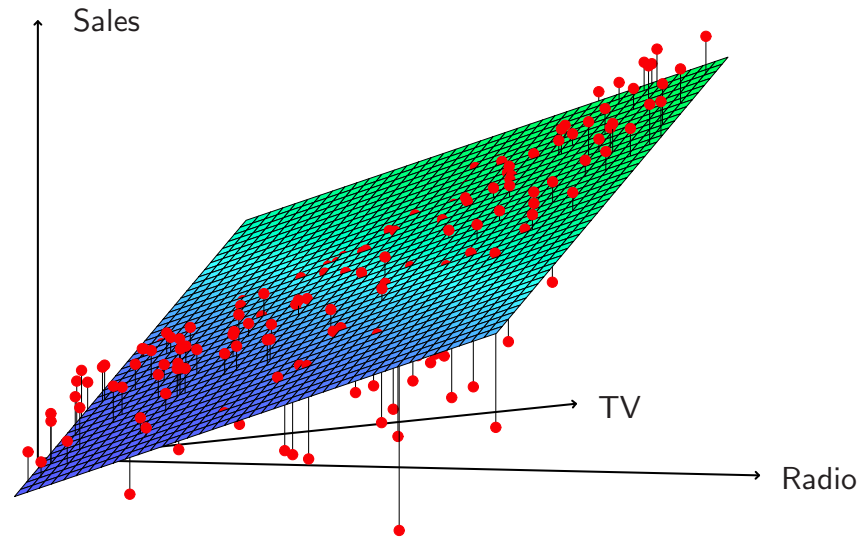
$$\widehat{\text{sales}} = \beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \beta_3 \times \text{newspaper}$$

states that the average effect on **sales** of a one-unit increase in **TV** is always  $\beta_1$ , 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.

# Interaction in the Advertising data?



When levels of either **TV** or **radio** are low, then the true **sales** are lower than predicted by the linear model.

But when advertising is split between the two media, then the model tends to underestimate **sales**.

# 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  $\text{TV} \times \text{radio}$  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  $\text{sales}$  using  $\text{TV}$  and  $\text{radio}$  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  
 $(\hat{\beta}_1 + \hat{\beta}_3 \times \text{radio}) \times 1000 = 19 + 1.1 \times \text{radio}$  units.
- An increase in radio advertising of \$1,000 will be associated with an increase in sales of  
 $(\hat{\beta}_2 + \hat{\beta}_3 \times \text{TV}) \times 1000 = 29 + 1.1 \times \text{TV}$  units.

# Hierarchy

- Sometimes it is the case that an interaction term has a very small p-value, but the associated main effects (in this case, **TV** and **radio**) 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.*

## Hierarchy — continued

- The rationale for this principle is that interactions are hard to interpret in a model without main effects — their meaning is changed.
- Specifically, the interaction terms also contain main effects, if the model has no main effect terms.

# Interactions between qualitative and quantitative variables

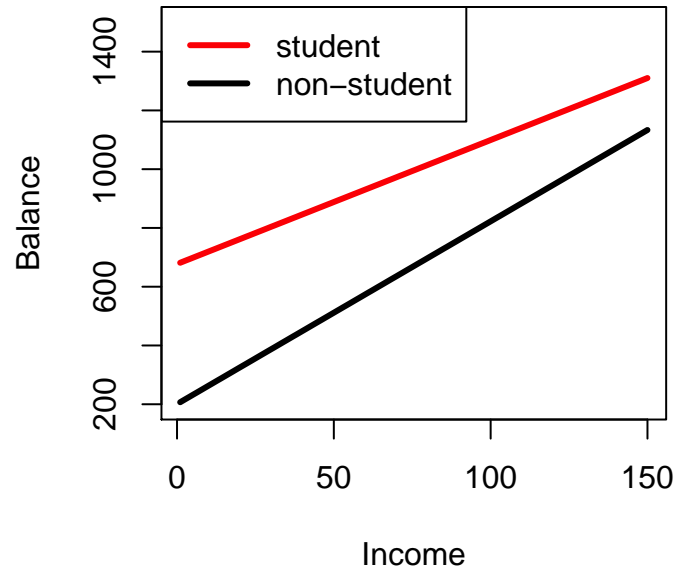
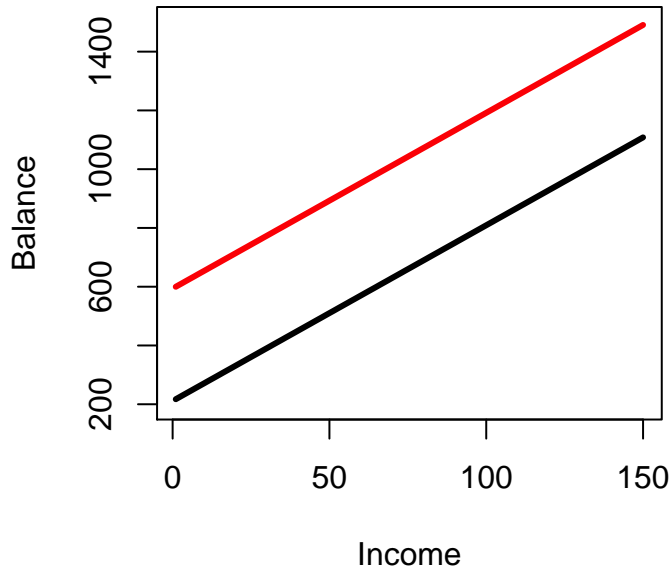
Consider the **Credit** data set, and suppose that we wish to predict **balance** using **income** (quantitative) and **student** (qualitative).

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

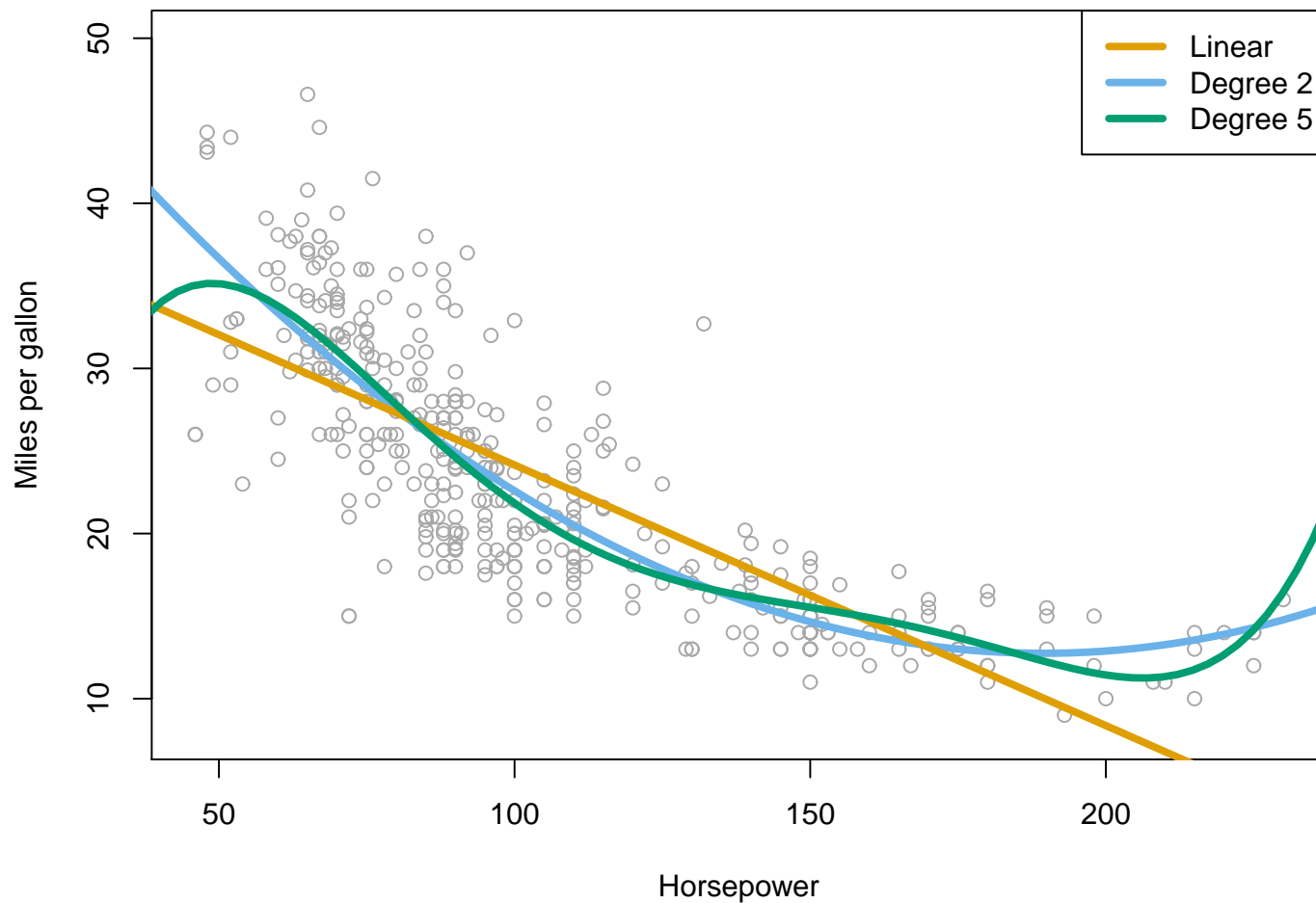
$$\begin{aligned}\text{balance}_i &\approx \beta_0 + \beta_1 \times \text{income}_i + \begin{cases} \beta_2 + \beta_3 \times \text{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\ &= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times \text{income}_i & \text{if student}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



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 <sup>2</sup>	0.0012	0.0001	10.1	< 0.0001

# What we did not cover

Outliers

Non-constant variance of error terms

High leverage points

Collinearity

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