Predictive Analytics

Week 2: Linear Regression and Statistical Thinking

Semester 2, 2018

Discipline of Business Analytics, The University of Sydney Business School

QBUS2820 content structure

1. **Statistical and Machine Learning foundations and applications**.

2. Advanced regression methods.

3. Classification methods.

4. Time series forecasting.

Before the lecture 2, review linear algebra, especially matrix multiplication, rank, determinant and inverse.

Week 2: Linear Regression and Statistical Thinking

1. Introduction
2. The least squares algorithm
3. The MLR model
4. Statistical properties
5. Interpreting a linear regression model
6. Regression modelling

Introduction

Linear regression

The linear regression is a simple and widely used method for supervised learning. There are several important reasons for developing an in-depth understanding of this method.

- It is very useful for prediction in many settings.

- It is extremely useful conceptually. Many advanced statistical learning methods can be understood as extensions and generalisations of linear regression.

- Due to its simplicity, linear regression is often a useful jumping-off point for model building and analysis.

- Interpretability.

Example: advertisement data

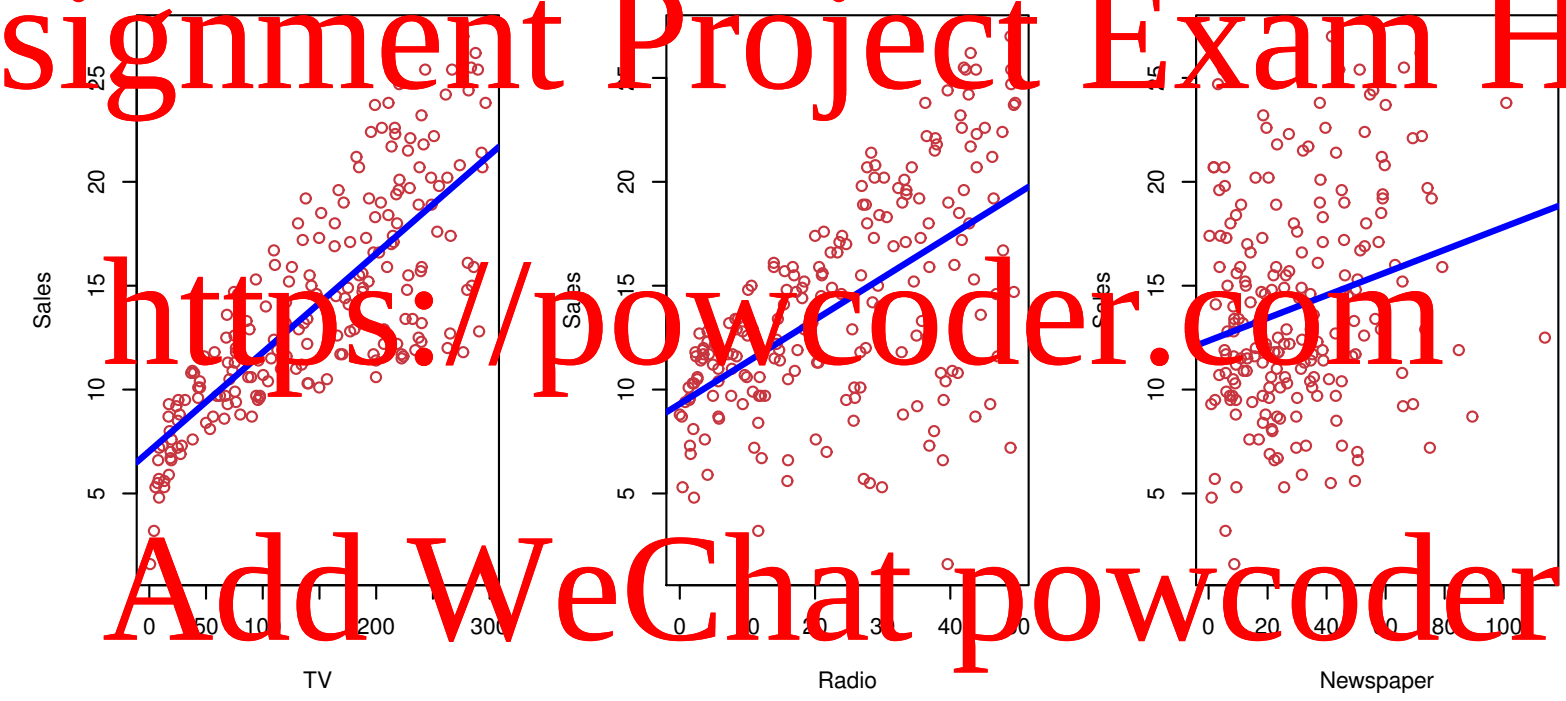
Consider from example the advertisement data from the ISL textbook (see next slide). Possible questions:

- 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 there synergy among the advertisement media?

Example: advertisement data



(Figure from ISL)

Example: advertisement data

To answer our questions, we can use a model such as

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

Statistical thinking

Statistical thinking is using statistical models, statistical theory, and critical thinking to learn from data.

- How do I design a study to answer a certain question?
- How relevant and representative are my data?
- What is the variability in my data? Can I reliably draw conclusions in light of this variability?
- How do I correctly interpret my results?
- Can I generalise my conclusions in the way that I would like to?
- What are the limitations of my analysis?

The least squares algorithm

Linear regression

In the linear regression method for prediction, we consider a regression function of the form

$$f(\boldsymbol{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p$$

We learn the prediction coefficients $\widehat{\beta}_0, \widehat{\beta}_1, \ldots \widehat{\beta}_p$ by fitting the model to the training data using the least squares method.

Least squares

Let $\mathcal{D} = \{(y_i, \boldsymbol{x}_i)\}_{i=1}^N$ be the training data. We define the **residual sum of squares** as a function of parameter values β as

$$\mathsf{RSS}(\boldsymbol{\beta}) = \sum_{i=1}^N (y_i - f(\boldsymbol{x}_i; \boldsymbol{\beta}))^2$$

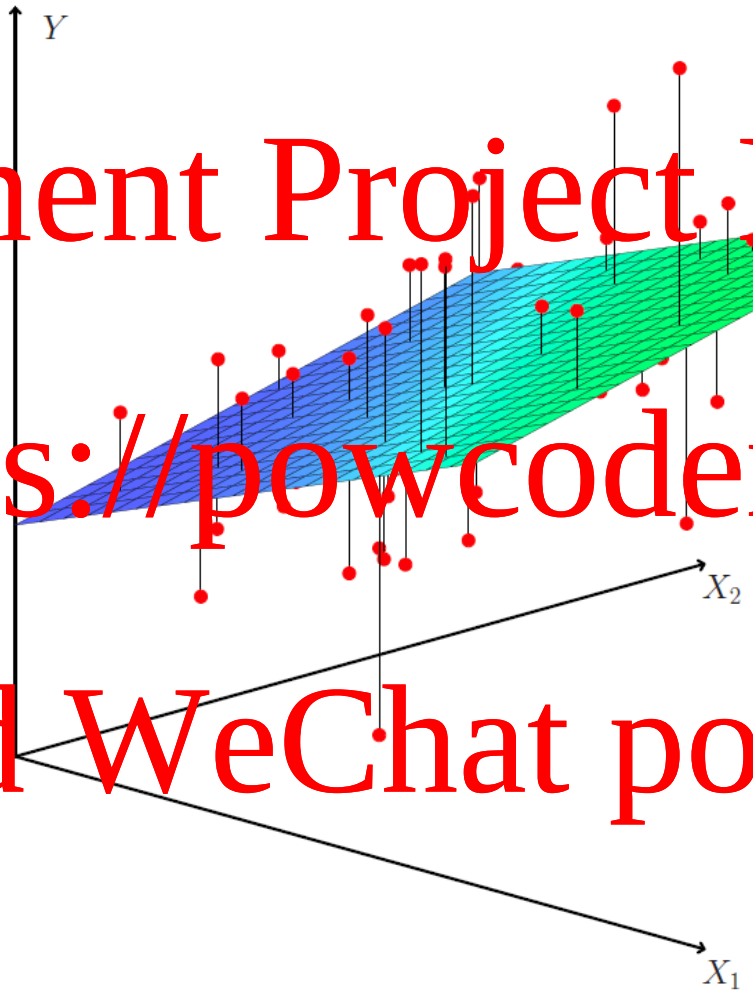
$$= \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^p \beta_j x_{ij} \right)^2$$

Least squares

The **ordinary least squares** (OLS) method selects the coefficient values that minimise the residual sum of squares

$$\widehat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

Least squares



(Figure from ISL)

Interpretation

If our loss function $L(y, f(\boldsymbol{x}))$ is the squared error loss, the OLS algorithm consists of minimising the empirical loss for our choice of predictive function:

$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(\boldsymbol{x}_i))$$

Least squares and linear algebra

In order to obtain a solution to the OLS minimisation problem, we need linear algebra.

https://xkcd.com/1838/

Design matrix

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & x_{N2} & \dots & x_{Np} \end{pmatrix}$$

Least squares and linear algebra

We equivalently write the RSS as

$$\begin{aligned}\text{RSS}(\beta) &= (\boldsymbol{y} - \boldsymbol{X}\beta)^T(\boldsymbol{y} - \boldsymbol{X}\beta) \\ &= \boldsymbol{y}^T\boldsymbol{y} - 2\beta^T\boldsymbol{X}^T\boldsymbol{y} + \beta^T\boldsymbol{X}^T\boldsymbol{X}\beta\end{aligned}$$

We optimise the RSS by taking the $p+1$ partial derivatives and setting them to zero.

Vector differentiation rules

Let $\boldsymbol{x}$ and $\boldsymbol{a}$ be vectors of equal dimension and $\boldsymbol{A}$ a matrix with column dimension the same as number of rows in $\boldsymbol{x}$. Then:

$$\frac{d(\boldsymbol{x}^T\boldsymbol{a})}{d\boldsymbol{x}} = \boldsymbol{a}$$

$$\frac{d(\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x})}{d\boldsymbol{x}} = (\boldsymbol{A} + \boldsymbol{A}^T)\boldsymbol{x}$$

Partial derivatives

$$RSS(\beta) = \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{y}^T\boldsymbol{X}\beta + \beta^T\boldsymbol{X}^T\boldsymbol{X}\beta$$

The vector of partial derivatives is

$$\frac{d(RSS(\beta))}{d\beta} = \frac{d(\boldsymbol{y}^T\boldsymbol{y})}{d\beta} - \frac{d(2\beta^T\boldsymbol{X}^T\boldsymbol{y})}{d\beta} + \frac{d(\beta^T\boldsymbol{X}^T\boldsymbol{X}\beta)}{d\beta} =$$

$$= \mathbf{0} - 2\boldsymbol{X}^T\boldsymbol{y} + 2\boldsymbol{X}^T\boldsymbol{X}\beta$$

OLS estimates

The first order condition is:

$$\frac{d(\text{RSS}(\beta))}{d\beta} = -2\boldsymbol{X}^T\boldsymbol{y} + 2\boldsymbol{X}^T\boldsymbol{X}\beta = 0$$

The least squares estimate $\widehat{\beta}$ therefore satisfies

$$\boldsymbol{X}^T\boldsymbol{X}\widehat{\beta} = \boldsymbol{X}^T\boldsymbol{y}$$

If $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$ is invertible, left multiplication with $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$ gives the unique solution

$$\widehat{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}.$$

OLS for big data?

The OLS solution is $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$, given that you can compute the matrix $\boldsymbol{X}^T\boldsymbol{X}$.

$\boldsymbol{X}$ is a matrix of size $N \times (p+1)$. If N is very large, then $\boldsymbol{X}$ is so large that it is impossible to compute $\boldsymbol{X}^T\boldsymbol{X}$ or it is close to being singular.

For big data, it's challenging to compute this matrix! Solutions?

$\boldsymbol{X}^T\boldsymbol{X}$ non-invertible?

- Reason: Multicollinearity problem or redundant predictors. Rank and determinant of $\boldsymbol{X}^T\boldsymbol{X}=$?
  - Solution: Drop one or more highly correlated predictors from the model or collect more data.

- Reason: The number of predictors is too large, e.g. $N \ll p$. Rank and determinant of $\boldsymbol{X}^T\boldsymbol{X}=$?
  - Solution: Drop some predictors or collect more data; Add regularization term into the model. More details later.

- For real matrices $\boldsymbol{X}$:
  $\text{rank}(\boldsymbol{X}^T\boldsymbol{X}) = \text{rank}(\boldsymbol{X}\boldsymbol{X}^T) = \text{rank}(\boldsymbol{X}) = \text{rank}(\boldsymbol{X}^T)$

Fitted values

The fitted values based on the training inputs are

$$\widehat{y}_i = \widehat{\beta}_0 + \sum_{j=1}^{p} \widehat{\beta}_j x_{ij}$$

The vector of fitted values for the entire sample is:

$$\widehat{\boldsymbol{y}} = \boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

We refer to $\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T$ as the **hat matrix**.

Residuals

The regression **residuals** are:

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

$$= y_i - \widehat{\beta}_0 - \sum_{j=1}^{p} \widehat{\beta}_j x_{ij}$$

The vector of residuals is:

$$\boldsymbol{e} = \boldsymbol{y} - \widehat{\boldsymbol{y}}$$

$$= \boldsymbol{y} - \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

$$= \left(\boldsymbol{I} - \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\right)\boldsymbol{y}.$$

Measuring fit

We can show that

$$\text{TSS} = \text{RegSS} + \text{RSS}$$

$$\sum_i (y_i - \bar{y})^2 = \sum_i (\hat{y}_i - \bar{y})^2 + \sum_i e_i^2$$

- TSS: total sum of squares.
- RegSS: regression sum of squares.
- RSS: residual sum of squares.

Measuring fit

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

Interpretation:

- The R^2 measures the proportion of the variation in the response data that is accounted for by the estimated linear regression model.

- The R^2 can only increase when you add another variable to the model.

- The R^2 is an useful part of the regression toolbox, but it does not measure the predictive accuracy of the estimated regression, or more generally how good the model is.

Prediction

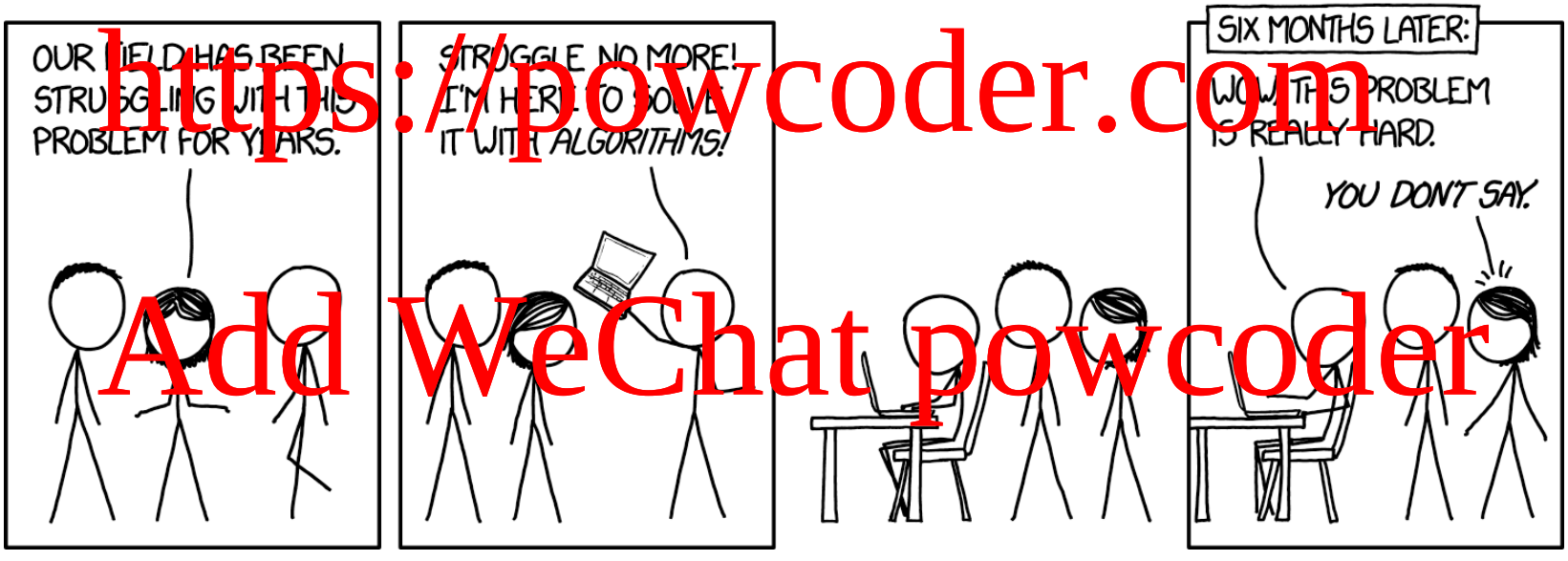
Let $\widehat{\beta}$ be the OLS coefficients obtained from the training sample.

$$\widehat{y}_0 = \widehat{\beta}_0 + \sum_{j=1}^{p} \widehat{\beta}_j x_{0j}$$

The MLR model

Models and algorithms

So far, we have talked about the least squares algorithm and even arrived at predictions without reference to a model. The current practice of data science places large emphasis on **algorithmic thinking** towards problem solving.



https://xkcd.com/1831/

Statistical models

A **statistical model** is a description of a data generating process based on a set of mathematical assumptions about the population and the sampling process.

A **regression model** is a description of the relationship between a response variable Y and predictors $X_1, \ldots, X_p$. More formally, it is a model of the form $p(y|\boldsymbol{x}; \theta)$.

Formulating statistical models and making assumptions allow us to say more about a problem.

The Multiple Linear Regression (MLR) model

1. Linearity: if $X = \boldsymbol{x}$, then

$$Y = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p + \varepsilon$$

for some population parameters $\beta_0, \beta_1, \ldots, \beta_p$ and a random error ε.

2. The conditional mean of ε given X is zero: $E(\varepsilon|X) = 0$.

3. Constant error variance: $\text{Var}(\varepsilon|X) = \sigma^2$.

4. Independence: all the error pairs ε_i and ε_j $(i \neq j)$ are independent.

5. The distribution of $X_1, \ldots, X_p$ is arbitrary.

6. There is no perfect multicollinearity.

Checking the assumptions

It is fundamental to check the assumptions with data. We do this with **residual diagnostics**. The following plots are often useful:

- Fitted values against residuals.
- Predictors against residuals.

- Fitted values against squared or absolute residuals.
- Predictors against squared or absolute residuals.

- Residual distribution.
- If the observations are ordered: residuals against coordinates (time and/or space).

Statistical properties

Sampling distribution of an estimator

In classical statistics, the population parameter β is fixed and the data is a random sample from the population. We estimate β by applying an **estimator** $\widehat{\beta}(\mathcal{D})$ to data (in our case the OLS algorithm).

We study the uncertainty of an estimate by computing the **sampling distribution** of the estimator.

Sampling distribution of an estimator

Imagine that we draw many different datasets $\mathcal{D}^{(s)}$ $(s = 1, \ldots, S)$ from the true model $p(\boldsymbol{y}|\boldsymbol{X}; \boldsymbol{\beta})$. Each dataset has size N.

For each of these datasets, we apply the estimator $\widehat{\boldsymbol{\beta}}(\cdot)$ and obtain a set of estimates $\{\widehat{\boldsymbol{\beta}}(\mathcal{D}^{(s)})\}$. The sampling distribution is the induced distribution on $\widehat{\boldsymbol{\beta}}(\cdot)$ as $S \to \infty$.

This concept is not necessarily intuitive since it refers to hypothetical datasets rather than data that we do have.

Sampling distribution of an estimator

Establishing the sampling distribution allows us to answer questions such as:

- Is there a significant relationship between the response and the predictors?
- Are all the predictors related to the response, or only a subset?
- How accurate are our coefficient estimates?
- How accurate are our predictions?

Sampling distribution

Under the Gaussian MLR model with $\varepsilon \sim N(0, \sigma^2)$, we can obtain an exact sampling distribution for the OLS estimator,

$$\widehat{\boldsymbol{\beta}} \sim N\left(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}\right)$$

When estimating σ^2, we have

$$\frac{\widehat{\beta}_j - \beta_j}{\mathrm{SE}(\widehat{\beta}_j)} \sim ?,$$

We can then rely on this distribution for hypothesis testing.

Review your study notes of previous units or the reference book for: OLS estimator sample distribution, regression coefficient significance testing, confidence interval, ANOVA, etc.

Interpreting a linear regression model

Advertisement data

We now estimate the linear regression model

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

To interpret the results, we need to note the following:

- The observational units in the data are markets.
- The response variable (sales) is in thousands of units.

- The predictors are in thousands of dollars.

What is the population of interest? (You always need to be able to answer this question)

Advertisement data

OLS Regression Results

Dep. Variable:	Sales	R-squared:	0.897
Model:	OLS	Adj. R-squared:	0.896
Method:	Least Squares	F-statistic:	570.3
Date:		Prob (F-statistic):	1.58e-96
Time:		Log-Likelihood:	-386.18
No. Observations:	200	AIC:	780.4
Df Residuals:	196	BIC:	793.6
Df Model:	3		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
Intercept	2.9389	0.312	9.422	0.000	2.324	3.554
TV	0.0458	0.001	32.809	0.000	0.043	0.049
Radio	0.1885	0.009	21.893	0.000	0.172	0.206
Newspaper	-0.0010	0.006	-0.177	0.860	-0.013	0.011

Omnibus:	60.414	Durbin-Watson:	2.084
Prob(Omnibus):	0.000	Jarque-Bera (JB):	151.241
Skew:	-1.327	Prob(JB):	1.44e-33
Kurtosis:	6.332	Cond. No.	454.

Interpreting coefficients

$$\widehat{\text{sales}} = \underset{(0.312)}{-2.9389} + \underset{(0.001)}{0.0458} \times \text{TV} + \underset{(0.009)}{0.1885} \times \text{radio} - \underset{(0.006)}{0.0010} \times \text{newspaper}$$

Interpretation (TV):

If we select two markets from the population, where the radio and newspaper budgets are the same, but the TV budget differs by 100 dollars, we would expect 4.58 more units sold in the market with higher TV budget.

Interpreting coefficients

Mathematically:

$$\beta_j = E(Y|X_1 = x_j + 1, X_{\neq j} = x_{\neq j}) - E(Y|X_j = x_j, X_{\neq j} = x_{\neq j})$$

For example, with $p = 2$ and focusing on the first predictor:

$$\begin{aligned}
&E(Y|X_1 = x_1 + 1, X_2 = x_2) - E(Y|X_1 = x_1, X_2 = x_2) \\
&= E[\beta_0 + \beta_1(x_1 + 1) + \beta_2 x_2 + \varepsilon] - E[\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon] \\
&= [\beta_0 + \beta_1(x_1 + 1) + \beta_2 x_2] - [\beta_0 + \beta_1 x_1 + \beta_2 x_2] \\
&= \beta_1
\end{aligned}$$

Omitted variables

With observational data, the assumption that $E(\varepsilon|X = \boldsymbol{x})$ is generally not satisfied. In this case, there are **omitted variables**: variables that are correlated with both the predictor and the response. This leads to **omitted variable bias** when estimating regression coefficients.

Here is an example: if we regress wealth on the number of luxury cars owned, the slope is positive (luxury cars predict wealth). However, we can imagine that buying more luxury cars will not make you richer.

Example: education and wages

OLS Regression Results

Dep. Variable:	Hourly wage	R-squared:	0.162
Model:	OLS	Adj. R-squared:	0.162
Method:	Least Squares	F-statistic:	1729.
Date:		Prob (F-statistic):	0.00
Time:		Log-Likelihood:	-57425.
No. Observations:	17919	AIC:	1.149e+05
Df Residuals:	17916	BIC:	1.149e+05
Df Model:	2		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
Intercept	-7.5017	0.337	-22.278	0.000	-8.162	-6.842
Education	1.1937	0.024	50.255	0.000	1.147	1.240
Experience	0.1513	0.011	13.772	0.000	0.130	0.173

Omnibus:	10774.032	Durbin-Watson:	0.744
Prob(Omnibus):	0.000	Jarque-Bera (JB):	237446.384
Skew:	2.484	Prob(JB):	0.00
Kurtosis:	20.128	Cond. No.	117.

Causal analysis

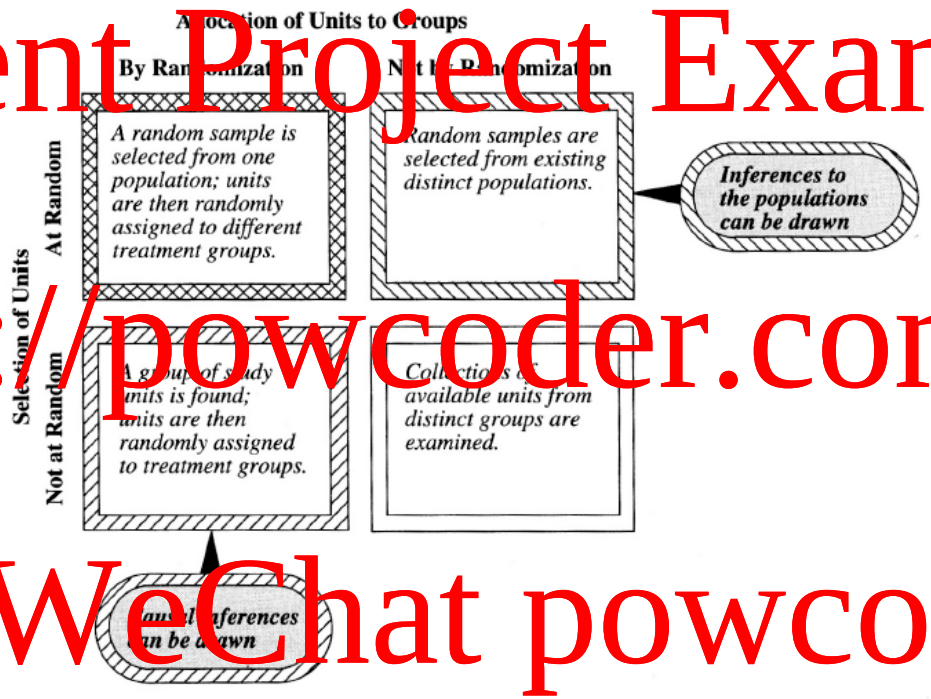
Causal analysis means to estimate a model of the type $E(Y|\text{do } X = \boldsymbol{x})$. This is an explicit intervention: "if we do $X = \boldsymbol{x}$, then we predict $E(Y|X = \boldsymbol{x})$".

This is different from predictive modelling: "if we observe $X = \boldsymbol{x}$, then we predict $E(Y|X = \boldsymbol{x})$".

Causal analysis requires an appropriate **study design** (such as A/B testing).

Study designs

Display 1.5 Statistical inferences permitted by study designs



Ramsey and Shafter (2002).

Study note

- For our purposes, the textbook is not sufficiently rigorous regarding the interpretation of linear regression coefficients.

- While our interpretation is less simple than the one provided by most textbooks, it is the correct one for observational data that is prevalent in business.

Regression modelling

Regression modelling

- All the material from Statistical Modelling for Business continues to be relevant in Predictive Analytics.
- In particular, constructing a helpful set of predictor variables is extremely important for supervised learning as it is often essential to improving performance. Constructing a helpful set of predictor variables possible is extremely important for supervised learning. This is known in machine learning and data science as **feature engineering**.. This is known in machine learning and data science as **feature engineering**.
- It is also useful to build models that fit as much as possible the assumptions on data (for example, constant error variance).

Regression modelling

- Data transformation (in particular log and power transformations).
- Categorical predictors.
- Interactions.
- Polynomial regression.
- Regression splines.
- Robust regression.

Potential problems

- Nonlinearity.
- Non-constant error variance.
- Correlated errors.
- Outliers and high leverage points.
- Multicollinearity.
- Non-Gaussianity.

Review questions

- How do we obtain the OLS estimates? Go through the full process.
- What is a sampling distribution?
- We formulated several questions about the advertisement data. Answer some of these questions based on the Python output in the slides.
- What is the correct interpretation of a linear regression model coefficient with observational data?
- What is the difference between predictive and causal analysis?