Business Analytics and Machine Learning

Regression Analysis

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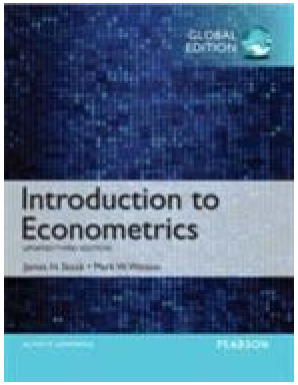
Course Content

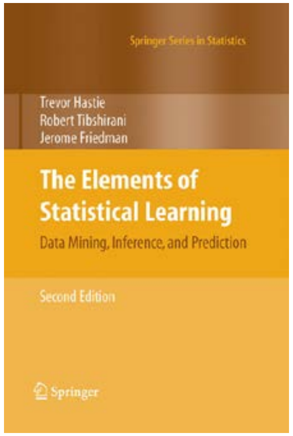
- Introduction
- **Regression Analysis**
- Regression Diagnostics
- Logistic and Poisson Regression
- Naive Bayes and Bayesian Networks
- Decision Tree Classifiers
- Data Preparation and Causal Inference
- Model Selection and Learning Theory
- Ensemble Methods and Clustering
- High-Dimensional Problems
- Association Rules and Recommenders
- Neural Networks

Recommended Literature

- **Introduction to Econometrics**
  - Stock, James H., and Mark W. Watson
  - Chapter 2 – 7, 17, 18



- **The Elements of Statistical Learning**
  - Trevor Hastie, Robert Tibshirani, Jerome Friedman
  - http://web.stanford.edu/~hastie/Papers/ESLII.pdf
  - Section 3.1-3.2: Linear Methods for Regression

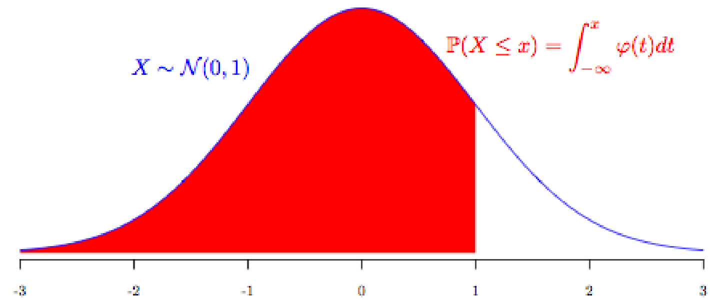


- **Any Introduction to Statistics**
  (e.g.: Statistical Inference by George Casella, Roger L. Berger
  or online course http://onlinestatbook.com/)

Today we revisit three important elements of statistical inference:

- Estimation, testing, regression

Question



What is the probability that a sample of 100 randomly selected elements with a mean of 300 or more gets selected if the true population mean is 288 and the population standard deviation is 60?

	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09
0.0	0.5000	0.5040	0.5080	0.5120	0.5160	0.5199	0.5239	0.5279	0.5319	0.5359
0.1	0.5398	0.5438	0.5478	0.5517	0.5557	0.5596	0.5636	0.5675	0.5714	0.5753
0.2	0.5793	0.5832	0.5871	0.5910	0.5948	0.5987	0.6026	0.6064	0.6103	0.6141
0.3	0.6179	0.6217	0.6255	0.6293	0.6331	0.6368	0.6406	0.6443	0.6480	0.6517
0.4	0.6554	0.6591	0.6628	0.6664	0.6700	0.6736	0.6772	0.6808	0.6844	0.6879
0.5	0.6915	0.6950	0.6985	0.7019	0.7054	0.7088	0.7123	0.7157	0.7190	0.7224
0.6	0.7257	0.7291	0.7324	0.7357	0.7389	0.7422	0.7454	0.7486	0.7517	0.7549
0.7	0.7580	0.7611	0.7642	0.7673	0.7704	0.7734	0.7764	0.7794	0.7823	0.7852
0.8	0.7881	0.7910	0.7939	0.7967	0.7995	0.8023	0.8051	0.8078	0.8106	0.8133
0.9	0.8159	0.8186	0.8212	0.8238	0.8264	0.8289	0.8315	0.8340	0.8365	0.8389
1.0	0.8413	0.8438	0.8461	0.8485	0.8508	0.8531	0.8554	0.8577	0.8599	0.8621
1.1	0.8643	0.8665	0.8686	0.8708	0.8729	0.8749	0.8770	0.8790	0.8810	0.8830
1.2	0.8849	0.8869	0.8888	0.8907	0.8925	0.8944	0.8962	0.8980	0.8997	0.9015
1.3	0.9032	0.9049	0.9066	0.9082	0.9099	0.9115	0.9131	0.9147	0.9162	0.9177
1.4	0.9192	0.9207	0.9222	0.9236	0.9251	0.9265	0.9279	0.9292	0.9306	0.9319
1.5	0.9332	0.9345	0.9357	0.9370	0.9382	0.9394	0.9406	0.9418	0.9429	0.9441
1.6	0.9452	0.9463	0.9474	0.9484	0.9495	0.9505	0.9515	0.9525	0.9535	0.9545
1.7	0.9554	0.9564	0.9573	0.9582	0.9591	0.9599	0.9608	0.9616	0.9625	0.9633
1.8	0.9641	0.9649	0.9656	0.9664	0.9671	0.9678	0.9686	0.9693	0.9699	0.9706
1.9	0.9713	0.9719	0.9726	0.9732	0.9738	0.9744	0.9750	0.9756	0.9761	0.9767
2.0	0.9772	0.9778	0.9783	0.9788	0.9793	0.9798	0.9803	0.9808	0.9812	0.9817
2.1	0.9821	0.9826	0.9830	0.9834	0.9838	0.9842	0.9846	0.9850	0.9854	0.9857
2.2	0.9861	0.9864	0.9868	0.9871	0.9875	0.9878	0.9881	0.9884	0.9887	0.9890
2.3	0.9893	0.9896	0.9898	0.9901	0.9904	0.9906	0.9909	0.9911	0.9913	0.9916
2.4	0.9918	0.9920	0.9922	0.9925	0.9927	0.9929	0.9931	0.9932	0.9934	0.9936
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2.6	0.9953	0.9955	0.9956	0.9957	0.9959	0.9960	0.9961	0.9962	0.9963	0.9964
2.7	0.9965	0.9966	0.9967	0.9968	0.9969	0.9970	0.9971	0.9972	0.9973	0.9974
2.8	0.9974	0.9975	0.9976	0.9977	0.9977	0.9978	0.9979	0.9979	0.9980	0.9981
2.9	0.9981	0.9982	0.9982	0.9983	0.9984	0.9984	0.9985	0.9985	0.9986	0.9986
3.0	0.9987	0.9987	0.9987	0.9988	0.9988	0.9989	0.9989	0.9989	0.9990	0.9990

Question

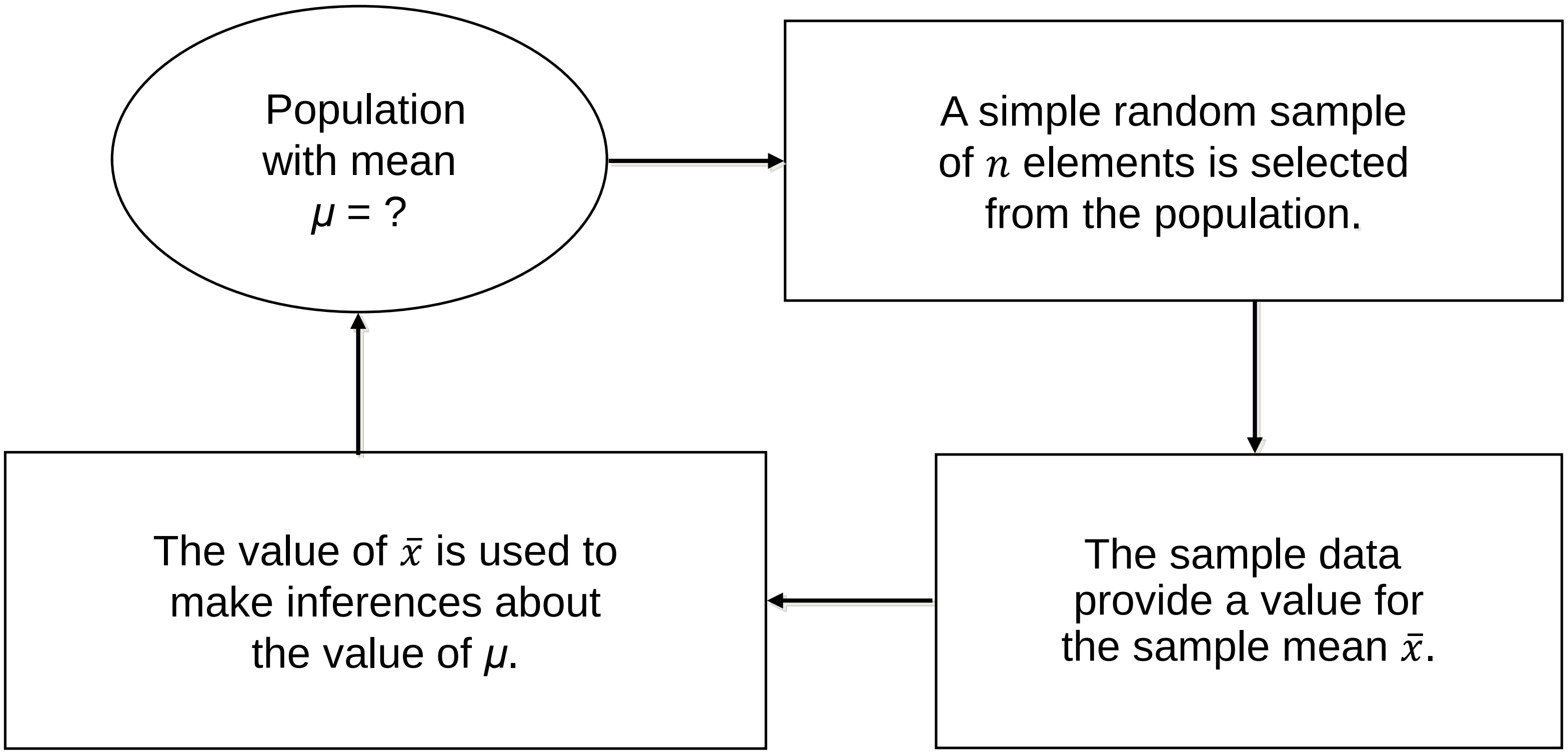
- What is the probability that a sample of 100 randomly selected elements with a mean of 300 or more get selected if the true population mean is 288 and the population standard deviation is 60?

  - The sample was randomly selected and we draw on the Central Limit Theorem.
  - We need to take the standard dev. of the sample mean.

$$Z = \frac{\overline{X} - \mu}{\sigma_{\overline{X}}} = \frac{\overline{X} - \mu}{\sigma / \sqrt{n}} = \frac{300 - 288}{60 / \sqrt{100}} = 2$$

  - Check out the table of the standard normal distribution.
  - There is a 2.28% chance of selecting a sample with a mean > 300.

Statistical Estimation



Statistical Estimation

Estimate

Point estimate

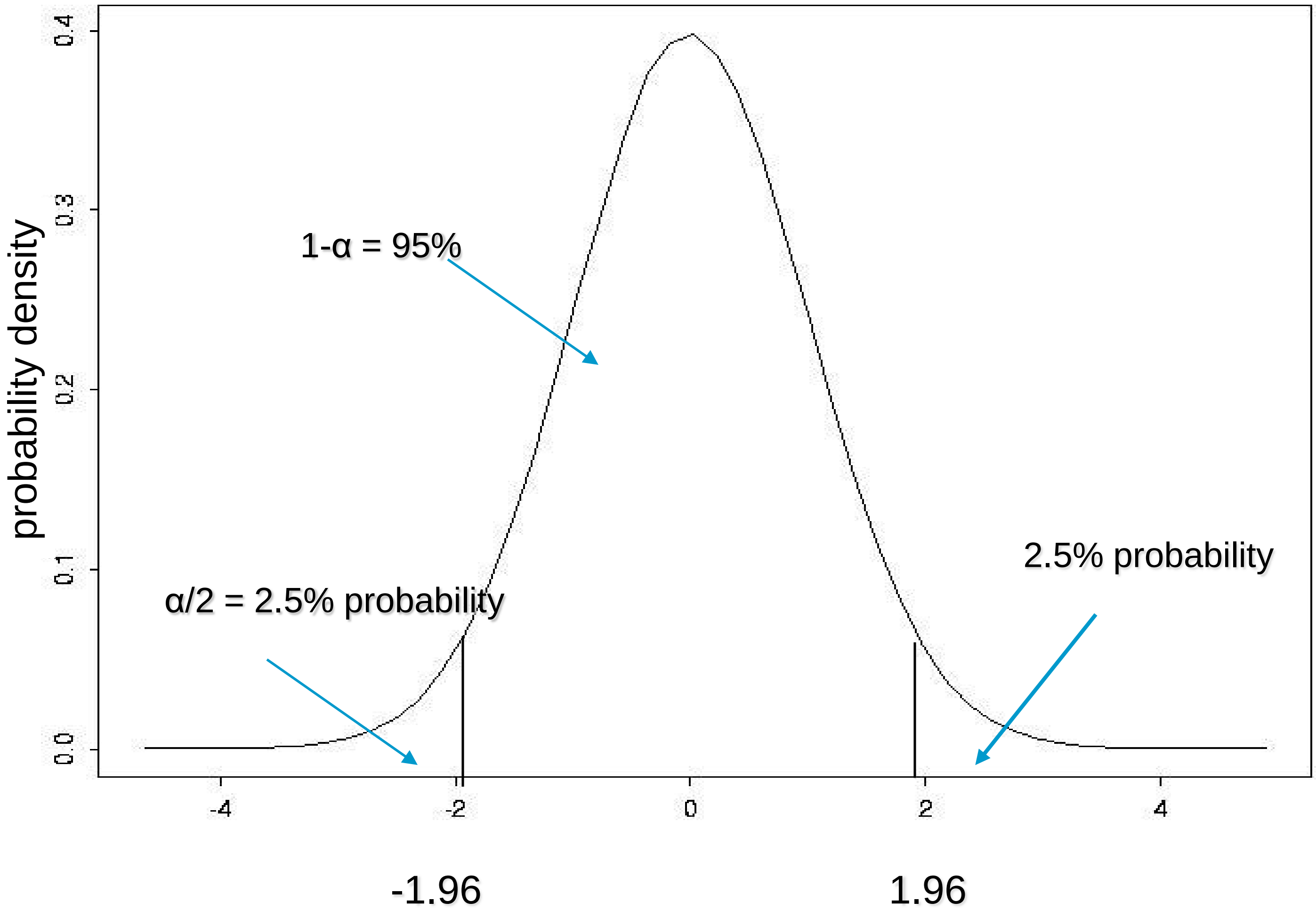
- sample mean
- sample proportion

Interval estimate

- confidence interval for mean
- confidence interval for proportion

Point estimate is always within the interval estimate

Confidence Interval



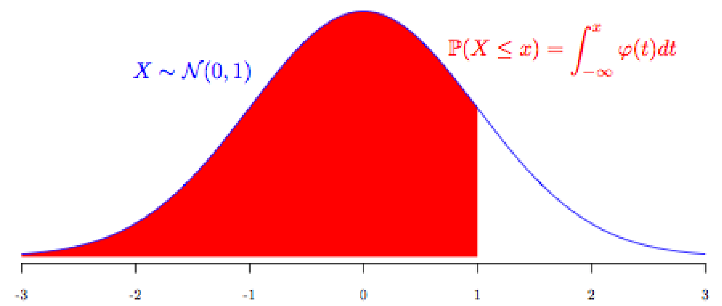
Confidence Interval (CI)

Suppose the samples are drawn from a normal distribution. The CI provide us with a range of values that we believe, with a given level of confidence, contains a population parameter:

$$\Pr\ (\bar{X} - z_{(1-\frac{\alpha}{2})}\ \frac{\sigma}{\sqrt{n}} < \mu < \bar{X} + z_{(1-\frac{\alpha}{2})} \frac{\sigma}{\sqrt{n}})$$

There is a 95% chance that your interval contains μ.

$$\Pr(\bar{X} - 1.96\, SD < \mu < \bar{X} + 1.96\, SD) = 0.95$$



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3.0	0.9987	0.9987	0.9987	0.9988	0.9988	0.9989	0.9989	0.9989	0.9990	0.9990

Example

Suppose we have a sample of n = 100 persons

mean = 215, standard deviation = 20

95% CI = $\bar{X} \pm 1.96 * \sigma/\sqrt{n}$

Lower Limit: 215 – 1.96*20/10

Upper Limit: 215 + 1.96*20/10

= (211, 219)

“We are 95% confident that the interval 211-219 contains μ.”

If the population standard deviation σ is unknown, use the sample standard deviation s and the *t*-distribution. If n is large enough, you might also use s and the standard Normal distribution.

Effect of Sample Size

Suppose we had only 10 observations

What happens to the confidence interval?

$$\bar{X} \pm 1.96 * \frac{\sigma}{\sqrt{n}}$$

For $n = 100,\ 215 \pm 1.96 * (20)/\sqrt{100} \approx (211{,}219)$

For $n = 10,\ 215 \pm 1.96 * (20)/\sqrt{10} \approx (203{,}227)$

Larger sample size = smaller interval

Effect of Confidence Level

Suppose we use a 90% confidence level
What happens to the confidence interval?

$$\bar{X} \pm 1.645 * s / \sqrt{n}$$

90%: $215 \pm 1.645 * (20) / \sqrt{100} \approx (212,218)$

Lower confidence level = smaller interval
(A 99% interval would use 2.58 as multiplier and the interval would be larger)

Effect of Standard Deviation

Suppose we had a *s* of 40 (instead of 20)

What happens to the confidence interval?

$$\bar{X} \pm 1.96 * \frac{\sigma}{\sqrt{n}}$$

$$215 \pm 1.96 * (40) / \sqrt{100} \approx (207, 223)$$

More variation = larger interval

Estimation for Population Mean μ

Point estimate: $\bar{X} = \frac{\sum X}{n}$

Estimate of variability in population $s = \sqrt{\frac{1}{n-1}\sum_i (X_i - \bar{X})^2}$

(<u>if σ is unknown, use s</u>)

True standard deviation of sample mean $SD = \sigma/\sqrt{n}$

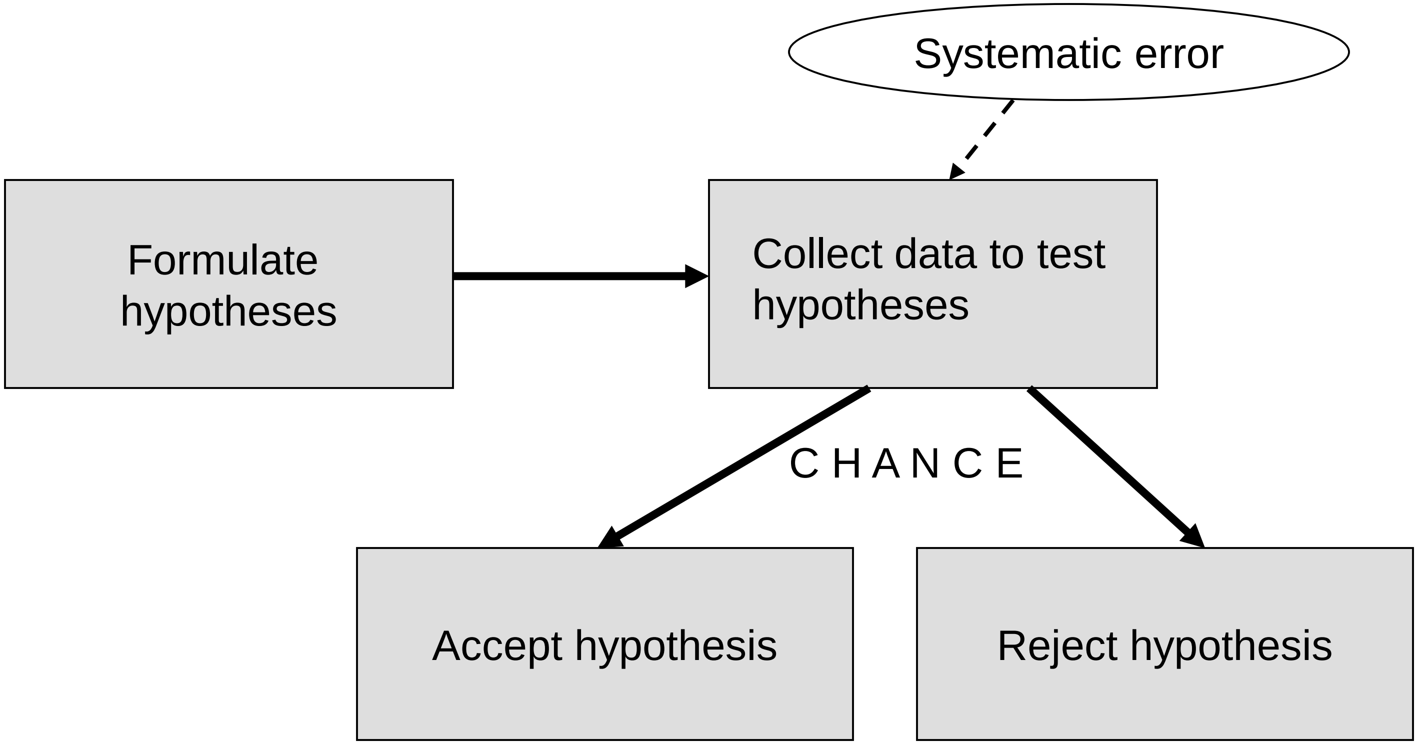
<u>Standard error</u> of sample mean $SE = s/\sqrt{n}$

95% confidence interval $\bar{X} \pm 1.96\,SD$

, or $\bar{X} \pm 1.96\,SE$

How does the size of the random sample impact the size of a confindence interval?

Statistical Tests



Random error (chance) can be controlled by statistical significance or by confidence interval

Hypothesis Testing

- State null and alternative hypothesis (H_0 and H_1)
  - H_0 usually a statement no difference between groups
- Choose α level (related to confidence level)
  - Probability of falsely rejecting H_0 (Type I error), typically 0.05 or 0.01
- Calculate test statistic, find p-value (p)
  - Measures how far data are from what you expect under null hypothesis
- State conclusion:

$p \leq \alpha$, reject H_0

$p > \alpha$, insufficient evidence to reject H_0

Hypothesis Testing

Hypothesis: A statement about parameters of population or of a model ($\mu = 200$?)

Test: Does the data agree with the hypothesis? (sample mean 220)
Simple random sample from a normal population
(or n large enough for CLT)

H_o: $\mu = \mu_o$
H_1 : $\mu \neq \mu_o$, pick α

Z-Test

Problem of interest:

- Population mean μ and population standard deviation σ are known

Z-confidence interval: $\bar{X} \pm z_{(1-\alpha/2)} \frac{\sigma}{\sqrt{n}}$

Z-test: $z = \frac{\bar{X}-\mu_0}{\sigma/\sqrt{n}}$

$\underline{H_1}$	<u>Rejection region</u>
$\mu \neq \mu_0$	$\lvert z\rvert \geq z_{1-\alpha/2}$
$\mu > \mu_0$	$z \geq z_{1-\alpha}$
$\mu < \mu_0$	$z \leq z_{\alpha} = -z_{1-\alpha}$

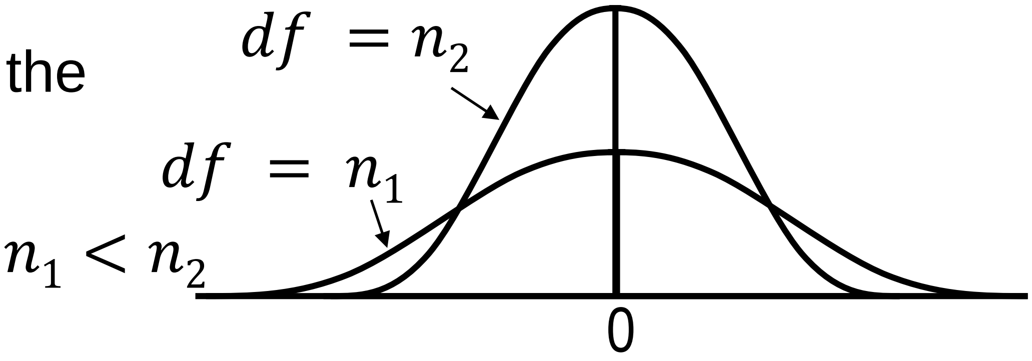
Student t-Distribution: Test Statistic for a mean μ with unknown σ

$$t(df = n - 1) = \frac{\bar{X} - \mu}{s/\sqrt{n}}$$

When the population is normally distributed, the statistic t is *Student t* distributed.

The "degrees of freedom (df)", a function of the sample size, determines how spread the distribution is (compared to the normal distribution)

The t distribution is bell-shaped, and symmetric around zero.

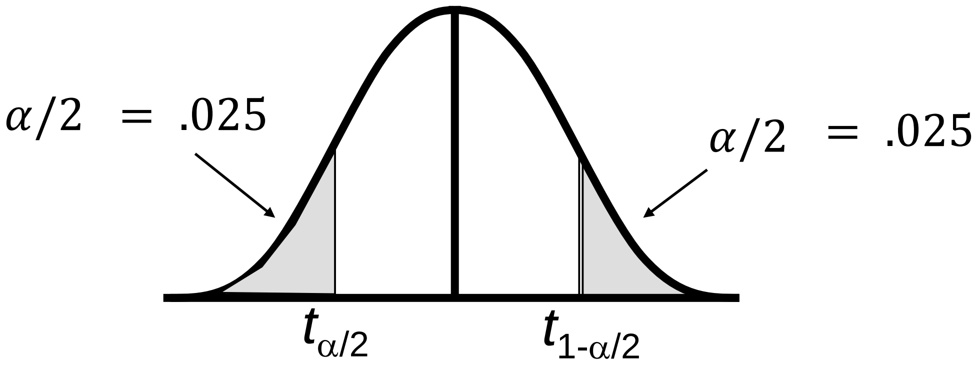


CI and 2-Sided Tests

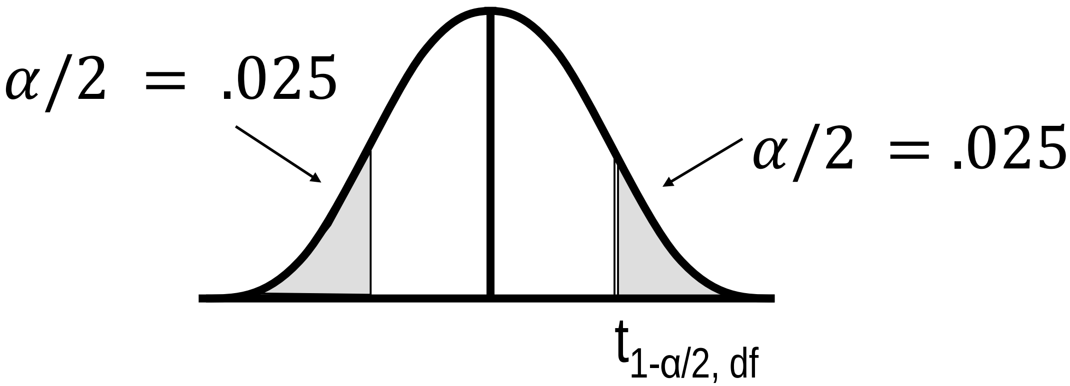
- A level α 2-sided test rejects $\mathrm{H}_0: \mu = \mu_0$ exactly when the value μ_0 falls outside a level $1-\alpha$ confidence interval for μ.
- Calculate $1-\alpha$ level confidence interval, then
  - if μ_0 within the interval, do not reject the null hypothesis,

$$|\mathrm{t}| < \mathrm{t}_{1-\alpha/2}$$

  - otherwise, $|\mathrm{t}| \geq \mathrm{t}_{1-\alpha/2}$ => reject the null hypothesis.



Student t-Distribution for α=0.05



Degrees of Freedom	$t_{.9}$	$t_{.95}$	$t_{.975}$	$t_{.99}$	$t_{.995}$
1	3.078	6.314	12.706	31.821	63.657
2	1.886	2.92	4.303	6.965	9.925
.	.	.	.	.	.
.	.	.	.	.	.
24	.	1.711	2.064	2.492	.
.	.	.	.	.	.
.	.	.	.	.	.
200	1.286	1.653	1.972	2.345	2.601
∞	1.282	1.645	1.96	2.326	2.576

t-distribution critical values

Possible Results of Tests

		What we decide	
		Reject null	Fail to reject null
Reality	Null true	Type I Error (α) (false positive)	Correct
	Null false	Correct	Type II Error (β) (false negative)

Type I error - You reject the null hypothesis when the null hypothesis is actually true.

Type II error - You fail to reject the null hypothesis when the the alternative hypothesis is true.

t-Tests

Formula is slightly different for each:

- *Single sample:*
  - tests whether a sample mean is significantly different from a pre-existing value
- *Paired samples:*
  - tests the relationship between 2 linked samples, e.g. means obtained in 2 conditions by a single group of participants
- *Independent samples:*
  - tests the relationship between 2 independent populations

The Paired t -Test with 2 Paired Samples

Null hypothesis: $\mathrm{H}_0\!: \mu_d = \mu_1 - \mu_2 = \Delta_0$

Test statistic: $t = \frac{\bar{d} - \Delta_0}{s/\sqrt{n}}$

H_1	Rejection region
$\mu_d \neq \Delta_0$	$\lvert t \rvert \geq t_{1-\alpha/2,\, n-1}$
$\mu_d > \Delta_0$	$t \geq t_{1-\alpha,\, n-1}$
$\mu_d < \Delta_0$	$t \leq t_{\alpha,\, n-1} = -t_{1-\alpha,\, n-1}$

Observations are dependent, e.g., pre and post test, left and right eyes, brother-sister pairs

The Paired t -Test with 2 Paired Samples

Subjects: random sample of 25 students from TUM

Mean grades of the students on two subsequent exams A and B

Is there a significant difference between the two exams?

Null Hypothesis: $E(A) = E(B)$

Answer can be given based on significance testing

No.	*A*	*B*	d=*A-B*
1	3.7	3.5	0.2
2	2.2	2.3	-0.1
...			
25	4.8	4.4	0.4

$\bar{d} = 0.093$

$s = 0.150$

$n = 25$

$s/\sqrt{n} = 0.03$

$t_{0.975;24} = 2.064$

$$t = \frac{\bar{d}}{s/\sqrt{n}} = \frac{0.093}{0.03} = 3.1$$

$$p = \Pr\{|\mathrm{t}| > 3.1 | DF = 24\} = 0.005$$

The p-Value

The p-value describes the probability of having $t = 3.1$ (or larger), given the null hypothesis. The smaller the p-value, the more unlikely it is to observe the corresponding sample value (or more extreme) by chance under H_0.

```
> # R code
> x = c(3, 0, 5, 2, 5, 5, 5, 4, 4, 5)
> y = c(2, 1, 4, 1, 4, 3, 3, 2, 3, 5)
> t.test(x,y,alt="two.sided", paired=TRUE)

           Paired t-test

data:  x and y
t = 3.3541, df = 9, p-value = 0.008468
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 0.325555 1.674445
sample estimates:
mean of the differences
```

Independent Samples

2 independent samples (possibly different size and variance):

Does the amount of credit card debt differ between households in rural areas compared to households in urban areas?

Population 1	Population 2
All Rural Households	All Urban Households
m_1	m_2

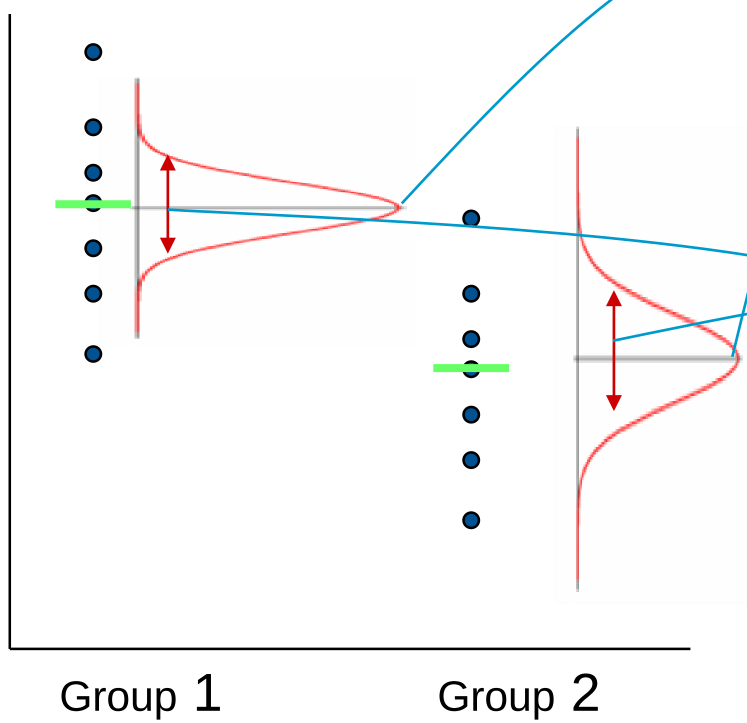
Null Hypothesis: $\mathrm{H}_0 : m_1 = m_2$

Alternate Hypothesis: $\mathrm{H}_1 : m_1 \neq m_2$

Independent Two-Sample t -Test (Welch's t -Test)

Two-sample unpaired t-test with (un)equal sample sizes, assuming unequal variance

Under $\mathrm{H_o}$ t follows a t-distribution with $\dfrac{(s_1^{\ 2}/n_1 + s_2^{\ 2}/n_2)^2}{(s_1^{\ 2}/n_1)^2/(n_1-1) + (s_2^{\ 2}/n_2)^2/(n_2-1)}$ degrees of freedom (df)



$$t = \frac{\bar{x}_1 - \bar{x}_2}{s_{\bar{x}_1 - \bar{x}_2}}$$

$$s_{\bar{x}_1 - \bar{x}_2} = \sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}$$

Independent Two-Sample t –Test: Example

Group 1	Group 2
21	22
19	25
18	27
18	24
23	26
17	24
19	28
16	26
21	30
18	28
$\bar{x}_1 = 19$	$\bar{x}_2 = 26$
$s_1 = \sqrt{40/9}$	$s_2 = \sqrt{50/9}$

$df = 18$ (rounded to integer)

$$t = \frac{\bar{x}_1 - \bar{x}_2}{s_{\bar{x}_1 - \bar{x}_2}} = \frac{19 - 26}{1} = -7$$

$$s_{\bar{x}_1 - \bar{x}_2} = \sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}} = \sqrt{\frac{40/9}{10} + \frac{50/9}{10}}$$
$$= 1$$

$$t_{(0.975,18)} = 2.101$$

$$|t| \geq t_{(0.975,18)}$$

→ Reject H_0 $(\mu_1 - \mu_2 = 0)$

Selected Statistical Tests

- **Parametric Tests**
  - The family of t-tests
    - Compares two sample means or tests a single sample mean
  - F-test
    - Compares the equivalence of variances of two samples

- **Non-parametric Tests**
  - Wilcoxon signed-rank test for 2 *paired* i.i.d samples.
  - Mann-Whitney-U test is used for 2 *independent* i.i.d samples
  - Kruskal-Wallis-Test for several i.i.d non-normally distributed samples

- **Tests of the Probability Distribution**
  - Kolmogorov-Smirnov and Chi-square test
    - used to determine whether two underlying probability distributions differ, or whether an underlying probability distribution differs from a hypothesized distribution

Please explain the role of confidence intervals in a single-sample t-test.

Linear Regression

- **Regressions identify relationships between dependent and independent variables**
  - Is there an association between the two variables
  - Estimation of impact of an independent variable
  - Formulation of the relation in a functional form
  - Used for numerical prediction and time series forecasting

- **Regression as an established statistical technique:**
  - Sir Francis Galton (1822-1911) studied the relationship between a father’s height and the son’s height

Terminology

- Data streams X and Y, forming the measurement tuples $(x_1, y_1), \dots, (x_n, y_n)$
- x_i is the predictor (regressor, covariate, feature, independent variable)
- y_i is the response (dependent variable, outcome)
- Denote the *regression function* by: $\eta(x) = E\,(Y\,|x)$
- The linear regression model assumes a specific linear form

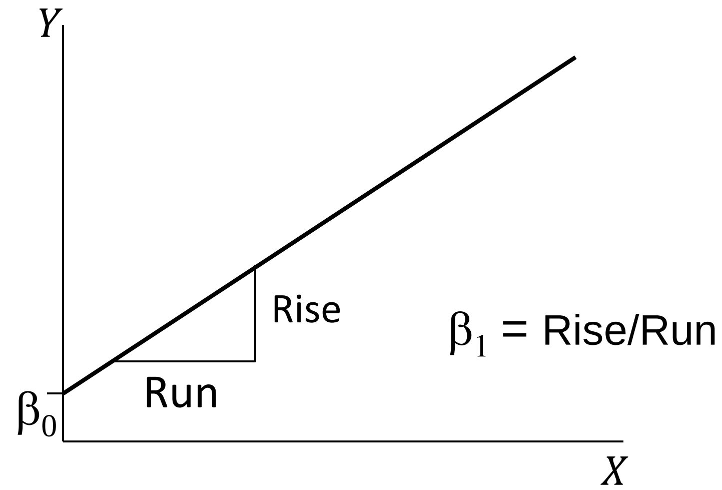
The Simple Linear Regression Model

- Linear regression is a statistical tool for numerical predictions
- The first order linear model

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

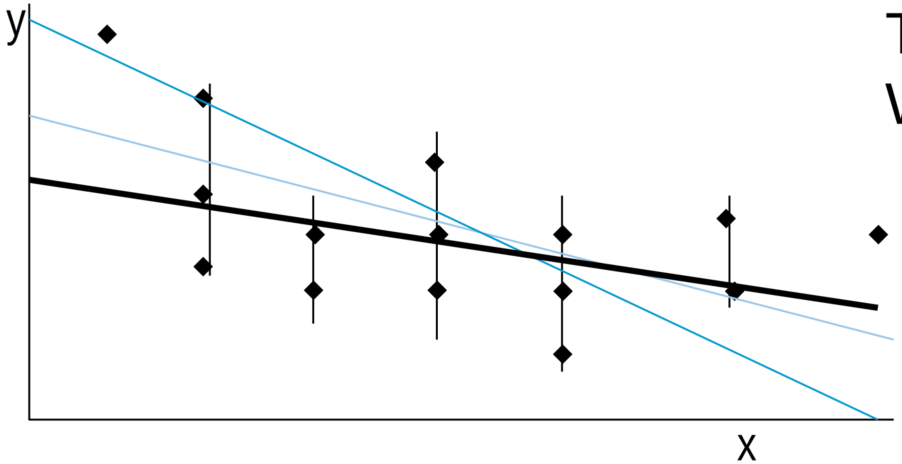
β_0 and β_1 are unknown, therefore, are estimated from the data

Y = response variable
X = predictor variable
β_0= y-axis intercept
β_1 = slope of the line
ε = random error term (residual)



Estimating the Coefficients

- Coefficients are random variables
- (Ordinary Least Squares) estimates are determined by
  - drawing a sample from the population of interest
  - calculating sample statistics
  - producing a straight line that cuts into the data



The question is:
Which straight line fits best?

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

OLS Estimators

- Ordinary Least Squares (OLS) approach:
  - Minimize the sum of squared residuals (aka. loss function)

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

$$\min \sum_{\mathrm{i}} e_{\mathrm{i}}^2 = \min \sum_{\mathrm{i}} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2$$

$$\hat{\beta}_1 = \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sum_i (x_i - \overline{x})^2} = \frac{Cov(x, y)}{Var(x)}$$

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

Example

- A car dealer wants to find the relationship between the odometer reading and the selling price of used cars.
- A random sample of 100 cars is selected, and the data recorded.
- Find the regression line.

Car	Odometer	Price
1	37388	5318
2	44758	5061
3	45833	5008
4	30862	5795
5	31705	5784
6	34010	5359
.	.	.
.	.	.
.	.	.

Independent/predictor variable x

Dependent/respond variable y

Solving a Simple Regression

- To calculate β_0 and β_1 we can calculate several statistics first:

$$\bar{x} = 36009.45; \qquad s_x^2 = \frac{\sum (x_i - \bar{x})^2}{n-1} = 43{,}528{,}688$$

$$\bar{y} = 5411.41; \qquad \operatorname{cov}(X,Y) = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n-1} = -1{,}356{,}256$$

where $n = 100$:

$$\hat{\beta}_1 = \frac{\operatorname{cov}(X,Y)}{s_x^2} = \frac{-1{,}356{,}256}{43{,}528{,}688} = -.0312$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = 5411.41 - (-.0312)(36{,}009.45) = 6{,}533$$

$$\boxed{\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x = 6{,}533 - 0.0312x}$$

Residual Sum of Squares (RSS)

- This is the sum of squared differences between the points and the regression line
- It can serve as a measure of how well the line fits the data (fits well, if statistic is small)
- An unbiased estimator of the RSS of the population is given by

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Total Deviation

- The Total Sum of Squares (TSS) is the sum of the Explained Sum of Squares (ESS) and the RSS.

$$\boxed{\sum(y-\bar{y})^2 \qquad = \sum(\hat{y}-\bar{y})^2 \qquad + \sum(y-\hat{y})^2}$$

TSS = ESS + RSS

Total deviation = explained deviation + unexplained deviation

Coefficient of Determination

- R^2 measures the proportion of the variation in y that is explained by the variation in x

$$ESS = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 \ , TSS = \sum_{i=1}^{n} (y_i - \bar{y})^2 = ESS + RSS$$

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

- R^2 takes on any value between zero and one
  - $R^2 = 1$: Perfect match between the line and data points
  - $R^2 = 0$: There is no linear relationship between x and y

Testing the Coefficients

- Test the significance of the linear relationship

  $\mathrm{H}_0\colon \beta_1 = 0$

  $\mathrm{H}_1\colon \beta_1 \neq 0$
- The test statistic is

$$t = \frac{\hat{\beta}_1}{\mathrm{SE}(\hat{\beta}_1)} = \frac{\hat{\beta}_1}{\sqrt{\frac{\mathrm{RSS}}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \cdot \frac{1}{n-2}}}$$

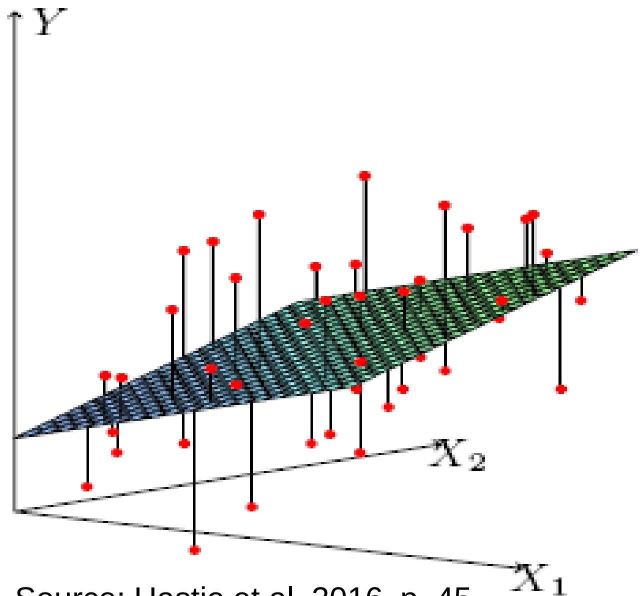
Variance of $\hat{\beta}_1$

- If $SE(\hat{\beta}_1)$ is large, then $\hat{\beta}_1$ must be large to reject H_0
- $SE(\hat{\beta}_1)$ is smaller, if the x_i are more spread out
- If the error variable is normally distributed, the statistic is a Student t –distribution with $n-2$ degrees of freedom (if n is large, draw on the CLT)
- Reject H_0, if: $t < t_{\alpha/2}$ or $t > t_{1-\alpha/2}$

The Multiple Linear Regression Model

- A p-variable regression model can be expressed as a series of equations
- Equations condensed into a matrix form, give the general linear model
- β coefficients are known as partial regression coefficients
- X_1, X_2, for example,
  - X_1='years of experience'
  - X_2='age'
  - Y='salary'
- Estimated equation:

$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 = \mathbf{X}\hat{\beta}$



Source: Hastie et al. 2016, p. 45

Matrix Notation

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

y	$\boldsymbol{X}$	β	+ ε
$(n \times 1)$	$(n \times (p+1))$	$((p+1) \times 1)$	$(n \times 1)$

OLS Estimation

- Sample-based counter part to population regression model:

$$y = \mathbf{X}\beta + \varepsilon$$
$$y = \mathbf{X}\hat{\beta} + e$$

- OLS requires choosing values of the estimated coefficients, such that Residual Sum of Squares (RSS) is as small as possible for the sample

$$RSS = e^T e = (y - \mathbf{X}\hat{\beta})^T (y - \mathbf{X}\hat{\beta})$$

- Need to differentiate with respect to the unknown coefficients

Least Squares Estimation

$\mathbf{X}$ is $n \times (p+1)$, y is the vector of outputs

RSS(β) = $(y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta)$

If $\mathbf{X}$ is full rank, then $\mathbf{X}^T\mathbf{X}$ is positive definite

$$RSS = \left(y^T y - 2\beta^T \mathbf{X}^T \mathrm{y} + \beta^T \mathbf{X}^T \mathbf{X}\beta\right)$$

$$\frac{\partial RSS}{\partial \beta} = -2\mathbf{X}^T \mathrm{y} + 2\mathbf{X}^T\mathbf{X}\beta = 0$$ First-order condition

$$\beta = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T y$$

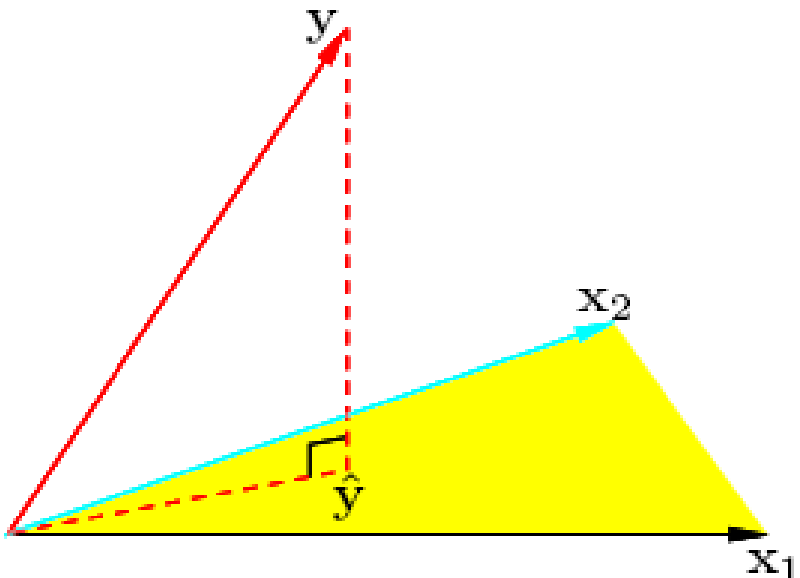
$$\hat{y} = \underbrace{\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T}_{\text{“Hat” or projection matrix } H} y$$

Geometrical Representation

- Least square estimates in $\mathbb{R}^n$
- Minimize RSS(β)=$||y - \mathbf{X}\beta||^2$, s.t. residual vector y – ŷ is orthogonal to this subspace.

Definition (Projection):
The set $C \subset \mathbb{R}^n$ is non-empty, closed and convex. For a fixed $y \in \mathbb{R}^n$ we search a point $\hat{y} \in C$, with the smallest distance to y (wrt. the Euclidean norm), i.e. we solve the minimization problem

$$P_C(y) = \min_{\hat{y} \in C} ||y - \hat{y}||^2$$



Source: Hastie et al. 2016, p. 46

Example

y:	2.6	1.6	4.0	3.0	4.9
x:	1.2	3.0	4.5	5.8	7.2

$y = \mathbf{X}\hat{\beta} + e$

$$\begin{pmatrix} 2.6 \\ 1.6 \\ 4.0 \\ 3.0 \\ 4.9 \end{pmatrix} = \begin{pmatrix} 1 & 1.2 \\ 1 & 3.0 \\ 1 & 4.5 \\ 1 & 5.8 \\ 1 & 7.2 \end{pmatrix} \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{pmatrix} + \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \end{pmatrix}$$

$\hat{\beta} = \left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-\mathbf{1}}\mathbf{X}^{\mathbf{T}}\mathrm{y}$

$$\left(\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1.2 & 3.0 & 4.5 & 5.8 & 7.2 \end{pmatrix} \begin{pmatrix} 1 & 1.2 \\ 1 & 3.0 \\ 1 & 4.5 \\ 1 & 5.8 \\ 1 & 7.2 \end{pmatrix} \right)^{-1} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1.2 & 3.0 & 4.5 & 5.8 & 7.2 \end{pmatrix} \begin{pmatrix} 2.6 \\ 1.6 \\ 4.0 \\ 3.0 \\ 4.9 \end{pmatrix} =$$

$$\begin{pmatrix} 5 & 21.7 \\ 21.7 & 116.17 \end{pmatrix}^{-1} \begin{pmatrix} 16.1 \\ 78.6 \end{pmatrix} = \begin{pmatrix} 1.0565 & -0.1973 \\ -0.1973 & 0.0455 \end{pmatrix} \begin{pmatrix} 16.1 \\ 78.6 \end{pmatrix} = \begin{pmatrix} 1.498 \\ 0.397 \end{pmatrix}$$

Check Results in R

```
> y <- c(2.6, 1.6, 4.0, 3.0, 4.9)
> x <- c(1.2, 3.0, 4.5, 5.8, 7.2)
> mod <- lm(y ~ x)
> summary(mod)

Call:
lm(formula = y ~ x)

Residuals:
      1       2       3       4       5
 0.6259 -1.0883  0.7165 -0.7993  0.5452

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   1.4980     1.0322   1.451    0.243
x             0.3968     0.2142   1.853    0.161

Residual standard error: 1.004 on 3 degrees of freedom
Multiple R-Squared: 0.5336,     Adjusted R-squared: 0.3782
F-statistic: 3.433 on 1 and 3 DF,  p-value: 0.1610
```

1. check coefficients
2. check significance
3. check coefficient of determination

Selected Statistics

Adjusted R²

- It represents the proportion of variability of y explained by X
  R² is adjusted so that models with a different number of variables can be compared

$$\bar{R}^2 = 1 - \frac{RSS/(n-p-1)}{TSS/(n-1)}$$

The F-test

- Significant F indicates a linear relationship between y and at least one of the xs: $\mathrm{H}_0\!: \ \beta_1 = \beta_2 \ldots \beta_p = 0$

The *t*-test of each partial regression coefficient

- Significant t indicates that the variable in question influences the response variable while controlling for other explanatory variables

Model Specification

In regression analysis the specification is the process of developing a regression model.

- This process consists of selecting an appropriate functional form for the model and choosing which variables to include.
- The model might include irrelevant variables or omit relevant variables

Non-linear models are challenging, but some nonlinear regression problems can be linearized.

- Dummy variables for discrete variables (e.g. 0/1 for gender)
- Quadratic models: $y = \beta_0 + \beta_1 x_1 + \beta_2 {x_2}^2 + \varepsilon$ use $z_2 = {x_2}^2$
- Models with interaction terms $y = \beta_0 + \beta_1 x_1 x_2$ use $z_1 = x_1 x_2$
- Exponential terms $y = \alpha x^{\beta} \varepsilon$ can be transformed using the logarithm to

$$\ln(y) = \ln(\alpha) + \beta \ln(x) + \ln(\varepsilon)$$

Subset Selection

- Setting: Possibly a large set of predictor variables, some irrelevant
- Goal: Fit a parsimonious model that explains variation in Y with a small set of predictors
  - Aka. subset selection or feature selection problem
- Automated procedures:
  - Best subset (among all exponentially many, computationally expensive)
  - Backward elimination (top down approach)
  - Forward selection (bottom up approach)
  - Stepwise regression (combines forward/backward)

- More in the context of the class on dimensionality reduction
  - Subset selection vs. shrinkage methods

Example: Backward Elimination

- Select a significance level to stay in the model (generally 0.05 is too low, causing too many variables to be removed)
- Fit the full model with all possible predictors
- Consider the predictor with lowest t-statistic (highest p-value).
  - If $p >$ sign. level, remove the predictor and fit model without this variable (must re-fit model here because partial regression coefficients change)
  - If $p \leq$ sign. level, stop and keep current model
- Continue until all predictors have p-values below sign. level

- Forward selection is similar: predictors with lowest p-value are added until none is left with $p >$ sign. level.

Please explain the term „ordinary least squares“ estimator and how it solves a convex optimization problem.