

# 1 Hypothesentest

## 1.1 Test Manual

1. Check samples
  - If 1 sample:  $\sigma_0$  known or unknown
  - If 2 sample: dependent or independent
2. State  $H_0$  and  $H_1$
3. Select and calculate the test statistics
4. Select  $\alpha$  (given)
5. Find the critical value in the table
6. Result

### 1.1.1 Step 1

**dependent:** A dependent variable is the variable being tested and measured in a scientific experiment.

**independent:** An independent variable is the variable that is changed or controlled in a scientific experiment to test the effects on the dependent variable.

### 1.1.2 Step 2

Hypothesis	$H_0$	$H_1$
Two-sided	$\mu_x = \mu_0$	$\mu_x \neq \mu_0$
One-sided	$\mu_x \leq \mu_0$	$\mu_x > \mu_0$
One-sided	$\mu_x \geq \mu_0$	$\mu_x < \mu_0$

### 1.1.3 Step 3

#### 1 Sample:

$\sigma_x$  known  $\rightarrow$  Gauss/z-test  $z_0 = \frac{\bar{x} - \mu_0}{\sigma_x} \sim N(0,1)$

$\sigma_x$  unknown  $\rightarrow$  t-test  $t_0 = \frac{\bar{x} - \mu_0}{s_x} \sqrt{n} \sim t_{n-1}$  with  $s_x^2 = \frac{1}{n-1} \sum (x_i - \bar{x})^2$

#### 2 Sample:

independent  $\rightarrow$  *Welch - Test*  $t_0 = \frac{\bar{x} - \bar{w} - \mu_0}{s_{\bar{x} - \bar{w}}} t_{df}$

dependent  $\rightarrow$  *Paired t - test*

### 1.1.4 Step 5

$t^c$  critical value in the table

Gauss/z-Test  $\rightarrow$  use normal distribution

t-test, Welch-Test and paired t-Test  $\rightarrow$  t-distribution

$H_1$	$t^{c}range$	$t^{c}range$
$\mu_x \neq \mu_0$	can be any	$ t_{1-\frac{\alpha}{2};df}^c  =  t_{\frac{\alpha}{2};df}^c $
$\mu_x > \mu_0$	must be positive	$ t_{1-\alpha;df}^c $
$\mu_x < \mu_0$	must be negative	$ t_{\alpha;df}^c $

### 1.1.5 Step 6

Reject  $H_0$ :

$H_1$	$t^{c}range$	$t^{c}range$
$\mu_x \neq \mu_0$	$p < \alpha$	$ t_0  >  t_{1-\frac{\alpha}{2};df}^c $
$\mu_x > \mu_0$	$p < \alpha$	$t_0 > t_{1-\alpha;df}^c$
$\mu_x < \mu_0$	$p < \alpha$	$t_0 < t_{\alpha;df}^c$

$\sigma$  - Standard Deviation for variable

s - Standard Deviation for sample

## 1.2 Welch-Test

$\mu_0$  - Value of Null-Hypothesis

$\bar{x}$  - Mean of first set

$\bar{w}$  - Mean of second set

$t_0$  - P-Value of Welch-Test

$t^c$  - P-Value from from T-Table

## 1.3 T-Test

H1	Rejection Region
$\bar{x} \neq \mu_0$	$ t_0  \geq t_{1-\alpha/2,n-1}$
$\bar{x} > \mu_0$	$t_0 > t_{1-\alpha,n-1}$
$\bar{x} < \mu_0$	$t_0 < t_{1-\alpha,n-1}$

## 1.4 Gauss/z-Test

H1	Rejection Region
$\mu \neq \mu_0$	$ z_0  \geq z_{1-\alpha/2}$
$\mu > \mu_0$	$z_0 > z_{1-\alpha}$
$\mu < \mu_0$	$z_0 < z_{1-\alpha}$

## 1.5 Confidence Intervals

$\sigma_x$  known:  $[\bar{x} - z_{1-\frac{\alpha}{2}}^c * \frac{\sigma_x}{\sqrt{n}}, \bar{x} + z_{1-\frac{\alpha}{2}}^c * \frac{\sigma_x}{\sqrt{n}}]$

$\sigma_x$  unknown, use  $S_x$  as estimate instead:  $[\bar{x} - t_{1-\frac{\alpha}{2}; n-1}^c * \frac{s_x}{\sqrt{n}}, \bar{x} + t_{1-\frac{\alpha}{2}; n-1}^c * \frac{s_x}{\sqrt{n}}]$

## 2 Linear Regression

Fit through linear function:  $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 * x_i$

Residual  $e$  is the difference between observed and predicted value:  $\hat{e}_i = y_i - \hat{y}_i$

**Residual Sum Squares:** Sum of all squared errors

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

$$\hat{\beta}_1 = \frac{Cov(x,y)}{Var(x)}$$

**Interpretation:**

$\hat{\beta}_0$ : Output of linear regression model when all predictor variables are set to 0. Also called the intercept on y.

$\hat{\beta}_1$ : Change in y for each unit increase in x.

**Hypothesis test:**

$$t_0 = \frac{\hat{\beta}_1}{SE(\hat{\beta}_1)} \quad t_n - 2$$

$$SE(\hat{\beta}_1) = \sqrt{\frac{RSS}{\sum(x_i - \bar{x})^2} * \frac{1}{n-2}}$$

**Evaluation of Model:**

RSS

Mean Squared Error (MSE) =  $\frac{RSS}{n}$

Root Mean Squared Error (REMSE) =  $\sqrt{MSE}$

**R Code:**

```
model=lm(demand~t_a)
pm=predict(model)
```

## 3 Naïve Bayes, 0 Rule, 1 Rule

### 3.1 1 Rule

1. Build table with pos/neg for each Attribute with every class
2. Find **Error Rate** for each **class** of each **attribute**.
3. Calculate total error rate (Lowest error rate wins)

$$\text{Error Rate: } \frac{\sum \text{Lowest values of class}}{\sum \text{All classes}}$$

Windy	Playing	Not Playing	Error Rate
True	3	3	$\frac{3}{6}$
False	6	2	$\frac{2}{8}$

$$\text{Total Error Rate: } \frac{3+2}{6+8}$$

### 3.2 Naïve Bayes

1. Count each **class** for target **attribute**. Calculate **prior**.
2. If a **used class** is = 0, increment all classes by one.
3. Calculate **likelihood of prior** given a certain **attribute**.
4. Calculate the normalized **likelihood of prior** given an **attribute**
5. Highest normalized **likelihood of prior** given an **attribute** wins

$$\text{Prior: } \Pr(h_l) = \frac{\text{Amount of class}}{\sum \text{class}}$$

$$\text{Likelihood of prior given an attribute: } \Pr(e_i|h_l) = \prod_{i=1}^n \Pr(e_i|h_l) \cdot \Pr(h_l)$$

$$\text{Normalized } \Pr(e_i|h_l) = \frac{\Pr(e_i|h_l)}{\sum_{i=1}^l \Pr(e_i|h_l)}$$

## 4 Decision Trees

### Classification:

- Internal *node* is a test on an attribute
- *Branch* represents an outcome of the test
- *Leaf* represents a class
- New *Instance* is classified by following a matching path to a leaf node

### Optimal Tree

- For  $n$  attributes there are  $2^{2^n}$  possible trees. Finding optimal tree is NP-complete. Solution: **Greedy Algorithm** for tree construction:

- Top down approach: Start with root
- Every split is assessed with a measure
- Best split is chosen
- Repeat until all leaf nodes are pure or all attributes have been used

## 4.1 Information and Entropy

**Entropy** measures information content in bits  $\rightarrow$  **Uncertainty of nodes**

$$\text{entropy}(p_1, \dots, p_n) = -\sum_{c=1}^n p_c * \log_2(p_c)$$

**Information** necessary to classify for  $C = \sum c_i$

$$\text{info}([c_1, \dots, c_n]) = \text{entropy}(\frac{c_1}{C}, \dots, \frac{c_n}{C})$$

### Average Information

Information weighted with the amount of outcomes on one leaf

**Information Gain:** Quality is split equal to the gained information gain

$$\text{gain}(\text{attribute}) = \text{gain}(\text{before split by attribute}) - \text{info}(\text{after split by attribute})$$

Problem with information gain:

- Biased against attributes with a lot of edges like IDs
- Results in overfitting

$\rightarrow$  Solution: Measurement that takes number and size of leafes into account

**Intrinsic Information:** ( $s$  is size of a leaf)

$$\text{intrinsic info}([s_1, \dots, s_n]) = \text{info}([s_1, \dots, s_n])$$

**Gain Ratio:**

$$\text{gainRatio}(\text{attribute}) = \frac{\text{gain}(\text{attribute})}{\text{intrinsicInfo}(\text{attribute})}$$

**Log Calculation:**

$$\log_2 x = \frac{\log x}{\log 2}$$

**Example (Figure 1):**

**Salary:**

**Leaf 1:**

$$\text{info}([2, 4]) = \text{entropy}(2/6, 4/6) = -2/6 * \log_2 2/6 - 4/6 * \log_2 4/6 = 0,918 \text{ bit}$$

**Leaf 2:**

$$\text{info}([3, 1]) = \text{entropy}(3/4, 1/4) = -3/4 * \log_2 3/4 - 0,25 * \log_2 0,25 = 0,811 \text{ bit}$$

**Average Information**

$$\text{info}([2, 4], [3, 1]) = \frac{6}{10} * 0,918 + \frac{4}{10} * 0,811 = 0,875 \text{ bit}$$

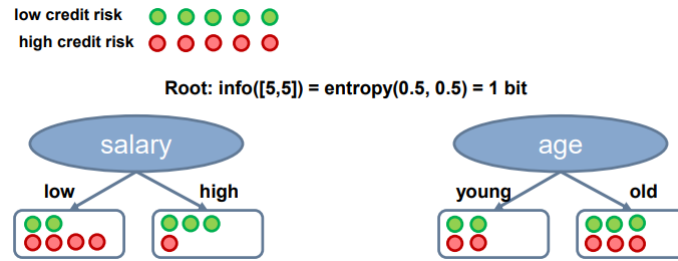


Figure 1: Decision Tree example

### Information Gain:

$$\text{gain}(\text{salary}) = \text{info}([5, 5]) - \text{info}([2, 4], [3, 1]) = 1\text{bit} - 0.875\text{bit} = 0.125\text{bit}$$

### Gain Ratio:

$$\text{intrinsicInfo}(\text{salary}) = \text{info}([6, 4]) = 0.9709$$

$$\text{gainRatio}(\text{salary}) = 0.125 / 0.9709 = 0.128$$

## 4.2 Construct a tree:

1. Calculate the information gain / gain ratio for the remaining attributes
2. Choose attribute with **highest** information gain
3. Remove attribute from list of attributes
4. Repeat if attributes are left

## 4.3 Pruning

- Shortening, simplifying, optimizing
- avoid overfitting

### Types of pruning:

- Prepruning (during construction of the tree)
  - Abort construction before the tree becomes too complex
  - Hard to decide because of the number of possible combinations
- Postpruning
  - Construct tree and prune afterwards
  - "Waste of computing time"

### 4.3.1 Subtree replacement

Replace a subtree with a leaf node.

→ Decreases accuracy on the training set

→ May increase accuracy on the test set

#### Criterion for replacement:

- error rate of a node and error rate of a leaf is estimated
- Replace if:

$$- e_{Node} < e_{Leaf}$$

#### Estimating the error rate:

- Estimate error based on the training set → Bad Choice!
- Withhold part of the training set and use it as test set
- **Method of C4.5**
  - Pessimistic estimation of error rate  $e$
  - Based on observed error rate  $f=E/N \rightarrow E = \text{error and } N = \text{instances}$
  - Confidence level:  $c$  (e.g. 25%) is called confidence limit
  - Formula → Not important! Table is given

#### Example (Figure 2):

##### Leaf 1:

$$N = 2 + 4 = 6, E = 2, f = 1/3$$

Look in table at row 6 (N) and column 2 (E) →  $e = 0,474$

##### Leaf 2:

$$N = 1 + 1 = 2, E = 1, f = 1/3$$

Look in table at row 2 (N) and column 1 (E) →  $e = 0,719$

##### Leaf 3:

$$N = 2 + 4 = 6, E = 2, f = 1/3$$

Look in table at row 6 (N) and column 2 (E) →  $e = 0,474$

#### Calculate $e$ for all leafs together:

$$e = \frac{6}{14} * 0,474 + \frac{2}{14} * 0,719 + \frac{6}{14} * 0,474 = 0.51$$

$\frac{6}{14} \rightarrow$  Sum of outcomes of one leaf (leaf 1 - 4+2=6) divided by the sum of outcomes of the node (health plan contribution - 6+2+6=14)

#### Calculate $e$ of the node:

Sum all positive/negative entries:  $[2,4] + [1,1] + [2,4] = [5,9]$

$$N = 5 + 9 = 14, E = 5, f = 5/14$$

Look in table at row 14 (N) and column 5 (E) →  $e = 0,449$

#### Replace if necessary:

$e_{Node} < e_{Leaf} \rightarrow$  Replace Node with one leaf! See Figure 3

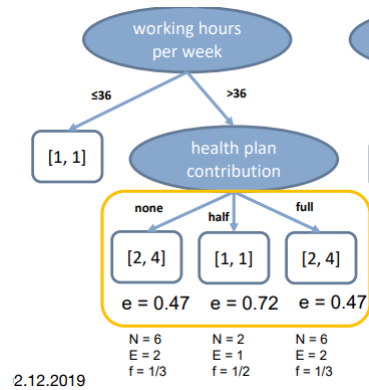


Figure 2: DT before pruning

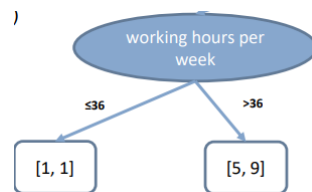


Figure 3: DT after pruning

## 5 Data preparation

Important R code:

- *mutate()* → adds new variables and preserves existing ones. New variables with the same name overwrite existing ones.

```
CPS1988 <- CPS1988 %>% mutate(wage = wage*2)
```

- *select()* → Is used to select certain columns from a DF. Can be used to rename:

```
df <- df %>% select(newName=column1)
```

- *factor()* → Encode vector as a vector. Gives a number to nominal values like a enumeration.

```
#Gives the numbers 2,3,4 in salutation the names
  Company, Mr and Mrs. and saves column as fct.
salutation = factor(salutation, labels = c("Company",
      "Mr.", "Mrs."))
```

- *toupper()* → Makes all characters to uppercase.
- *mutate\_at* → Used to apply multiple functions on selected variables.



```
df <- df %>% mutate_at(vars(order_date, delivery_date,
                             date_of_birth), as_date)
```

- *mutate\_all* → same as *mutate\_at* but for all variables.
- *as\_date()* → transfers data to date format
- *is.na()* → checks if a value is NA.
- *na.omit* → removes all entries which contain NA values.

```
df <- df %>% na.omit()
```

- *if\_else()* → takes condition, yes, no
- ```
if_else(is.na(price), mean(price, na.rm = T), price)
```
- *case\_when()* → Like switch case in Java

```
delivery_time_discrete = case_when(
  is.na(delivery_time) ~ "NA",
  delivery_time <= 5 ~ "5d",
  delivery_time > 5 ~ ">5d"
)
```

## 6 Data Evaluation

### 6.1 Holdout

Holding out certain values for evaluation, not training:

- Reduce number of training instances
- Composition influence results

**Solution:**

- More reliable results using stratification
- Some instances may never be used for training/testing

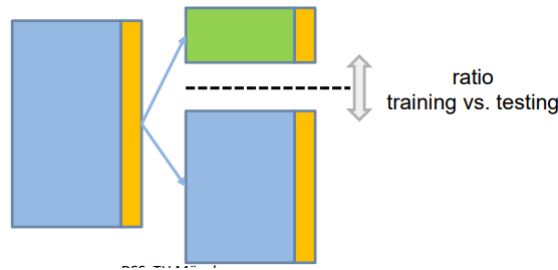


Figure 4: Holdout Example

## 6.2 k-fold Cross Validation

- Partition the data set into  $k$  complementary subsets (make  $k$  groups)
- Train with  $k-1$  subsets and test on one subset
- Every subset is used  $k-1$  times for training and 1 time for testing

### Example:

Dataset:  $[+, +, +, +, -, +, +, -, -, -, +, +, +, -, -]$

3-fold Cross Validation:

- Divide the sample into 3 different partitions:  
 P1:(1,2,3,4,5)  
 P2:(6,7,8,9,10)  
 P3:(11,12,13,14,15)
- Create  $k$  Folds which each use  $k-1$  partitions for training and 1 for testing  
 Fold1: Train with P2 and P3 and test with P1  $\rightarrow$  classes[4,1]  
 Fold2: Train with P3 and P1 and test with P2  $\rightarrow$  classes[2,3]  
 Fold3: Train with P1 and P2 and test with P3  $\rightarrow$  classes[3,2]

**Stratified:** The splitting of data into folds may be governed by criteria such as ensuring that each fold has the same proportion of observations with a given categorical value, such as the class outcome value. This is called stratified cross-validation.

**Example:** Find partitions so that Folds result in the same class values: P1 = 1,2,3,5,8, P2 = 4,6,7,9,10, P3 = 11,12,13,14,15

Fold 1: Train: P2 & P3, Test: P1, classes: [3,2]

Fold 2: Train: P1 & P3, Test: P2, classes: [3,2]

Fold 3: Train: P1 & P2, Test: P3, classes: [3,2]

### 6.2.1 Leave One Out Validation

$k$ -fold validation with  $k=N \rightarrow N =$  Number of training instances

- Deterministic but requires a lot of time for computing
- extreme class distribution of test data

|                 |     | Actual class |     |
|-----------------|-----|--------------|-----|
|                 |     | Cat          | Dog |
| Predicted class | Cat | 5            | 2   |
|                 | Dog | 3            | 3   |

Figure 5: Example of an Confusion Matrix

## 7 Confusion Matrix

Used to test an algorithm. Is divided in (see Figure 5):

- True Class
- Predicted Class
- True Positive Rate:  $tpr = \frac{TP}{TP+FN}$   
'How many positive instances have been predicted positive?'
- False Positive Rate:  $fpr = \frac{FP}{TN+FP}$   
'How many negative instances have been predicted positive?'
- True Negative Rate:  $tnr = \frac{TN}{TN+FP}$   
'How many negative instances have been predicted negative?'
- Accuracy  $accuracy = \frac{TP+TN}{TP+FP+TN+FN}$   
'How many instances have been predicted correctly?'

**Example:**

| True Class | Pedicted Class |
|------------|----------------|
| 0          | 0              |
| 0          | 1              |
| 1          | 1              |
| 1          | 0              |
| 0          | 0              |
| 1          | 0              |
| 0          | 0              |
| 1          | 1              |
| 0          | 1              |
| 1          | 0              |

$$\begin{aligned}
 tpr &= \frac{2}{2+3} = 0,4 \\
 fpr &= \frac{2}{3+2} = 0,4 \\
 tnr &= \frac{3}{3+2} = 0,6 \\
 accuracy &= \frac{2+3}{2+2+3+3} = 0,5
 \end{aligned}$$

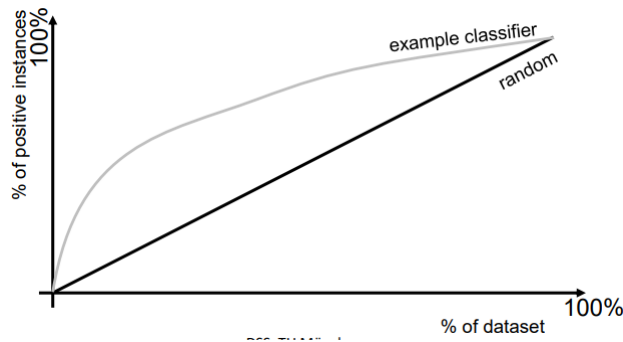


Figure 6: Gain Curve

## 8 t-Test

Paired t-Test to test if the difference between two classifiers is significant.

$$H_0 : d = 0$$

$$H_1 : d \neq 0 \text{ (depends on the question!)}$$

**Formulas:**

$$\bar{d} = \frac{1}{k} \sum_i d_i$$

$$s_d = \sqrt{\frac{1}{k-1} \sum_i (d_i - \bar{d})^2}$$

$$t = \frac{\bar{d}}{\frac{s_d}{\sqrt{k}}} t_{k-1}$$

## 9 Curves

### 9.1 Gain Curve

Used to show the difference between different cut-offs. **Instances are sorted descending by the probability!**

x-axis: percentage of the data set (0-100% meaning 10% of the instances in the data set)

y-axis: percentage of number of **positive** instances. Check the percentage of the positive instances **within the cut-off** of the X percent of the x-axis.

### 9.2 Lift Curve

Displays the factor between the classifier and random value

x-axis: Percentage of the data set

y-axis:  $\frac{Gainatx}{x}$

### 9.3 ROC Curve

Displays ratio of False Positive and True Positive

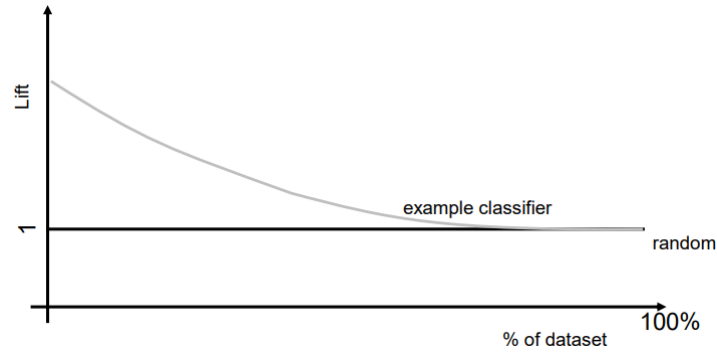


Figure 7: Lift Curve

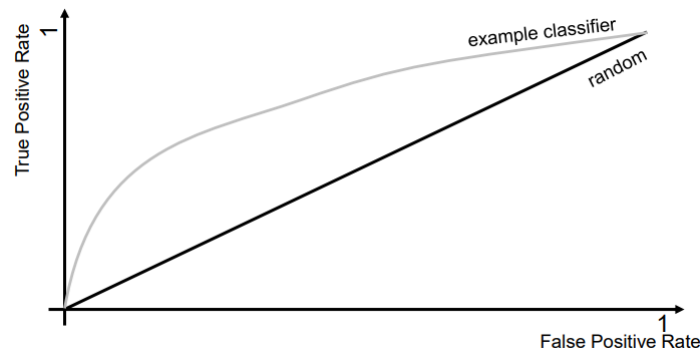


Figure 8: ROC Curve

## 10 Clustering

### Definition:

Given: A  $p$ -dimensional data set with  $n$  instances.

Want: Partition data set into a number of clusters.

- Items in the same cluster are identical: Intra-cluster similarity is maximized
- Items from different cluster are different: Inter-cluster similarity is minimized

### Difference between Classification and Clustering:

Classification:

- Supervised learning
- Target is known
- Training data
- Naive Bayes
- Decision Tree
- Ensemble Methods

Clustering:

- Unsupervised learning
- Target is unknown
- No labels meaning no true classes
- k-means
- Minimum spanning tree
- Expectation maximization

## 10.1 k-means

Divide instances into k clusters  $C_1, \dots, C_k$

- Randomly choose k centers or pick k instances as initial centers
- Repeat until no changes:

- Assign instances to the closes cluster
$$d(p, c) = \sqrt{(x(p) - x(c))^2 + (y(p) - y(c))^2}$$
- Recalculate the center of the clusters
$$x'(c_i) = \frac{\sum_{p \in C_i} x(p)}{|c_i|}$$
$$y'(c_i) = \frac{\sum_{p \in C_i} y(p)}{|c_i|}$$

## 10.2 Expectation Maximation (EM) - Fuzzy Clustering

Currently: Each item of the dataset is assigned to one cluster but sometimes a fuzzy or more flexible cluster can be more realistic!

Method:

- Start with guessing for cluster centers and define k
  - calculate the probability that instance p belongs to cluster c
$$f(x, \mu_A, \sigma_A) = \frac{1}{\sigma_A \cdot \sqrt{2\pi}} \cdot e^{-\frac{(x - \mu_A)^2}{2 \cdot \sigma_A^2}}$$
$$Pr[X] = f(x, \mu_A, \sigma_A) \cdot p_A + f(x, \mu_B, \sigma_B) \cdot p_B$$
$$Pr[A|x] =$$
  - optimize distribution parameters based on the likelihoods
$$\mu_A = \frac{w_1 + \dots + w_n}{w_1 + \dots + w_n}$$