NOVA IMS Information Management School

Data Mining

S3

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Fernando Lucas Bação

bacao@isegi.unl.pt

http://www.isegi.unl.pt/fbacao

Instituto Superior de Estatística e Gestão de Informação
Universidade Nova de Lisboa

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Agenda

- Data Mining
  - The data mining process
  - General aspects of problem definition
  - Input space
  - The curse of dimensionality
  - Input space coverage
  - Binary and multiclass classification
  - Separability and Bayes error
  - Different types of variables
  - Spurious correlations and confounding variables
  - Performance evaluation

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The Data Mining Process

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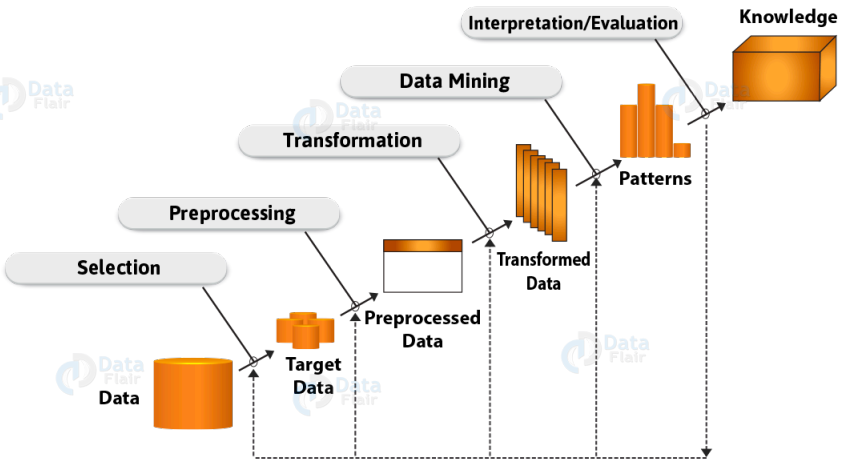
Data Mining and Knowledge Discovery Database (KDD) Process



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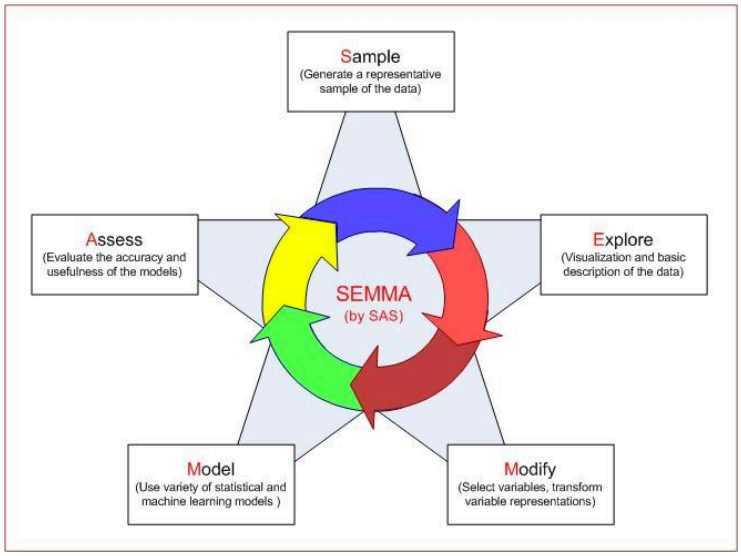
Sample, Explore, Modify, Model, and Assess (SEMMA)



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CRISP-DM, Cross Industry Standard Process for Data Mining

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General aspects of the problem definition

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Problem definition

- "We're doomed to complex theories that will never have the **elegance of physics equations**. But if that's so, we should stop acting as if our goal is to author extremely elegant theories, and instead **embrace complexity** and make use of the best ally we have: **the unreasonable effectiveness of data**."
- Invariably, **simple models** and a **lot of data** trump more elaborate models based on less data.

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Problem definition

- So, follow the data. Choose a representation that can use **unsupervised learning** on **unlabeled data**, which is so **much more plentiful than labeled data**.
- Represent all the data with a nonparametric model rather than trying to summarize it with a parametric model: **"let the data speak for themselves"**

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Problem definition

- Suppose you've constructed the **best set of features** you can, but the **classifiers you're getting are still not accurate enough**.
- What can you do now? There are **two main choices**:
  - design a **better learning algorithm**,
  - or **gather more data** (more examples, and possibly more raw features, subject to the curse of dimensionality).
- Machine learning researchers are mainly concerned with the former, but **pragmatically the quickest path to success is often to just get more data**.
- As a rule of thumb, **a dumb algorithm with lots and lots of data beats a clever one with modest amounts of it**. (After all, machine learning is all about **letting data do the heavy lifting**.)

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Input Space

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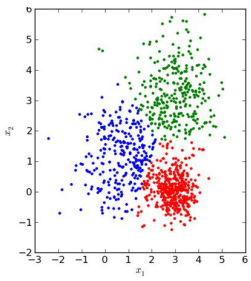
Problem definition

- **Input Space**
  - The input space is defined by the input feature vectors.
  - Where the algorithms will try to find a solution to the problem



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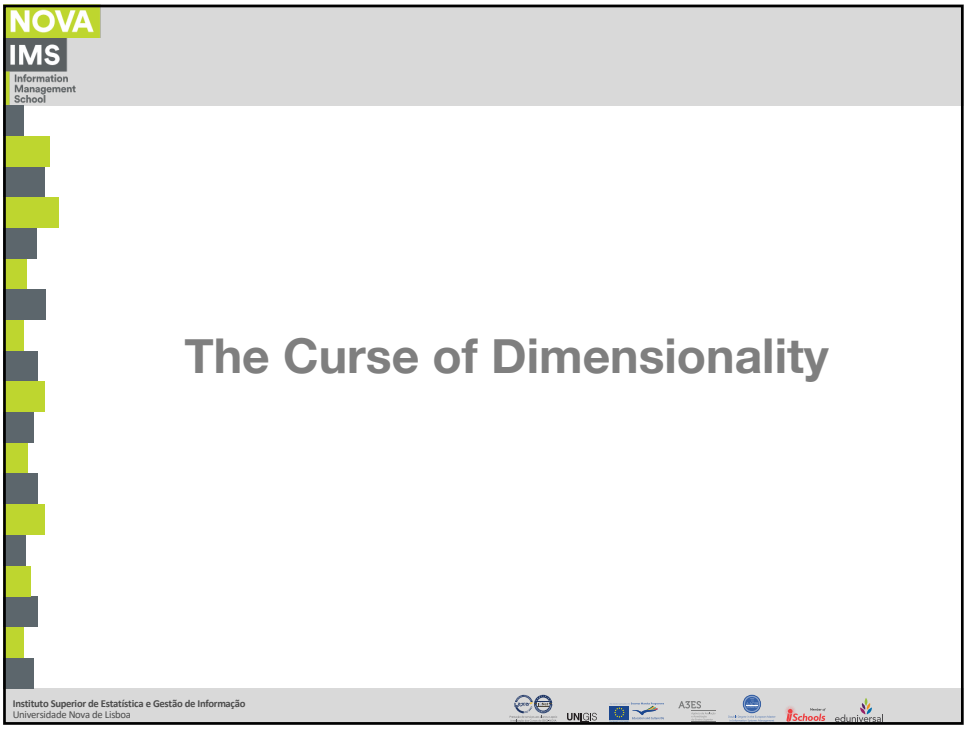
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The Curse of Dimensionality
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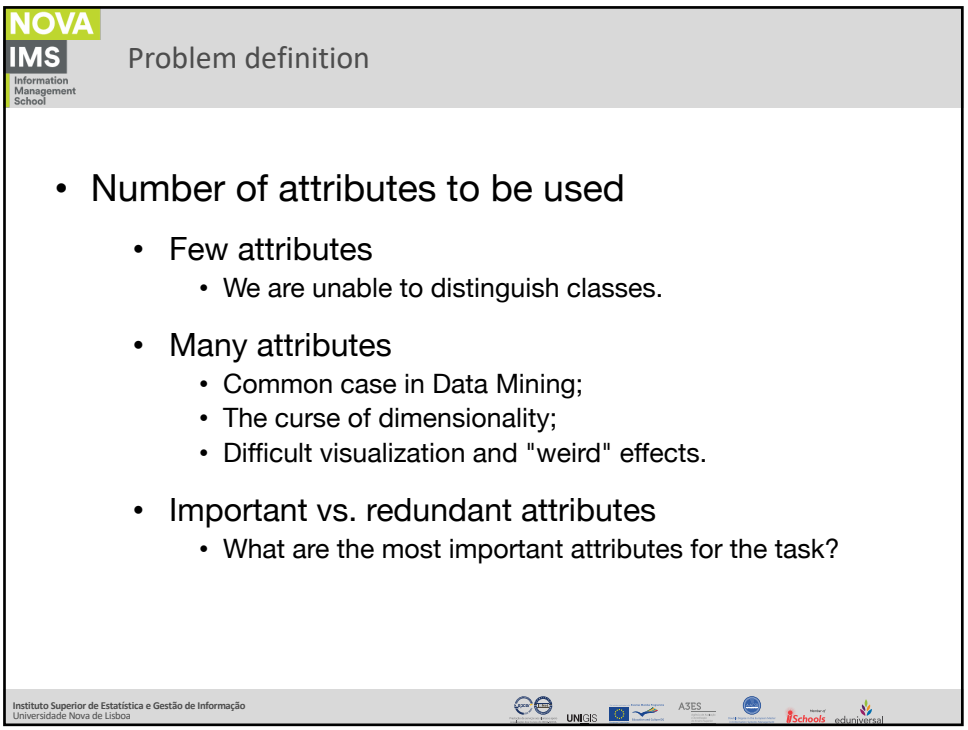
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Problem definition
• Number of attributes to be used
• Few attributes
• We are unable to distinguish classes.
• Many attributes
• Common case in Data Mining;
• The curse of dimensionality;
• Difficult visualization and "weird" effects.
• Important vs. redundant attributes
• What are the most important attributes for the task?
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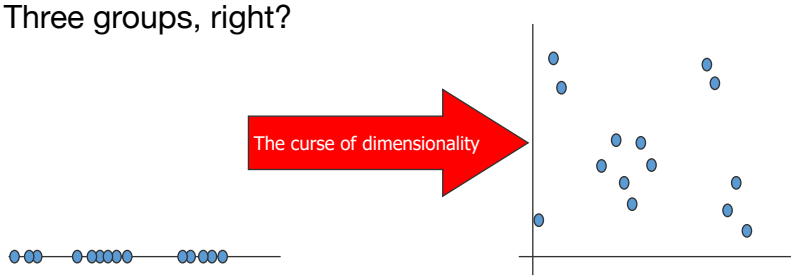
Problem definition

Three groups, right?



Well… not exactly.

When the dimensionality increases, the space becomes more sparse and it becomes more difficult to find groups (you need even more data)

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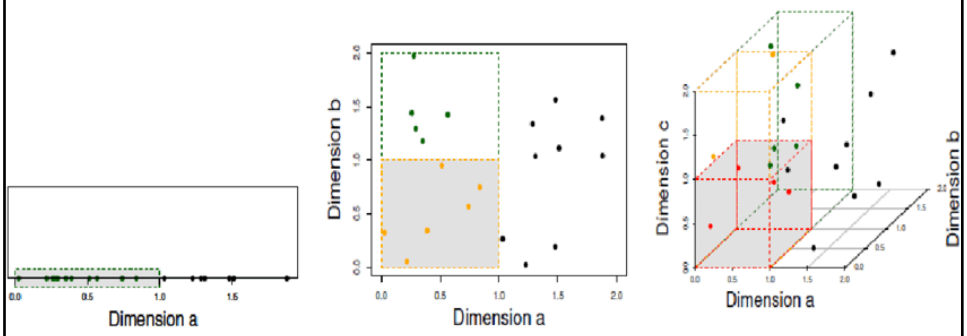
Problem definition



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Problem definition

- The curse of dimensionality
  - **Generalizing correctly becomes exponentially harder** as the dimensionality (number of features) of the examples grows, because a fixed-size training set covers a dwindling fraction of the input space.
  - With a **dimension of 100 and a huge training set of a trillion examples**, the latter covers only a fraction of about 10^{-18} of the input space. This is what makes machine learning both necessary and hard.

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Input Space Coverage

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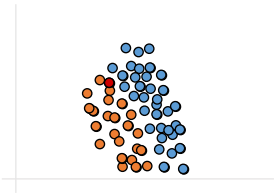
Problem definition



- Good coverage of the problem space increases confidence in the results and in its quality.

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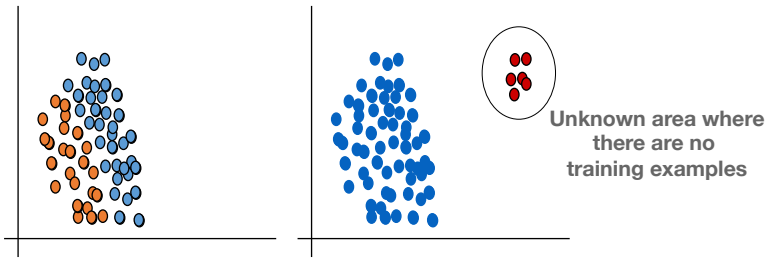
Space coverage



- If a model is developed based on a set of examples, but in fact the examples would be very different, it is natural that the results will be bad (@men women photo).

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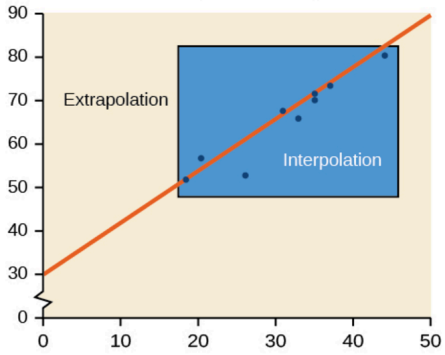
Extrapolation vs Interpolation



- **Interpolation** involves predicting a value inside the domain and/or range of the data.
- **Extrapolation** involves predicting a value outside the domain and/or range of the data.

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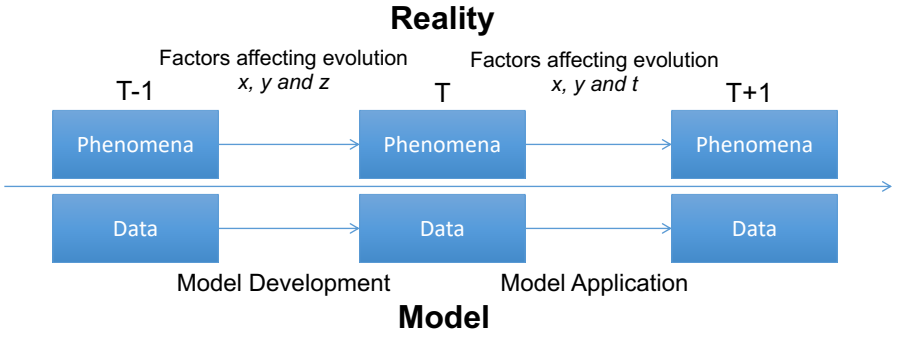
General aspects of data collection



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Binary and Multiclass Classification

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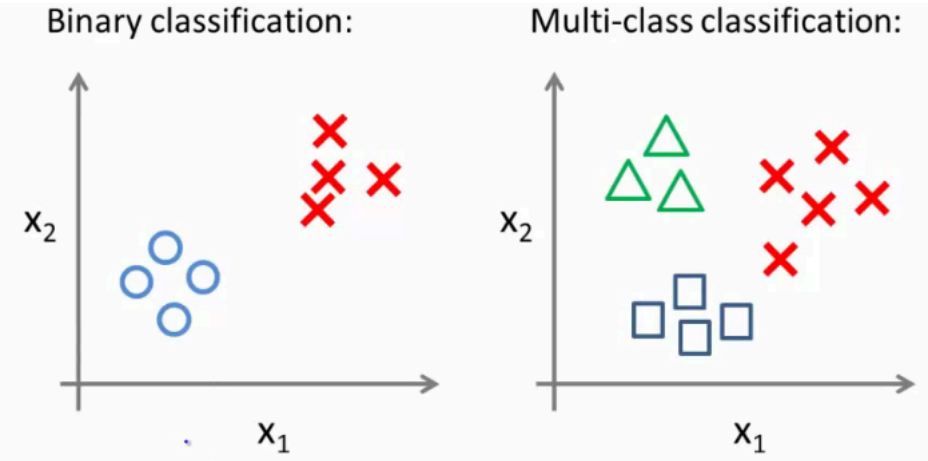
Binary and Multi-class



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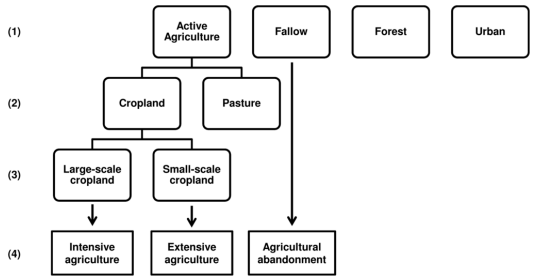
Granularity

- **Granularity of classification problems:**
  - Initially a small number of output classes;
  - The more output classes, the greater the number of data needed for training.



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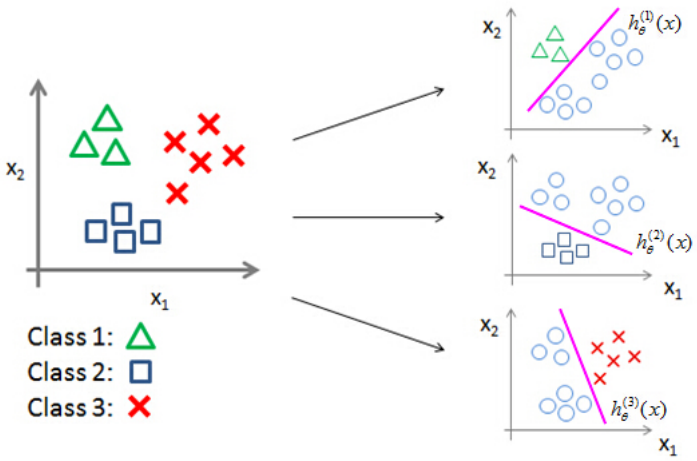
Multi-class strategies



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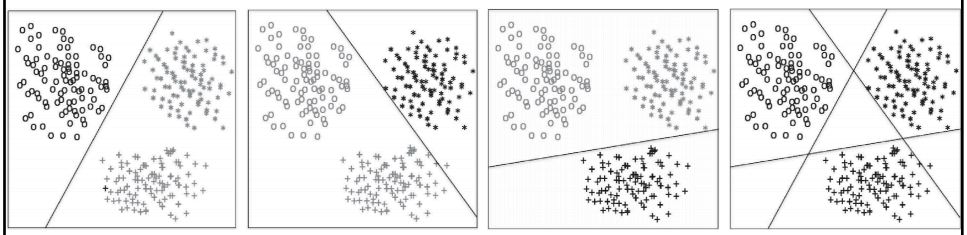
Multi-class strategies

- **One-vs-rest (OVR) strategy:**
  - Breaks the multi-class classification down into a series of binary classification
  - N-class classification problem is decomposed into N binary classification problems.



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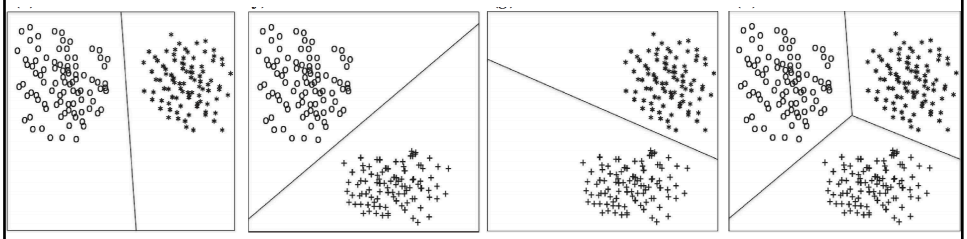
Multi-class strategies

- **One-vs-one (OVO) strategy:**
  - Enumerating all possible pairs of classes and then to develop a binary classifier for each pair of classes
  - Classification is then done by inputting the data point into each particular binary classifier and labelling by majority voting 1/2N(N-1)



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Separability and Bayes Error

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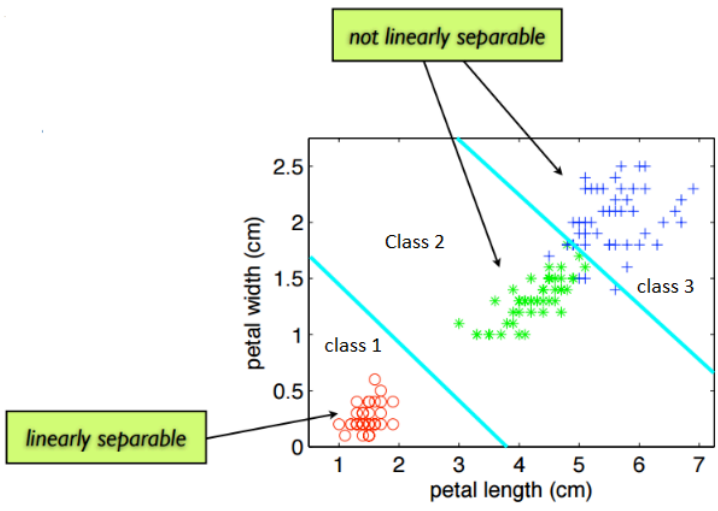
Separation and error



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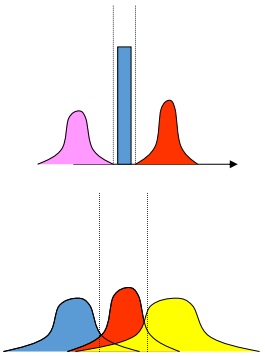
Problem definition

Separable

- Ø error possible

Not separable

- Always error > Ø
- Bayes error
  - Lowest possible error for a classifier



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Different Types of Variables

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Variables

- **Different types of variables:**
  - **Nominal** are just labels, e.g. ‘red’, ‘green’, ‘blue’, no particular order. Think in classes.
  - **Ordinal** have an order, e.g. ‘satisfied’, ‘very satisfied’, ‘extremely satisfied’. Think in ranks.
  - **Discrete** are just counting data, e.g. 0, 1, 2, ...
  - **Continuous** are just measurement data, e.g. 1.23, 0.001, etc

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Variables

- **Different types of variables:**
  - **Interval** data are measured and have constant, equal distances between values, but the zero point is arbitrary. The zero isn’t meaningful, it doesn’t mean a true absence of something.
  - When a **ratio** between two values of a quantitative variable is meaningful, it's a ratio scaled variable. Ratio measurement assumes a zero point where there is no measurement.

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Problem definition

Provides:	Nominal	Ordinal	Interval	Ratio
The "order" of values is known		✔	✔	✔
"Counts," aka "Frequency of Distribution"	✔	✔	✔	✔
Mode	✔	✔	✔	✔
Median		✔	✔	✔
Mean			✔	✔
Can quantify the difference between each value			✔	✔
Can add or subtract values			✔	✔
Can multiple and divide values				✔
Has "true zero"				✔

Summary of data types and scale measures

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Metadata

- **Metadata:**
  - Metadata is "data [information] that provides information about other data".
  - Three distinct types of metadata exist:
    - Descriptive metadata describes a resource for purposes such as discovery and identification.
    - Structural metadata is metadata about containers of data and indicates how compound objects are put together, for example, how pages are ordered to form chapters.
    - Administrative metadata provides information to help manage a resource, such as when and how it was created, file type and other technical information, and who can access it.

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Spurious Correlations and Confounding Variables

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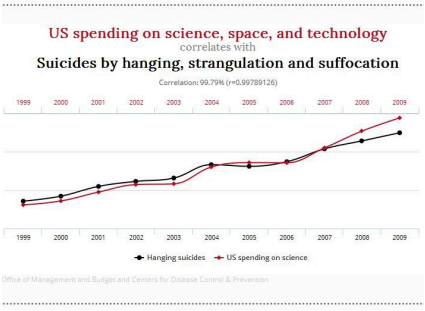
Problem definition

- **Input variables should be causally related to the outputs**
  - Spurious correlations
    - Low number of training examples;
    - Large number of input variables.
  - It is important that there is a plausible reason to chose the input variables.



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Causality and correlation

- **Input variables should be causally related to the outputs**
  - Confounding variables
    - In statistics, a confounding variable (also confounding factor) is an **extraneous variable** in a statistical model that **correlates** (directly or inversely) **with both the dependent variable and the independent variable**.
    - A **spurious relationship** is a perceived relationship between an independent variable and a dependent variable that has been **estimated incorrectly** because the estimate **fails to account for a confounding factor**.

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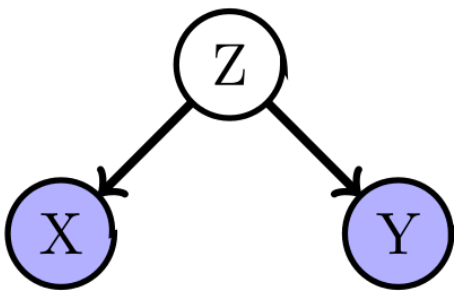
Problem definition

- **Input variables must be causally related to the outputs**
  - Confounding variables



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Causality and correlation

- **Spurious correlations**
  - Example n.º 1: Ice cream sales and the number of drowning's;
  - Example n.º 2: Correlation between the measuring of a patient's temperature on admission to hospital and the probability of his survival;

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Performance Evaluation

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Problem definition

- **Result Evaluation:**

		Actual Value: Positives	Actual Value: Negatives
Predicted Value	Positives	TP True Positives	FP False Positives
Predicted Value	Negatives	FN False Negatives	TN True Negatives

$$Accuracy = \frac{True\ Positives + True\ Negatives}{Total\ Population}$$

$$Specificity\ (true\ negative\ rate) = \frac{True\ Negatives}{Total\ Negatives}$$

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Problem definition

- **Result Evaluation:**

		Actual Value: Positives	Actual Value: Negatives
Predicted Value	Positives	TP True Positives	FP False Positives
Predicted Value	Negatives	FN False Negatives	TN True Negatives

$$Recall = \frac{True\ Positives}{Total\ Positives}$$

$$Precision = \frac{True\ Positives}{Predicted\ Positives}$$

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Problem definition

- **Result Evaluation:**

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$$

$$R^2 = 1 - \frac{MSE(model)}{MSE(baseline)}$$

$$MSE(baseline) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \bar{y})^2$$

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Problem definition

- **Result Evaluation:**
  - What is the level of accuracy required to consider the application a success?
  - How to compare the quality of an obtained solution?
  - What are the existing alternatives that can serve as a standard of comparison?
  - What type of data to use to evaluate the various models?

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