# Introduction to Machine Learning
## NPFL 054

http://ufal.mff.cuni.cz/course/npfl054

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# Outline

- **Organizational notes**
  - Brief overview of the course
  - Lectures and lab sessions
  - Credit and examination requirements
  - Related courses
- **Informal intro to Machine Learning**
  - Motivation example
  - Artificial intelligence – Machine Learning – Deep Learning – Neural Networks
- **Formal definition of Machine Learning**
  - Supervised Machine Learning
  - Features and target values
  - Prediction function
  - Loss function
  - Training and test data
  - Development cycle
- **Summary of the lecture**

# Organizational notes on the course

- `https://ufal.mff.cuni.cz/courses/npfl054`
  – the course web page with all important information and materials

- **Two parallel classes** – identical content

- **Brief overview of the course**
  - This is an introductory course
  - We teach general foundations of ML
    and "traditional" machine learning algorithms (no neural networks)
  - Main topics correspond to the exam requirements

- **Recommended literature**
  - ***An Introduction to Statistical Learning***
    by James, Witten, Hastie, and Tibshirani.
    Springer, New York, 2013. (available online)
  - ***Machine learning with R***
    by Brett Lantz.
    Packt Publishing Ltd. 2013. (available in the MFF library)

# Please, introduce briefly yourself

- What you study – faculty, your field?
- Machine Learning course – your motivation/expectations?
- Your experience with Machine Learning – at school, or in practice?

# Machine Learning Lab Sessions

**Goals of the lab sessions**

- to learn how to practically analyse example data and ML tasks
- to learn how to practically implement some ML methods
- to solve a particular task
- practical experience with R system for statistical computing and graphics

`http://www.r-project.org/`

# Why statistics and probability theory?

**Motivation**

- In machine learning, models come from data and provide insights for understanding data (unsupervised classification) or making prediction (supervised learning).
- A good model is often a model which not only fits the data but gives good predictions, even if it is not interpretable.

**Statistics**

- is the science of the collection, organization, and interpretation of data
- uses the probability theory

# Gentle introduction to R

**What is R?**

- a library of statistical tools
- an interactive environment for statistical analyses and graphics
- a programming language
- a public free software derived from the commercial system S

**R is becoming more and more popular** especially for its

- effective data handling and storage facility
- large, coherent, integrated collection of tools for data analysis
- well-developed, simple and effective programming language

**Recommended reading**

- *An Introduction to R*
  by W. N. Venables, D. M. Smith and the R core team
- also, an introduction available on the web:
  `http://cran.r-project.org/doc/manuals/R-intro.html`
- *R for Beginners* by Emmanuel Paradis

# Conditions for getting the credits

- **Obligatory participation in lab sessions**
  – you should take part in at least 2/3 of all practical classes
- **Two obligatory short presentations during lab sessions**
  – you should shortly present your solution of assigned homework
- **Obligatory written assignments**
  – you should submit one written homework in the middle of the semester, and finally a more demanding written report of your term project
- **Written tests**
  – you should pass one written test in the middle of the semester
  – and then a more demanding final written test
- **Scored assignments and written tests are necessary conditions for attending the oral exam!**

# What you *cannot* learn in this course

- **no advanced methods**
  ⟶ NPFL 097 Selected Problems in Machine Learning
- **no deep learning**
  ⟶ NPFL 114 Deep Learning
  ⟶ NPFL 122 Deep Reinforcement Learning
- **no very details on Neural Networks**
  ⟶ NAIL 002 Neural Networks
- **no special applications**
  ⟶ e.g. NDBI 023 Data Mining
- **no advanced theoretical aspects of ML**
  ⟶ NAIL 029 Machine Learning
- **no Weka, no Python libraries, etc.**
  – interested in Python?
    ⟶ NPFL 104 Machine Learning Methods
    ⟶ NPFL 129 Machine Learning for Greenhorns
      – a new course, very similar topics, exercises in Python

# Supportive course NPFL 081
# Practical Fundamentals of Probability and Statistics

- Intended and designed for students with weaker mathematical background
- We will go through **basics of probability theory and statistics**
- We will do **practical exercises using R system**
- Taught by Martin Holub and flexible for students' needs

Send a message to Holub@UFAL if you want to attend

# Informal explanation of ML – motivation examples

**Word-sense disambiguation (WSD)**
Assign the correct sense of a word in a sentence.
Let's work with the word *line*:

- I've got Inspector Jackson on the **line** for you.
- Outside, a **line** of customers waited to get in.
- He quoted a few **lines** from Shakespeare.
- He didn't catch many fish, but it hardly mattered.
  With his **line** out, he sat for hours staring at the Atlantic.
- ...

# Motivation example

**Word-sense disambiguation**
Assign the correct sense of a word in a sentence.
Let's work with the word *line* and its following senses:

- CORD
- DIVISION
- FORMATION
- PHONE
- PRODUCT
- TEXT

# Motivation example — Word-sense disambiguation

**?CORD ?DIVISION ?FORMATION ?PHONE ?PRODUCT ?TEXT**

| | |
|---|---|
| • I've got Inspector Jackson on the **line** for you. | `PHONE` |
| • Outside, a **line** of customers waited to get in. | `FORMATION` |
| • He quoted a few **lines** from Shakespeare. | `TEXT` |
| • He didn't catch many fish, but it hardly mattered. With his **line** out, he sat for hours staring at the Atlantic. | `CORD` |
| • The company has just launched a new **line** of small, low-priced computers. | `PRODUCT` |
| • Draw a **line** that passes through the points P and Q. | `DIVISION` |
| • This has been a very popular new **line**. | `PRODUCT? FORMATION?` |

# Motivation example

**Word-sense disambiguation**

- What knowledge do you use to assign the senses?
- What are the keys for the correct decision?

# Motivation example

- We – human beings – do word sense disambiguation easily using the **context in the sentence** and having our **knowledge of the world**.
- We want computers to master it as well.

**Let's prepare examples and guide computers to learn from them.**

That is Machine Learning!

# Classical vs. deep Machine Learning

Cited from: *Deep Learning*, MIT Press, 2016.

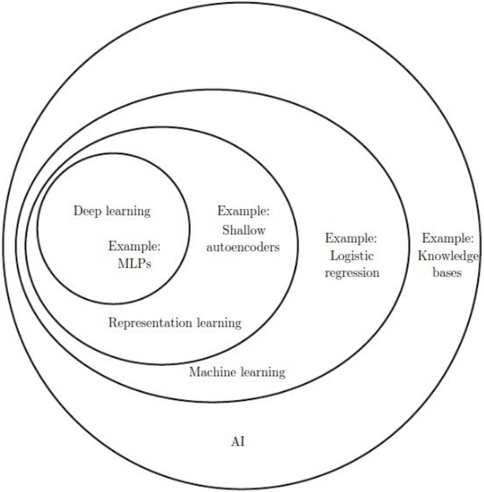
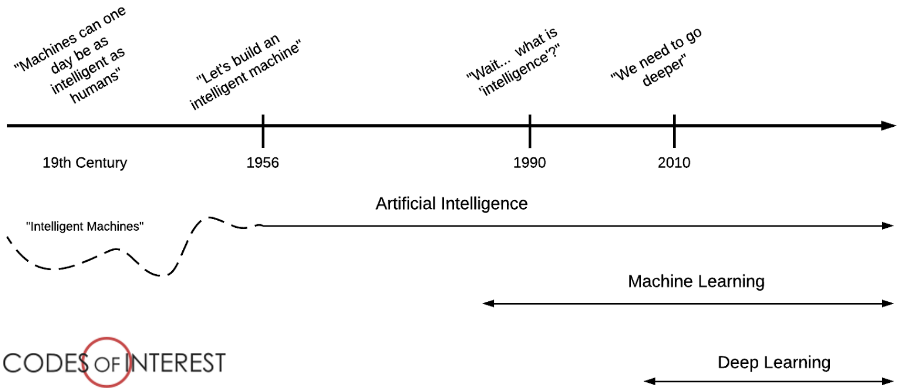


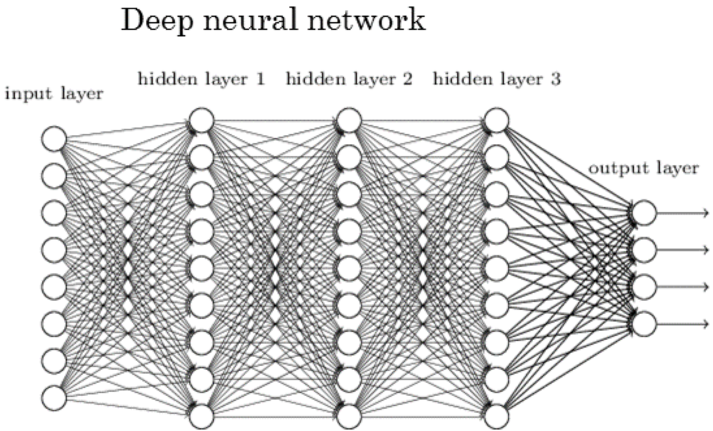

Figure 1.4: A Venn diagram showing how deep learning is a kind of representation learning, which is in turn a kind of machine learning, which is used for many but not all approaches to AI. Each section of the Venn diagram includes an example of an AI technology.

# Deep learning – history

Cited from: `www.codesofinterest.com/p/what-is-deep-learning.html`



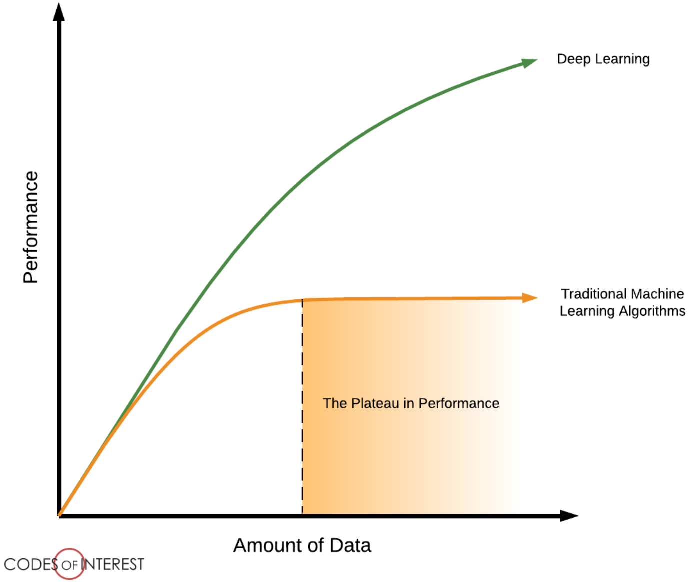
# Deep feedforward architecture



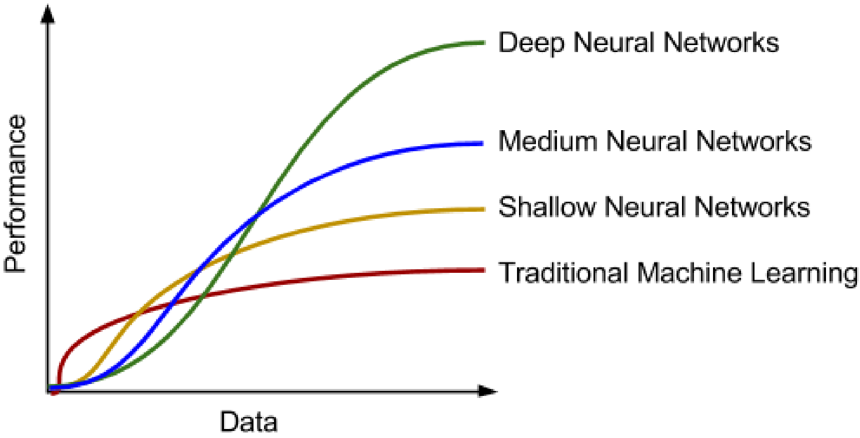

Fully connected layers have their own

- sets of parameters (weights and biases)
- outputs (activation values)

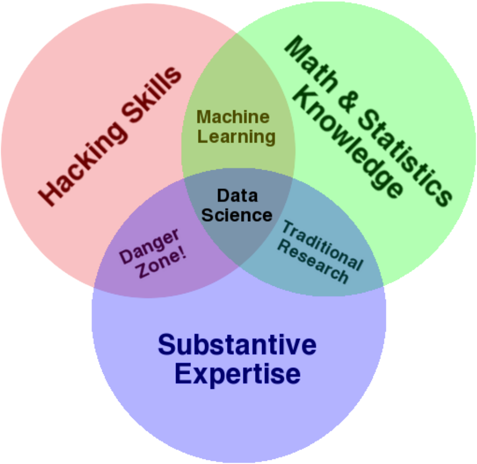
# ML performance – traditional vs. deep



# The deeper the better?



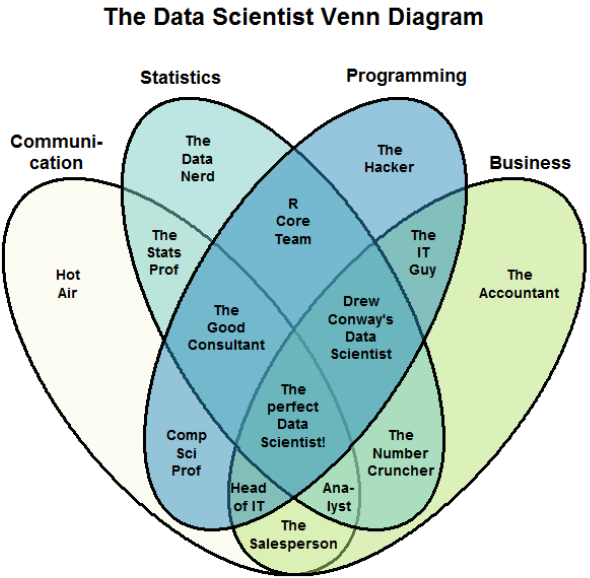
# Machine Learning in the context of Data Science




**How to read the Data Science Venn Diagram**

For more comments see `http://drewconway.com/zia/2013/3/26/the-data-science-venn-diagram`

# The perfect Data Scientist



# Formal definition of ML by Mitchell (1997)

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

# Machine learning needs examples

Intuitively we need a large set of recognized **examples** to learn the essential knowledge necessary to recognize correct output values. Examples used for learning are called **training data**.

| sentence | sense |
|---|---|
| I've got Inspector Jackson on the **line** for you. | PHONE |
| Outside, a **line** of customers waited to get in. | FORMATION |
| These companies rent private telephone **lines**. | PHONE |
| Please hold the **line**. | PHONE |
| He quoted a few **lines** from Shakespeare. | TEXT |
| He drew a **line** on the chart. | DIVISION |
| She hung the washing on the **line**. | CORD |

# What computers extract from examples

In the WSD task, both humans and computers need to know the **context of the target word** ("line") to recognize correct senses.

Humans use their reason, intuition, and their real world knowledge.

Computers need to extract a limited set of useful **context clues** that are then used for automatic decision about the correct sense.

- Formally, the context clues are called **attributes or features** and should be exactly and explicitly defined.
- Then each object (e.g. a sentence) is characterized by a list of features, which is called **feature vector**.

**Computer makes feature vectors from examples.**

# Intuitive feature extraction – examples

**To choose an effective set of features we always need our intuition. Only then all experiments with data can start.**

**A few example hints:**

| **class** | **a feature to recognize the class – will be useful?** |
|---|---|
| CORD | immediately preceding word |
| FORMATION | immediately following word |
| PHONE | can be often recognized by characteristic verbs |

# “Examples” in ML – two meanings

**1) Real examples** – Each real object that is already recognized or that we want to recognize is an example.

**2) Data instances** – In ML, each real example is represented as a data instance. In this sense

**example = feature vector + output value**

# Data instances

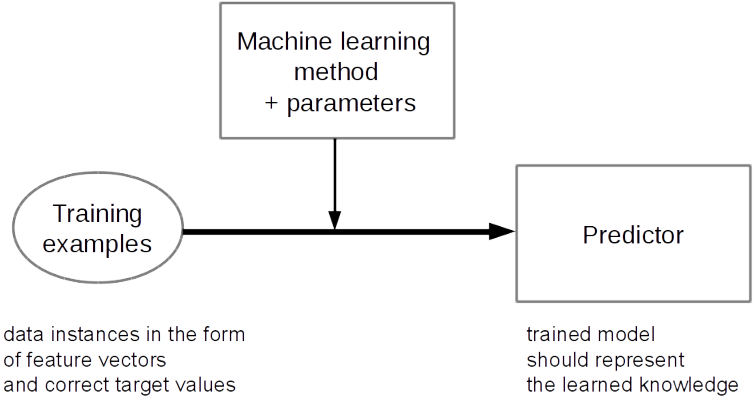
Sometimes we do not know the output value; in this case data instances are not different from feature vectors.

**data instance = feature vector (+ output value, if it is known)**

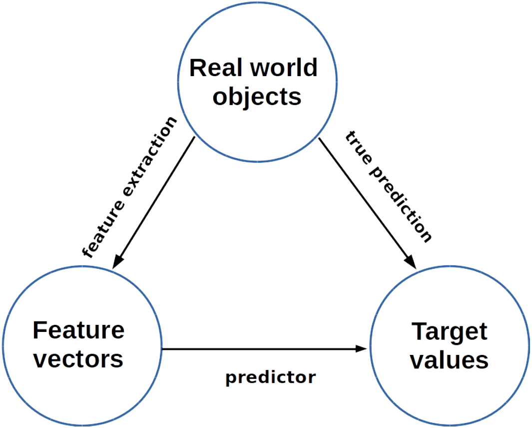
A data instance is either a feature vector or a complete example.

# Supervised learning process

**Supervised Machine Learning** = computer learns "essential knowledge" extracted from a (large) set of examples with known output values



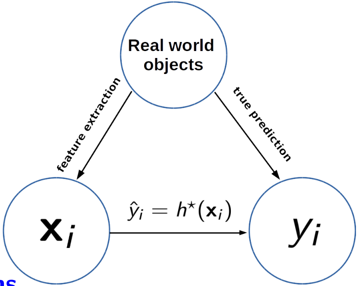
# Machine learning as building a prediction function




- if target values are *continuous* numbers, we speak about **regression**
  = estimating or predicting a continuous response
- if target values are *discrete/categorical*, we speak about **classification**
  = identifying group membership

# Prediction function and its relation to the data

**Idealized model of supervised learning**




- $\mathbf{x}_i$ are **feature vectors**, $y_i$ are true **predictions**
- **prediction function** $\hat{f}^\star$ is the "best" of all possible hypotheses $\hat{f}$
- **learning process** is searching for $\hat{f}^\star$, which means to search the **hypothesis space** and minimize a predefined **loss function**
- ideally, the learning process results in $\hat{f}^\star$ so that predicted $\hat{y}_i = \hat{f}^\star(\mathbf{x}_i)$ is equal to the true target values $y_i$

# Loss function

A loss function $\mathrm{L}(\hat{y}, y)$ measures the cost of predicting $\hat{y}$ when the true value is $y$. Commonly used loss functions are

- squared loss $\mathrm{L}(\hat{y}, y) = (\hat{y} - y)^2$
  for regression
- zero-one loss $\mathrm{L}(\hat{y}, y) = \mathrm{I}(\hat{y} \neq y)$
  for classifiation; *indicator variable* $\mathrm{I}$ is 1 if $\hat{y} \neq y$, 0 otherwise

**The goal of learning can be stated as producing a model with the smallest possible loss; i.e., a model that minimizes the average $\mathrm{L}(\hat{y}, y)$ over all examples.**

**Important notes**

- Loss function is sometimes also known as "cost function".
- In a broader sense, loss function means the value that summarizes the loss over a sample of examples, e.g. $\sum \mathrm{L}(\hat{y}, y)$ or $\mathsf{E}\left[\mathrm{L}(\hat{y}, y)\right]$.
- A more general term is "objective function", which is sometimes used for the function that should be optimized (minimized or maximized); yes, typically the objective function is in fact the loss function computed over a sample of development test examples.

# Training data vs. test data

- **Training data** = a set of examples
  – used for **learning process**

- **Test data** = another set of examples
  – used for **evaluation** of a trained model

- **Important**: the split of all available examples into the training and the test portions should be **random**!

# Supervised ML task and data instances

**Supervised machine learning necessarily requires learning examples**

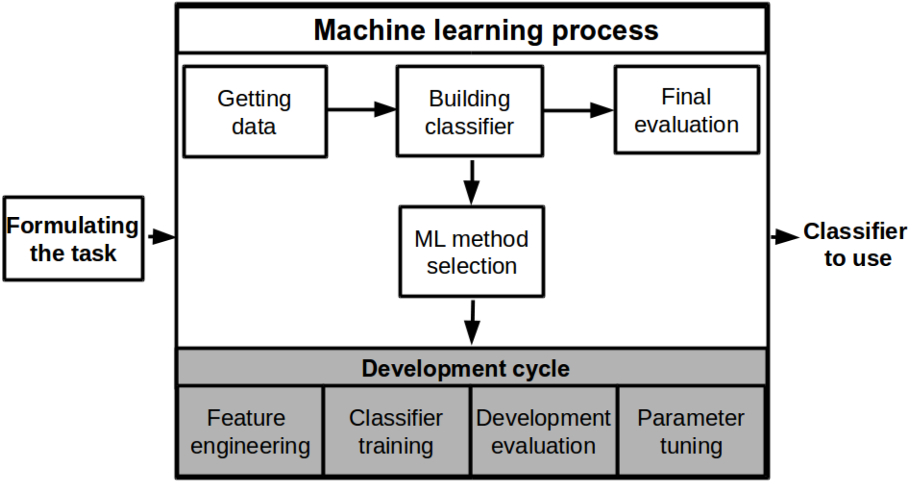
- **Features** are properties of examples that can be observed or measured
  – are numerical (discrete or continuous), or categorical (incl. binary)
- **Feature vector** is an ordered list of selected features
- **Data instance** = feature vector (+ target class, if it is known)
- **Training data** = a set of examples used for **learning process**
- **Test data** = another set of examples used for **evaluation**

# Terminology – features and target values

- **How different people call values that describe objects**

| | **observed (known) object characteristics** | **values or categories to be predicted** |
|---|---|---|
| **computer scientists** | **features** | **(target) value or class** |
| **mathematicians (statisticians)** | attributes or predictors | response (value) or output value |

# Machine learning process — development cycle



# Terminological notes on building predictors

**The purpose of the learning process is search for the best parameters of prediction function. – These parameters are the output of learning algorithms.**

| learning parameters (aka hyperparameters) | hypothesis parameters |
|---|---|
| = parameters of learning algorithm | = parameters of prediction function |

- **Method** = approach/principle to learning. i.e. to building predictors
- **Model** = method + set of features + learning parameters
- **Predictor** = trained model, i.e. an output of the machine learning process, i.e. a particular method trained on a particular training data.
- **Prediction function** = predictor (used in mathematics). It's a function calculating a response value using "predictor variables".
- **Hypothesis** = prediction function – not necessarily the best one (used in theory of machine learning).

# Practical procedures in the ML process

- Formulating the task
- Getting data, examples
- Data preprocessing and feature extraction/selection
- Learning and evaluation
- Model assessment

# Formulating the task – example

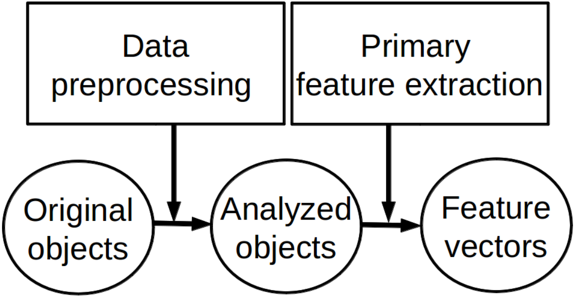
1. **Task description**
   WSD: Assign the correct sense to the target word "line"

2. **Object specification**
   WSD: Sentences containing the target word

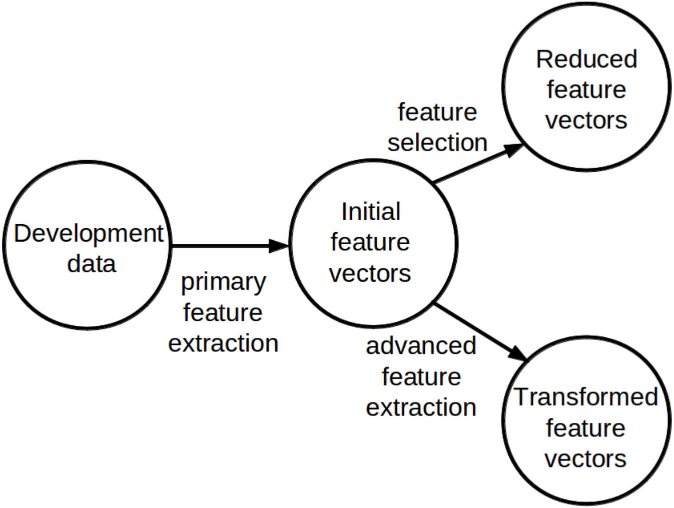
3. **Specification of desired output $Y$**
   WSD: $Y = \texttt{SENSE}$
   `SENSE = {CORD,DIVISION,FORMATION,PHONE,PRODUCT,TEXT}`

# Data preprocessing and feature extraction

**Step 1**: Getting feature vectors



# Feature extraction and feature selection



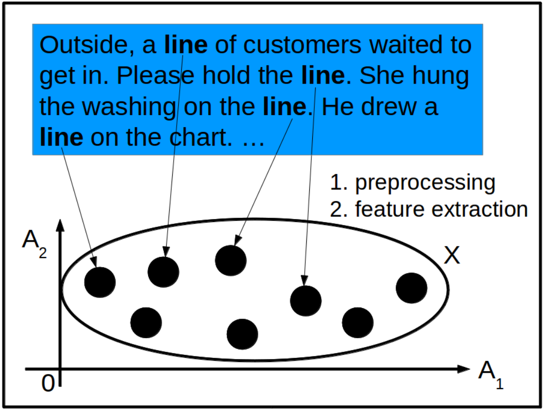
# Getting data

**Step 1**: Getting feature vectors – terminology and notation

- Features as variables $A_1$, ..., $A_m$
  - **numerical**
    – either discrete or continuous
  - **categorical**
    – any list of discrete values, non-numerical
  - **binary** (0/1, True/False, Yes/No)
    – can be viewed as a kind of categorical
- Feature values $x_1, ..., x_m$, $x_i \in A_i$
- Each object represented as feature vector $\mathbf{x} = \langle x_1, ..., x_m \rangle$
- Feature vectors are elements in an $m$-dimensional feature space
- Set of instances $X = \{\mathbf{x} : \mathbf{x} = \langle x_1, ..., x_m \rangle, x_i \in A_i\}$.

# Getting data

**Step 1**: Getting feature vectors – Example



# Example feature vectors – the WSD task

| A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 | A9 | A10 | A11 | A12 | A13 | A14 | A15 | A16 | A17 | A18 | A19 | A20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | safety | special | install | inside | NN | IN | DT | lines | dobj |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | class | across | reach | . | NN | . | X | lines | prep_across |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | fine | the | walk | between | JJ | IN | JJ | line | dobj |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | fine | `` | a | between | JJ | IN | VBG | line | dobj |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | a | draw | to | between | DT | IN | NNS | line | dobj |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | a | draw | to | between | DT | IN | NNS | line | dobj |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | long | when | , | of | JJ | IN | NNS | lines | nsubj |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | long | in | patiently | to | JJ | TO | VB | lines | prep_in |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | long | the | but | delay | JJ | VBD | DT | lines | nsubj |
| 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | car | the | X | affect | NN | VBN | IN | lines | nsubj |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | establish | of | marketing | such | VBN | JJ | IN | lines | prep_of |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | main | few | a | and | JJ | CC | RB | lines | prep_on |
| 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | computer | new | the | to | NN | TO | VB | line | dobj |

See the feature description `wsd.attributes.pdf` at
`https://ufal.mff.cuni.cz/course/npfl054/materials`

# Getting data

**Step 2**: Assigning true predictions

- Take *a number* of original objects and assign true prediction to each of them, e.g. **do manual annotation**.

- Take these objects and their true prediction, do preprocessing and feature extraction. It results in **Gold Standard Data**

$$Data = \{\langle \mathbf{x}, y \rangle : \mathbf{x} \in X, y \in Y\}.$$

# Getting data

**Step 2**: Assigning true prediction
**Example**: $Y$ = SENSE = {CORD,DIVISION,FORMATION,PHONE,PRODUCT,TEXT}

| SENSE | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 | A9 | A10 | A11 | A12 | A13 | A14 | A15 | A16 | A17 | A18 | A19 | A20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **cord** | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | safety | special | install | inside | NN | IN | DT | lines | dobj |
| **division** | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | class | across | reach | . | NN | . | X | lines | prep_across |
| **division** | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | fine | the | walk | between | JJ | IN | JJ | line | dobj |
| **division** | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | fine | `` | a | between | JJ | IN | VBG | line | dobj |
| **division** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | a | draw | to | between | DT | IN | NNS | line | dobj |
| **division** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | a | draw | to | between | DT | IN | NNS | line | dobj |
| **formation** | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | long | when | , | of | JJ | IN | NNS | lines | nsubj |
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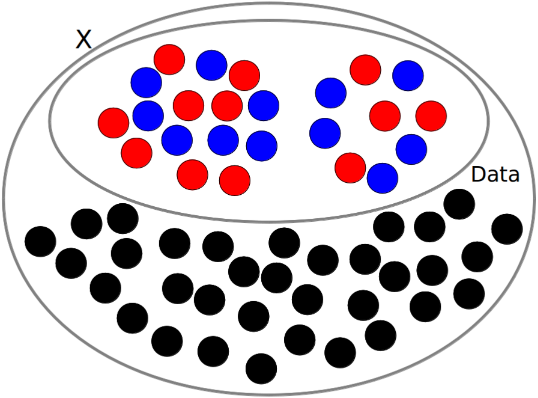
| **formation** | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | long | the | but | delay | JJ | VBD | DT | lines | nsubj |
| **product** | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | car | the | X | affect | NN | VBN | IN | lines | nsubj |
| **product** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | establish | of | marketing | such | VBN | JJ | IN | lines | prep_of |
| **product** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | main | few | a | and | JJ | CC | RB | lines | prep_on |
| **product** | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | computer | new | the | to | NN | TO | VB | line | dobj |

# Getting data

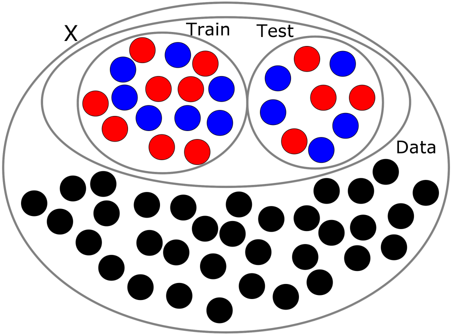
**Step 2**: Assigning true prediction
**Example**: $Y = \{\textit{red}, \textit{blue}\}$



# Getting data

**Step 3**: Selecting training set *Train* and test set *Test*

- $Train \subseteq Data$, $Test \subseteq Data$
- $Train \cap Test = \emptyset$
- $Train \cup Test = Data$



# Summary of Lecture #1
# Examination Requirements

**You should be familiar with the following key machine learning terms**

- Machine learning process
- Development cycle
- Examples, feature vectors, data instances
- Gold standard data, training data, test data
- Manual annotation (true predictions)
- Model, predictor, hypothesis optimization
- Supervised learning
- Classification, regression

# Homework – get ready for the first lab session!

- **Install R on your own computer and get familiar with its basic functions**

# What you will learn at the following Lab session #1

- **Annotation experiment**
  - Practical experience with manual annotation
- **Startup with R**
  - Elementary data processing and computation in R
  - Annotation data analysis