3.1 Introduction to Machine Learning and Potential Applications to Chemical Engineering

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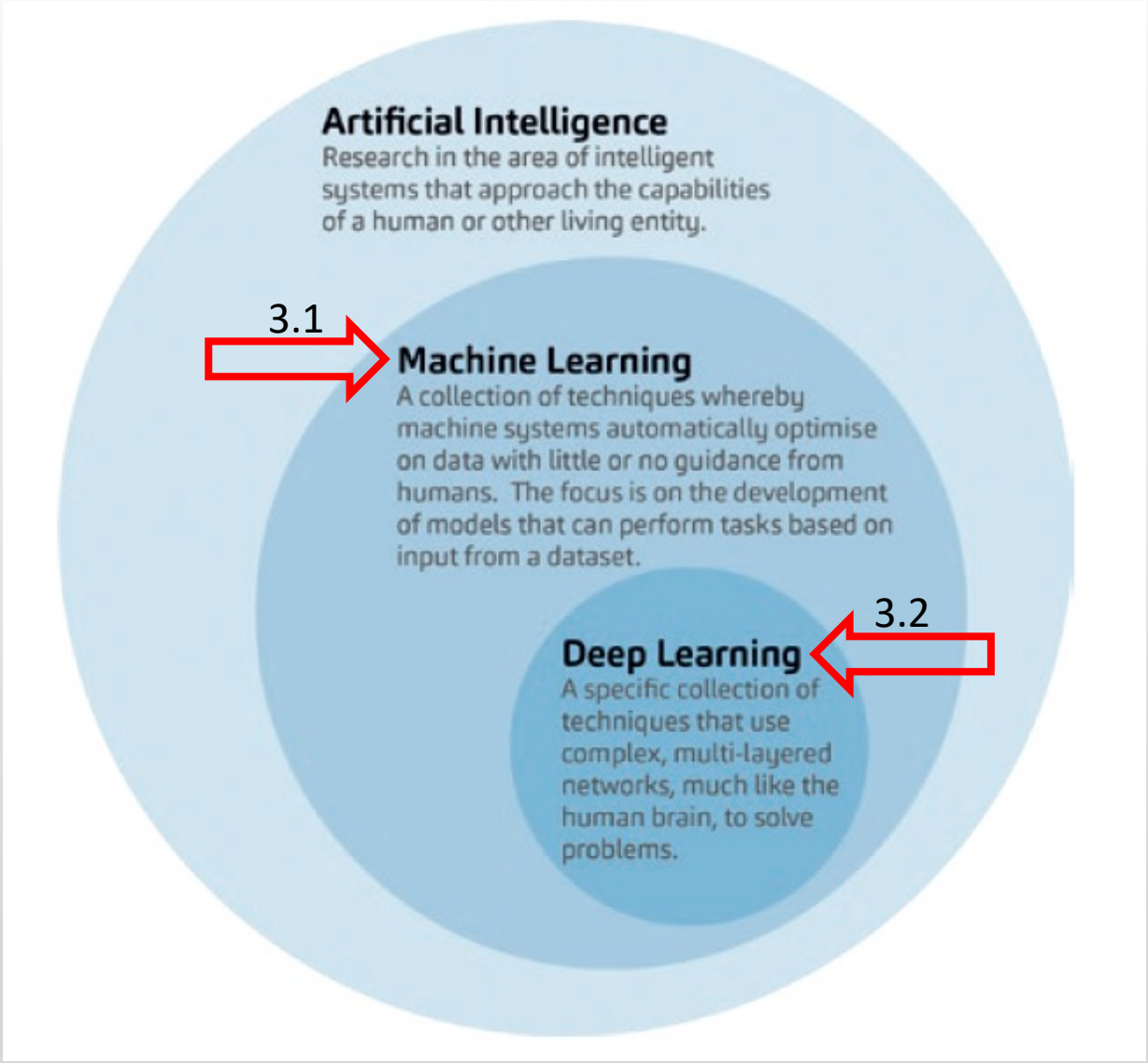
Outline

1. Introduction to Machine Learning
2. Classification
3. Regression
4. An application to chemical engineering

What is Machine Learning?

- The term "**Artificial Intelligence**" (**AI**) is colloquially used to describe the "ability" of machines to mimic cognitive functions of human mind, such as **learning** and **problem solving**.
- **Machine Learning** (**ML**) is the study of computer algorithms that improve automatically through experience.
  - Subfield of AI.
  - ML algorithms build models based on data (training examples) in order to make predictions or take decisions.
  - Several (and progressively increasing) **application fields**, e.g.:
    - communication, cyber-security, economics and finance, gaming, linguistics, **manufacturing**, marketing, medicine, robotics, satellite navigation, …
- **Deep Learning** (**DL**) is an important subfield of ML based on **Artificial Neural Networks** mimicking human brain operation (see 3.2).



Gertz F., Fleutsch G., Applications of Deep Learning in Medical Device Manufacturing. *ONdrugDelivery*, 110, 6-11, 2020.

A bit of history

- The term “Machine Learning” was used for the first time in 1959 by **Arthur Lee Samuel**[1].
  - Samuel had an electrical engineering degree from MIT.
  - In 1959, he used to work at IBM when he developed his **checkers program** on IBM701, which is considered the **world's first self-learning program**.
  - He was also among the developers of the TeX typesetting language.

- In 1997, Tom M. Mitchell gave an **operational definition** of ML[2]:
  - “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.*”
- Contemporary ML has **two possible objectives**:
  - **classification** of data based on models,
  - **prediction** for future outcomes based on data.

Introduction to ML 1

- To solve a problem on a computer, we typically need an **algorithm** → finite sequence of instructions that transform inputs into outputs.
  - For example, an algorithm for sorting numbers: the input is a set of numbers in random order, the output is the ordered list.
- For the same task, there might be different algorithms.
  - The choice is based on some optimization criteria: the one requiring the less instructions, memory, …
- Sometimes, the inputs and outputs are clearly defined, but there is **no algorithm**.
  - Example: sorting spam email from legitimate one.
    - Input: email messages, output: yes/no
    - How to transform input into output? This may change from person to person…
- When an algorithm is lacking, the problem can be solved anyways if we have **a lot of data**.
  - We feed a machine with thousands of messages, of which we know whether they are spam or not (**training data**), and we ask it to extract "automatically" the algorithm to classify them.

Introduction to ML 2

- ML is programming computers to optimise a performance criterion using example data.
- Given a model containing some parameters, learning is optimising the parameters of the model using the training data in order to
  - enhance the description of the data (descriptive model),
  - predict future data (predictive model).
- Since the core task is making inference from a sample, ML uses the **theory of statistics**.

ML approaches

- ML approaches are traditionally divided into **three categories**:
  - **supervised learning**: a "teacher" feeds the computer with examples of inputs and corresponding "correct" outputs with the aim of learning a general rule that maps inputs to outputs,
  - **unsupervised learning**: unlabelled inputs are given to a learning algorithm, leaving it "on its own" to find a structure among them,
  - **reinforcement learning**: in case the output of a system is a sequence of actions, the single action is not important. Instead, it is important to identify a correct sequence to reach a certain goal, also interacting with a **dynamic environment**.
    - Examples: game playing, driving vehicles, …
  - Intermediate approaches exist, like **semi-supervised learning**, where some of the training examples are unlabelled and some are labelled. The presence of the latter can produce a considerable improvement in learning accuracy.

Applications of ML 1

- Given many data, one application of ML is of finding **association rules** among them.
  - Association rules are **conditional probabilities** of the form $P(Y|X)$.
  - Example: from the data available to a supermarket chain, it emerges that 70 percent of customers who buy beer also buy chips → $P(\text{chips}|\text{beer}) = 0.7$.
- Another typical application is **classification** of inputs based on their features.
  - Classification rules are conditional structures based on **training with data**.
  - Example: in order to loan money, customers of a bank are classified according to the rule $IF\ [(\text{income} > X)\ AND\ (\text{savings} > Y)]\ THEN\ \text{low} - \text{risk}\ ELSE\ \text{high} - \text{risk}$.
  - Classification, in turn, is the basis for **prediction**: if the near future is similar to the past, a rule that fits the available data allows to make correct predictions for novel instances.
  - A more complex example of classification is **pattern recognition**, where there are multiple classes.
    - For example, character recognition, language translation, face recognition, medical diagnosis, ...

Applications of ML 2

- The data, in turn, can be used to learn **rules** from them → **knowledge extraction**.
  - Rules are models explaining the data.
  - This allows for **memory saving**.
  - **Outlier detection**: finding data that do not obey the rule.
- Another important ML application is **regression**.
  - Given input data X, output data Y, and a model $y = g(x, \theta)$, where θ denotes parameters, the ML algorithm optimizes the value of θ such that the approximation error is minimised, i.e., estimates are as close as possible to Y-values given in the training set.
  - Example: coffee consumers' satisfaction is measured at varying temperature, extraction time, and coffee bean type. To find the optimal setting, a regression model linking inputs to output is fitted. Then, new data are collected close to the optimum of the model and a new model is fitted to identify an even better configuration.

Applications of ML 3

- One aim of unsupervised learning is the identification of patterns in large data sets → **data mining**.
- In statistics, the evaluation of pattern recurrence is called **density estimation**.
- A method for density estimation is **clustering**, i.e., finding groupings of inputs.
  - **Example**: document clustering depending on the number of shared words.
    - Critical aspect: lexicon choice.

So, what is ML in the end?

- Given the successful application of ML in various domains, it may be claimed that what we needed was **not new algorithms**[3], but
  - a lot of data,
  - sufficient computational power to run algorithms on them.
- For example, support vector machines are based on **potential functions**, **linear classifiers**, and **neighbour-based methods** proposed in the 1950s and 1960s.
  - No fast computers or large storage devices were available for these algorithms to show their full potential at that time.
- Complicated tasks, e.g., machine translation, can be solved with relatively **simple learning algorithms**, but trained on large amounts of example data.
  - Recent successes with DL algorithms support this claim.
- AI seems not to originate from some outlandish formula, but rather from the patient, almost brute-force use of simple, straightforward algorithms[3].

ML for classification

- On of the main tasks of ML is **classification**.
- Let us go through an **example**: we want a machine decide if a car is a family car or not.
- We show a **set of examples** of cars to people, asking them to **label** them depending on whether they are family cars or not.
  - Yes → positive example
  - No → negative example
- This has two possible aims:
  - **prediction**: given a car not labelled before, is this a family car?
  - **knowledge extraction**: what do people expect form family cars?

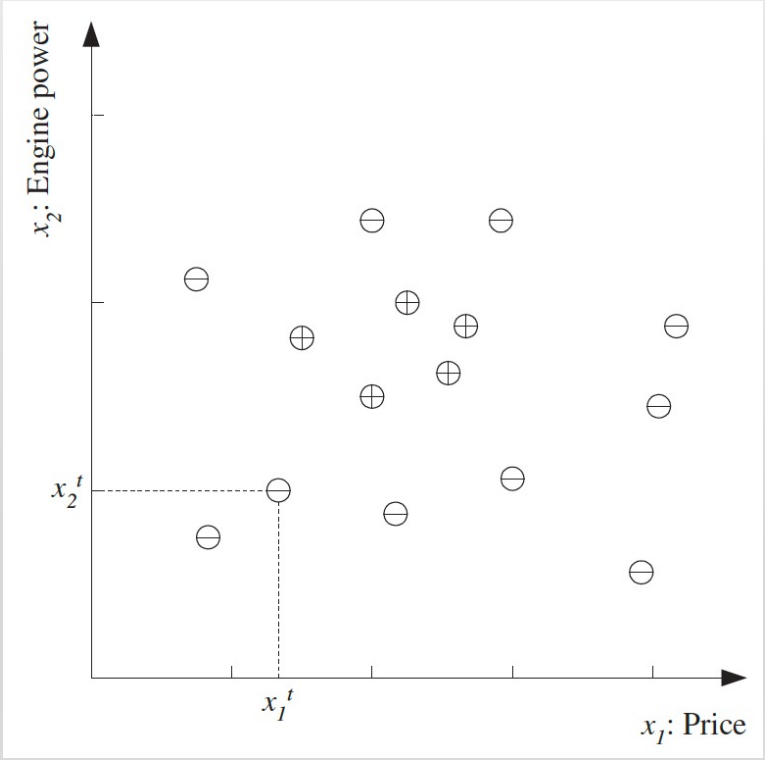
Training examples

- In order to label the examples, the **features** that identify the **class** must be selected, e.g.
  - price x_1,
  - engine power x_2.
- The **training dataset** contains N examples

$$\mathcal{X} = \{\boldsymbol{x}_t, r_t\}_{t=1}^{N}$$

where

- $\boldsymbol{x}_t = [x_1, x_2]$
- $r_t = \begin{cases} 1 \text{ if } \boldsymbol{x}_t \text{ is a positive example} \\ 0 \text{ if } \boldsymbol{x}_t \text{ is a negative example} \end{cases}$

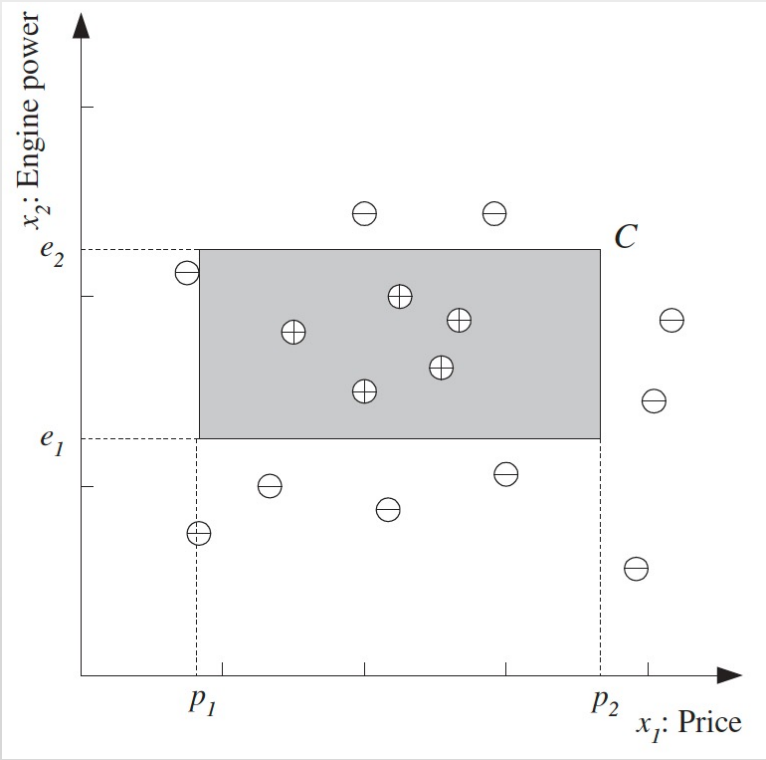


Hypothesis class selection

- After discussion with **"experts"**, we might state that a family car satisfies

$$(p_1 \leq x_1 \leq p_2) \cap (e_1 \leq x_2 \leq e_2)$$

- C is assumed (by the experts) to be a rectangle (with unknown boundaries) in the feature space.
  - C is drawn from an **hypothesis class** $\mathcal{H}$.
  - $\mathcal{H}$ is the class of all the rectangles in the feature space.
- The objective of the learning algorithm is to find $h \in \mathcal{H}$, specified by $\left(p_1^h, p_2^h, e_1^h, e_2^h\right)$, that approximates C as closely as possible.



Hypothesis selection 1

- The **hypothesis** h makes a prediction for an instance $\boldsymbol{x}$ such that

$$h(\boldsymbol{x}) = \begin{cases} 1 \text{ if } h \text{ classifies } \boldsymbol{x} \text{ as a positive example} \\ 0 \text{ if } h \text{ classifies } \boldsymbol{x} \text{ as a negative example} \end{cases}$$

- In “real life”, we do not know $C(\boldsymbol{x})$, so we cannot evaluate how well $h(\boldsymbol{x})$ matches $C(\boldsymbol{x})$.

- What we have is the training set $\mathcal{X}$, which is a small subset of all possible data.

Hypothesis selection 2

- The **empirical error** is the portion of training instances where predictions of h do not match the required values given in $\mathcal{X}$.
- It is defined as

$$E(h|\mathcal{X}) = \sum_{t=1}^{N} 1(h(\boldsymbol{x}_t) \neq r_t)$$

with $1(a \neq b) = \begin{cases} 1 \text{ if } a \neq b \\ 0 \text{ if } a = b \end{cases}$

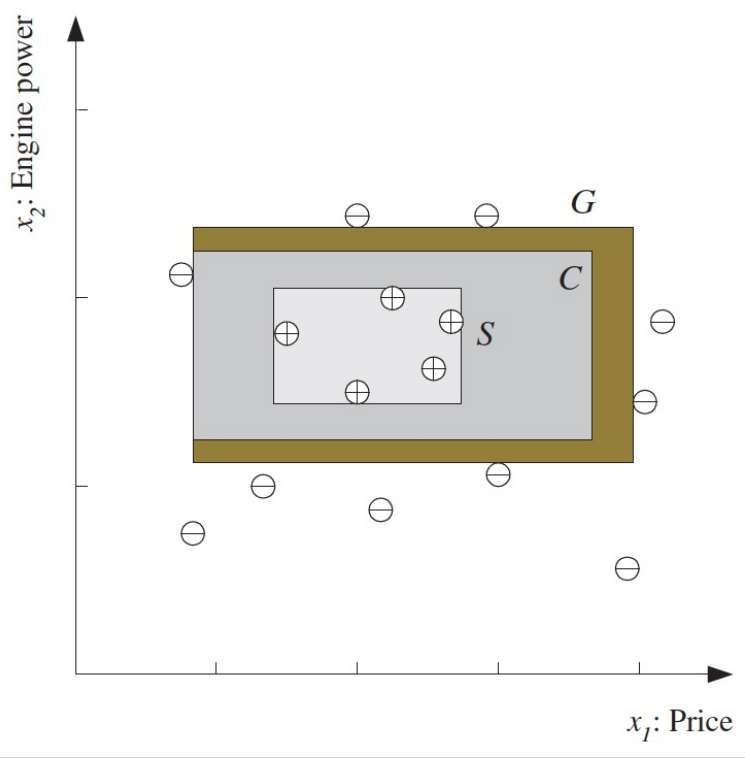
- In our example, $\mathcal{H}$ is the class of all rectangles, each quadruple $\left(p_1^h, p_2^h, e_1^h, e_2^h\right)$ defines an hypothesis h.
  - What is the **"best"** one?

Hypothesis selection 3

- Given the training set, $\left(p_1^h, p_2^h, e_1^h, e_2^h\right)$ should include all the positive examples and none of the negative examples.
- If x_1 and x_2 are real-valued, there are **infinite h-s** for which $E = 0$.
- On the other hand, different candidate hypotheses may make different **predictions** for a future example somewhere close to the boundary between positive and negative examples.
- This is the **problem of generalisation**: how well will our hypothesis classify future examples that are not part of the training set?

Hypothesis selection 4

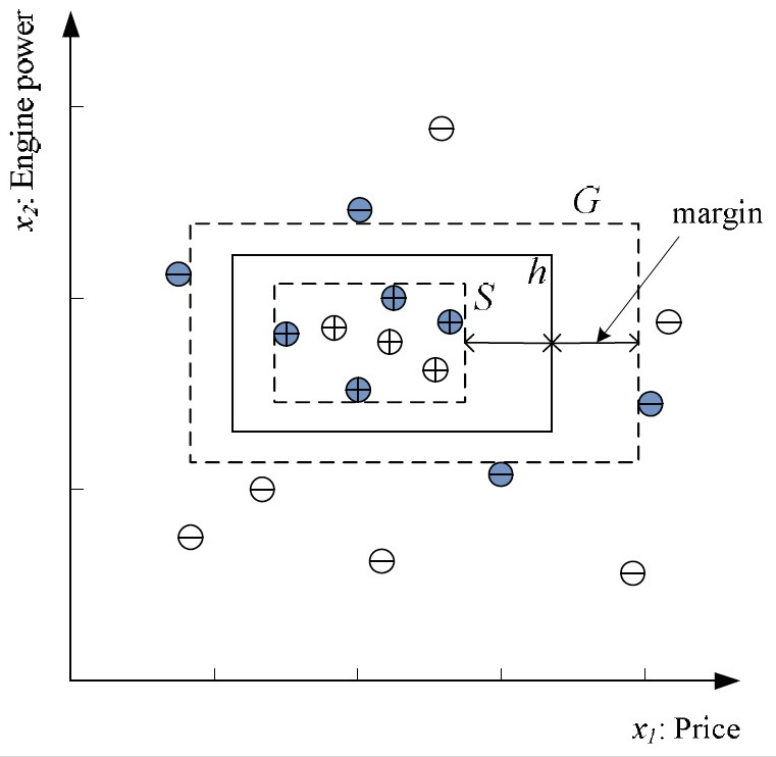
- We call the **most specific hypothesis**, S, the tightest rectangle that includes all the positive examples and none of the negative examples.
  - C may be larger than S but not smaller.
- We call the **most general hypothesis**, G, the largest rectangle that includes all the positive examples and none of the negative examples.
  - C may be smaller than G but not larger.



Hypothesis selection 5

- Any $h \in \mathcal{H}$ between S and G is a valid hypothesis **consistent with the training set**.
  - The set of all possible h consistent with the training set makes up the **version space**.
  - Given another training set, S, G, the version space, and the learned hypothesis h can be different.

- It could be intuitive to choose h **halfway** between S and G.
  - This increases the **margin**, which is the distance between the boundaries of h and the instances closest to it.

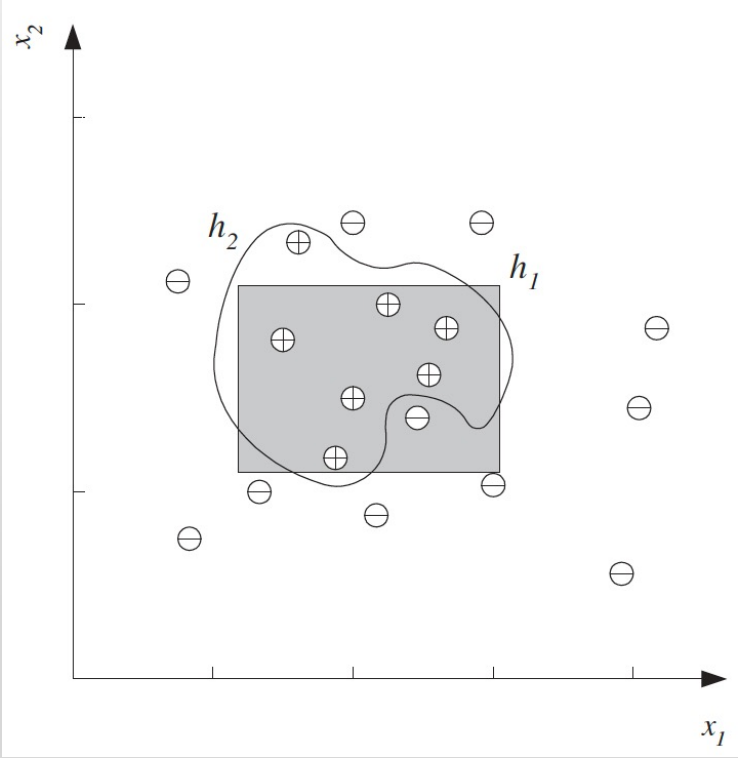


Hypothesis selection 6

- In order to choose h that minimises the empirical error while maximising the margin, we should use an **error** (**loss**) **function** that not only checks whether an instance is on the correct side of the boundary but also how far it is from it.
  - To do that, we need a hypothesis that returns a value carrying a measure of the distance to the boundary and we need a loss function using it, thus different from $E(h|\boldsymbol{\mathcal{X}}) = \sum_{t=1}^{N} 1(h(\boldsymbol{x}_t) \neq r_t)$.
- In some applications, a **wrong decision** may be **very costly**.
  - In such a case, any instance between S and G is a case of **doubt**, which cannot be labelled with certainty due to lack of data.
  - If so, the system **rejects** the instance and defers the decision to a human expert.

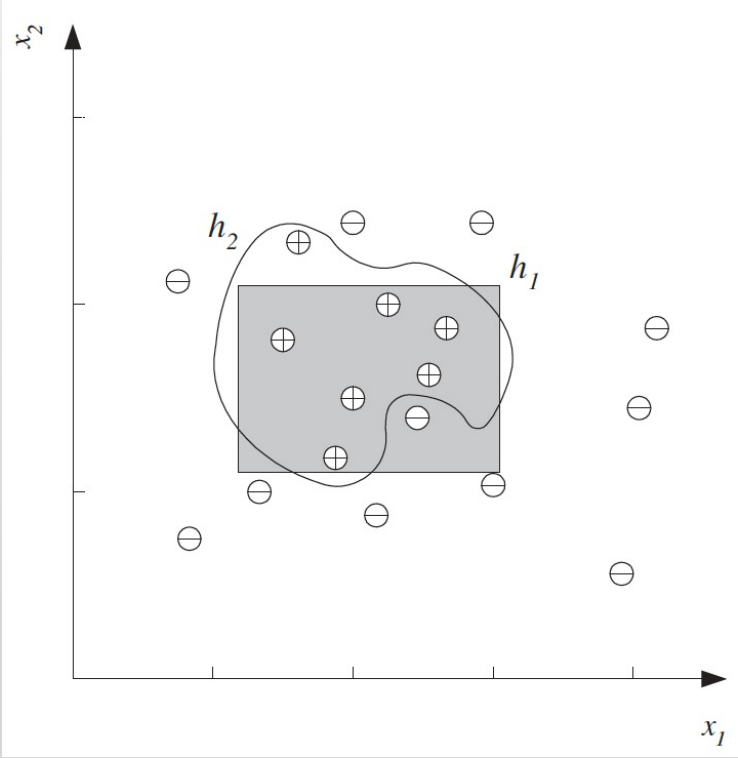
Noise 1

- **Noise** is any unwanted anomaly in the data.
  - Due to noise, a class may be more difficult to learn and **zero error** may be **unattainable** with a simple hypothesis class.
- Possible **causes** of noise:
  - imprecision in recording the input attributes
    - may shift the data in the input space
  - errors in labelling the data
    - may cause labelling of positive instances as negative and vice-versa
    - sometimes called “teacher noise”



Noise 2

- When there is noise, there is **no simple boundary** between the positive and negative instances.
- To separate them, one needs a **more complicated hypothesis**, having a **larger capacity**.
- With a complex model, a fit to the data with zero error can be made.
- Another possibility is to keep the model simple and allow some error.



Variance vs. bias

- In our example, using the simple rectangle makes sense because
  - it is easy to check whether a point is inside or outside a rectangle
  - it is **simple to train** as it has few parameters
    - easier to find the corner values of a rectangle than the control points of an arbitrary shape
  - if the training set is small, the rectangle will change less than a complex model with different training instances → a simple model has **less variance**
    - if there is noise, the rectangle is less affected by single instances than a wiggly shape
  - it is **simple to explain**: a rectangle corresponds to defining intervals on the two attributes
- Given comparable empirical error, a simple model will generalise better than a complex model.
  - **Occam's razor**: simpler explanations are more plausible and any unnecessary complexity should be shaved off.
- On the other hand, a simple model is based on **more rigid assumptions** and may fail if the underlying class is not that simple → it has **more bias**.

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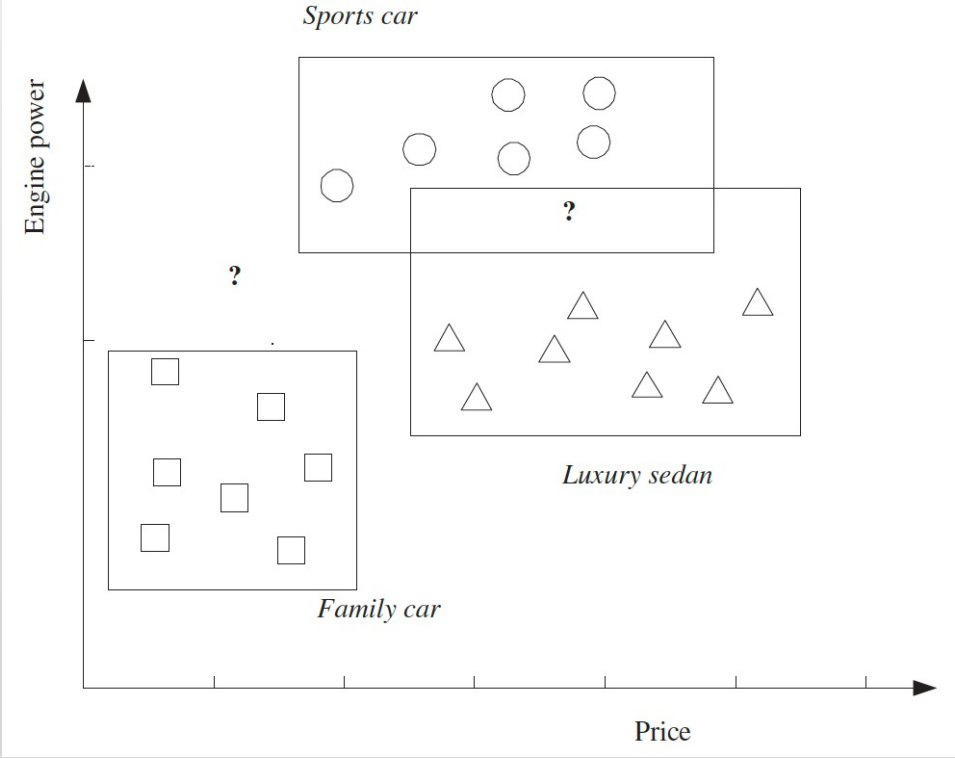
More general classification problems

- In the **general case**, we have K classes $C_i, i = 1, \ldots, K$, and each input instance belongs to one of them.
- In ML for classification, we would like to learn the boundaries separating the instances of one class from those of all the other classes.
- A K-class classification problem can be seen as K two-class problems.
- The training examples belonging to C_i are the positive instances of hypothesis h_i and the examples of all other classes are the negative instances of h_i.



Interpolation and extrapolation

- In classification, given an input, the output is Boolean: yes/no.
- When the output is a numeric value, we would like to learn an (**unknown**) **numeric function** linking it to the input.
- The **training set** of examples drawn from such function is

$$\boldsymbol{\mathcal{X}} = \{\boldsymbol{x}_t, r_t\}_{t=1}^{N}$$

  with $r_t \in \mathbb{R} = f(\boldsymbol{x}_t)$.
- If there is **no noise**, the function $f(\boldsymbol{x})$ can be found by **interpolation**.
  - Given N points, a $(N-1)^{\text{th}}$-degree polynomial passes through all the examples in the training set.
- Such function can be used to predict the output for any $\boldsymbol{x}$ out of the training set → **extrapolation**.

Regression 1

- If there is noise acting on the output of the unknown function, we have

$$r_t = f(\boldsymbol{x}_t) + \epsilon_t$$

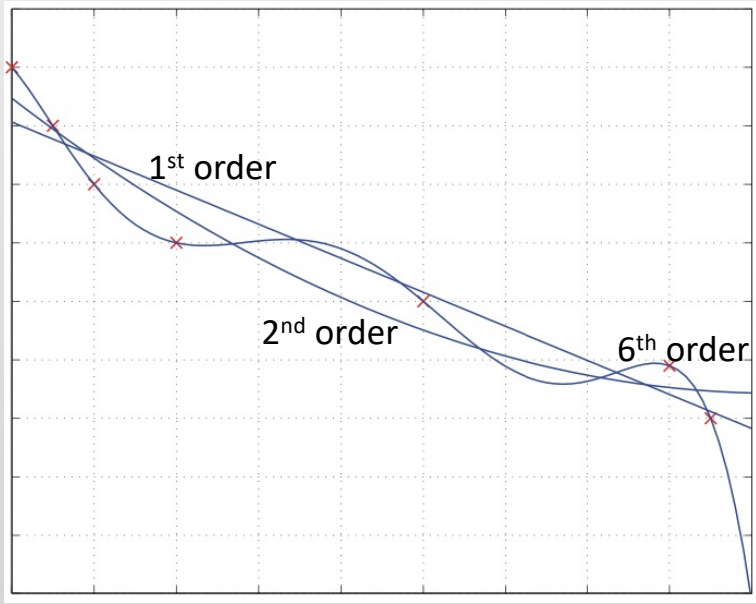
  where ϵ_t represents random noise.
- In this case, we would like to **approximate** the output by a **model** $g(\boldsymbol{x})$ → **regression**.
- A possible reassure of the **empirical error** on the training set $\boldsymbol{\mathcal{X}}$ is

$$E(g|\boldsymbol{\mathcal{X}}) = \frac{1}{N}\sum_{t=1}^{N}[r_t - g(\boldsymbol{x}_t)]^2$$

- Since r_t and $g(\boldsymbol{x}_t)$ are numeric quantities, we can define a **distance** between them.
  - The square of the difference is a possible **loss function**.
  - The absolute value of the difference is another possibility.

Regression 2

- Our aim is to find g that **minimises the loss function**.
- The approach is the same as for classification: we assume a **hypothesis class** for g with a small number of parameters, e.g., a linear function.
- If the linear model is too simple, the empirical error corresponding to the minimization of the loss function will be still too large: in such a case, the output may be taken as a **higher-order function** of the input, e.g., quadratic.
- When the order of the polynomial is increased, the error on the training data decreases.
- On the other hand, a high-order polynomial follows individual examples instead of capturing the general trend.
- **Occam's razor** applies also in the case of regression and we should be careful when fine-tuning the model complexity to match it with the complexity of the function underlying the data.



ML is an ill-posed problem

- Since the training set contains only a small subset of all possible instances, the solution is not unique → ML is an **ill-posed problem**.
  - Such issue appears both in classification and regression applications.

- As training examples increase, we learn more about the underlying function and we can remove inconsistent hypotheses from the hypothesis class.
  - However many consistent hypotheses are still there.

Inductive bias

- Since learning is ill-posed and data by themselves are not sufficient to find the solution, we should make some **extra assumptions** to have a unique solution.
- The set of assumptions we make to perform ML is called the "**inductive bias**" of the learning algorithm.
  - In the classification of cars, there are infinite ways of separating positive from negative examples.
    - Assuming the shape of a rectangle is an inductive bias.
    - Choosing the rectangle with the largest margin is another inductive bias.
  - In regression, there are infinite functions that could relate input to output.
    - Assuming a linear function is an inductive bias
    - Choosing the one that minimizes the squared error is another inductive bias.

Model capacity

- Each hypothesis class has a certain **capacity** and can learn only certain functions.
- The set of functions that can be learned can be extended by using a hypothesis class with larger capacity, containing more complex hypotheses.
  - In classification, a hypothesis class that is the union of two rectangles has higher capacity than a single rectangle, but its hypotheses are more complex → more parameters are needed.
  - In regression, as we increase the order of the polynomial, the capacity and complexity increase.
- The question is to decide where to stop.

Model selection

- Learning is not possible without inductive bias: how to choose the **“right” bias**?
  - This is called **model selection**.
- To answer, we should remember that the aim of ML is the prediction for new cases rather than the replication of the training data.
- We would like to be able to generate the right output for an input instance outside the training set.
- The measure of how well a model trained on a training set predicts the right output for new instances is called **generalisation**.

Model generalisation

- For the best generalisation, we should **match the complexity** of the hypothesis class $\mathcal{H}$ with the complexity of the function underlying the data.
- If $\mathcal{H}$ is less complex than the function, we have **underfitting**.
  - For example, if we fit a straight line to data sampled from a third-order polynomial.
  - In such a case, if we increase the model complexity, the training error decreases.
- If we choose a too complex $\mathcal{H}$, the data is not enough to constrain it and we may end up with a bad hypothesis $h \in \mathcal{H}$. This is called **overfitting**.
  - For example, if we fit two rectangles to data sampled from one rectangle.
  - If there is noise, an overcomplex hypothesis may learn not only the underlying function but also the noise in the data, yielding a bad fit.
- Given a training set and an hypothesis class $\mathcal{H}$, we can find $h \in \mathcal{H}$ that minimises the training error, but, if $\mathcal{H}$ is not chosen well, we will not have good generalization no matter what h we pick.

Triple trade-off

- In all ML algorithms that are trained from example data, there is a **triple trade-off**[4] among
  - the capacity of the hypothesis class (i.e., the complexity of the hypothesis we fit to data),
  - the amount of training data,
  - the generalisation error on new examples.
- As the amount of training data increases, the generalisation error decreases.
- As the complexity of the model class increases, the generalisation error first decreases, then it starts to increase.

Cross-validation 1

- We can measure the **generalisation ability** of a hypothesis if we have access to data outside the training set.
- We simulate this by dividing the dataset we have into two parts:
  - one part is used for training, i.e., to fit a hypothesis,
  - the remaining part is called the **validation set** and is used to test the generalisation ability.
- Given a set of possible hypothesis classes $\mathcal{H}_i, i = 1, \ldots, K$, for each we fit the best $h_i \in \mathcal{H}_i$ on the training set.
- Assuming large enough training and validation sets, the most accurate h_i on the validation set is the best one.
- This process is called **cross-validation**.

Cross-validation 2

- Let us consider, for example, the problem of finding the right order in polynomial regression.
- Given K candidate polynomials of different orders (corresponding to $\mathcal{H}_i, i = 1, \ldots, K$), we fit the coefficients of such polynomials on the training set.
- We calculate their errors on the validation set and take that with less validation error as the best polynomial.
- If we want to give an idea about the expected error of our best model, we should not use the error on the validation set, since this has become a part of the training set → we need a third dataset, said **test set** (or **publication set**), containing examples not used in training nor validation.

Cross-validation 3

- We should always remember that the training data we use are a random sample.
- Given an application, if we collect data again, we will get a slightly different dataset, a slightly different fitted h, and a slightly different validation error.
  - Or, if we have a fixed set which we divide for training, validation, and test, we will have different errors depending on how we do the division.
- We have to check if these differences are significant or due to chance.
- In choosing between two hypothesis classes $\mathcal{H}_i$ and $\mathcal{H}_j$, we will use both of them multiple times on different training and validation sets and check if the difference between average errors of h_i and h_j is larger than the average difference among multiple h_i.

An application to chemical engineering

- The Shell oil company has been collecting values of its operational variables in real time for decades → more than 10^7 data per minute are collected.
- In 2018[5], a model was fit to valve historical process data from two manufacturing sites in order to predict valves' behaviour.
- When the measured data of a valve did not match with the predicted behaviour, the valve was predicted to fail (and it actually happened).
- The model linking process inputs to outputs was not derived on a first-principle basis, yet it worked very well due to the large amount of data.

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Those who are interested in taking a little **self-assessment quiz** can do that through the Kahoot! App with Game PIN 09442651.