IB031 Úvod do strojového učení

Tomáš Brázdil

Course Info

Resources:

- Lectures & tutorials (the **main** source)
- Many books, few perfect for introductory level
  One relatively good, especially the first part:
  A. Géron. Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems. O'Reilly Media; 3rd edition, 2022
- (Almost) infinitely many online courses, tutorials, materials, etc.

Evaluation

The evaluation is composed of three parts:

- Mid-term exam: Written exam from the material of the first half of the semester.
- End-term exam: The "big" one containing everything from the semester (with possibly more stress in the second half).
- Projects: During tutorials, you will work on larger projects (in pairs).

Each part contributes the following number of points:

- Mid-term exam: 25
- End-term exam: 50
- Project: 25

To pass, you need to obtain at least 60 points.

Distinguishing Properties of the Course

- Introductory, prerequisites are held to a minimum
- Formal and precise: Be prepared for a complete and "mathematical" description of presented methods.

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I assume that you have basic knowledge of

- Elementary understanding of mathematical notation (operations on sets, logic, etc.)
- Linear algebra: Vectors in $\mathbb{R}^n$, operations on vectors (including the dot product). Geometric interpretation!
- Calculus: Functions of multiple real variables, partial derivatives, basic differential calculus.
- Probability: Notion of probability distribution, random variables/vectors, expectation.

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Machine learning is the field of study that allows computers to learn without being explicitly programmed.

And a more engineering-oriented one:

Tom Mitchell, 1997

A computer program is said to learn from experience E concerning some task T and some performance measure P if its performance on T, as measured by P, improves with experience E.

Example

In the context of spam filtering:

- The task T is to flag spam in new emails.
- The experience E is represented by a set of emails labeled either spam or ham by hand (the training data).
- The performance measure P could be the accuracy, which is the ratio of the number of correctly classified emails and all emails.

  There are many more performance measures; we will study the basic ones later.

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In the context of housing price prediction:

- The task T is to predict prices of new houses based on their basic parameters (size, number of bathrooms, etc.)
- The experience E is represented by information about existing houses.
- The performance measure P could be, e.g., an absolute difference between the predicted and real price.

Examples (cont.)

In the context of game playing:

- The task T is to play chess.
- The experience E is represented by a series of self-plays where the computer plays against itself.
- The performance measure P is winning/losing the game.

  Here, the trick is to spread the delayed and limited feedback about the result of the game throughout the individual decisions in the game.

Examples (cont.)

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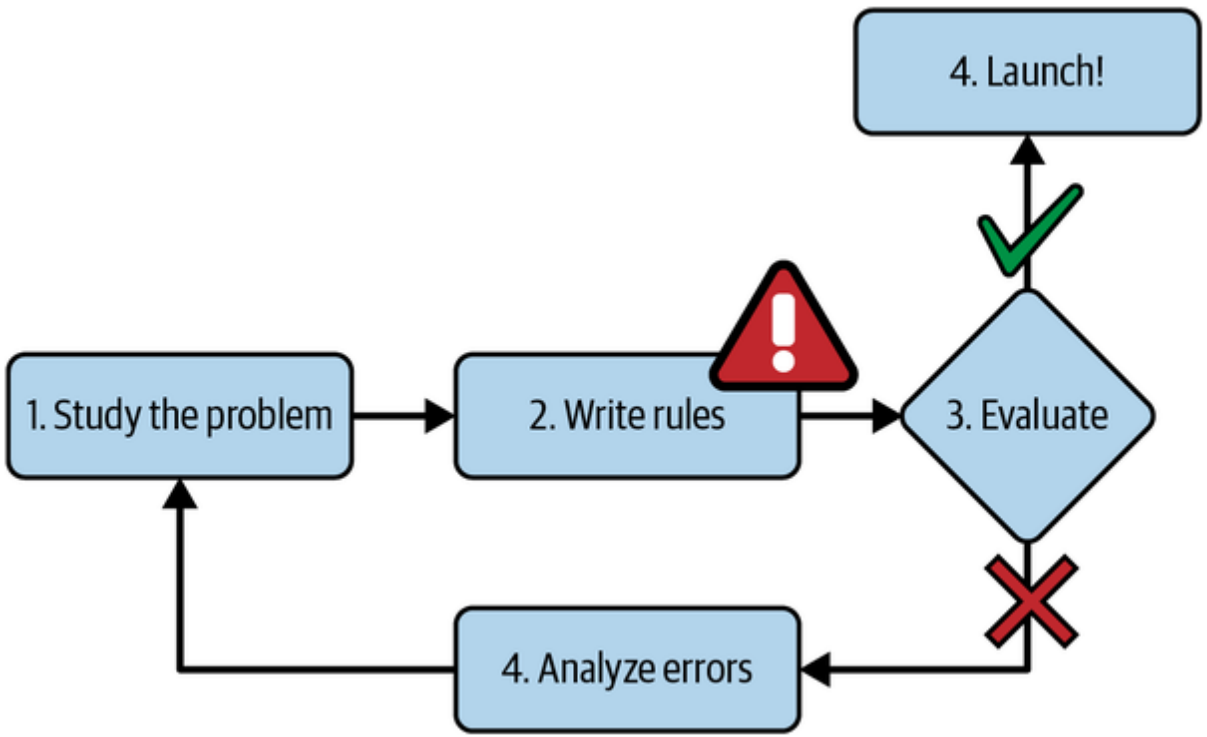
In the context of customer behavior:

- The task T is to group customers with similar shopping habits in an e-shop.
- The experience E consists of lists of items individual customers bought in the shop.
- The performance measure P?
  Measure how "nicely" the customers are grouped.
  (whether people with similar habits, as seen by humans, fall into the same group).

Comparison of Programming and Learning

How to code the spam filter?

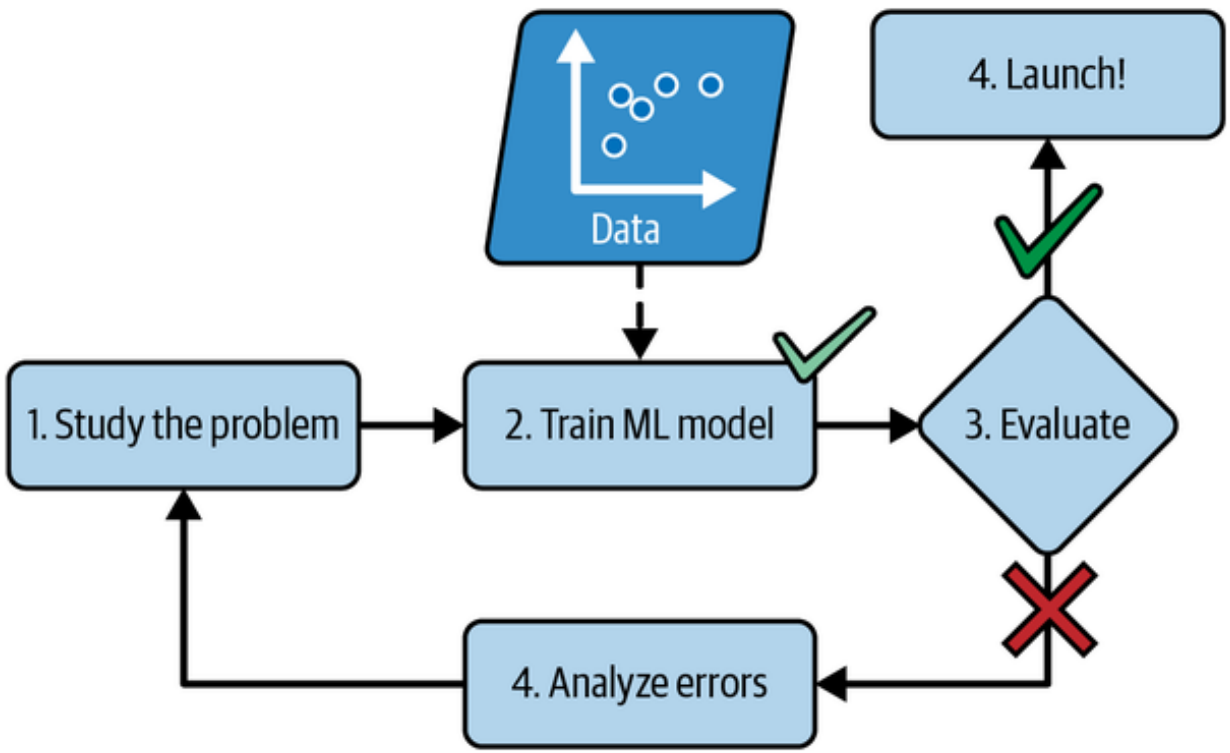
- Examine what spam mails typically contain: Specific words ("Viagra"), sender's address, etc.
- Write down a rule-based system that detects specific features.
- Test the program on new emails and (most probably) go back to look for more spam features.



Comparison of Programming and Learning

The machine learning way:

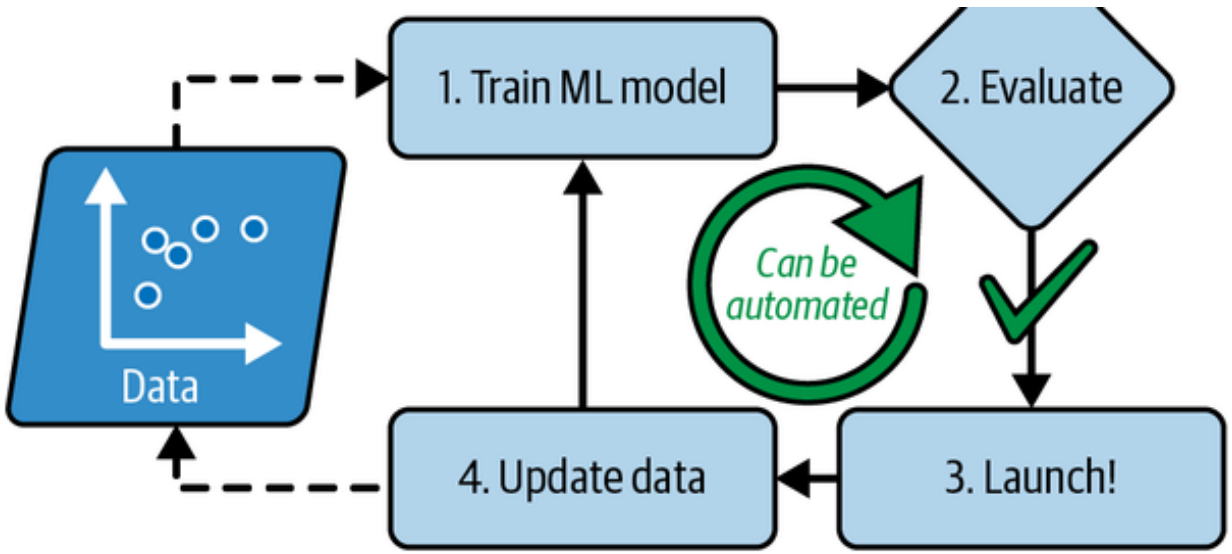
- Study the problem and collect lots of emails, labeling them spam or ham.
- Train a machine learning model that reads an email and decides whether it's spam or ham.
- Test the model and (most probably) go back to collect more data and adjust the model.



ML Solutions are Adaptive

Spam filter: Authors of spam might and will adapt to your spam filter (possibly change the wording to pass through).

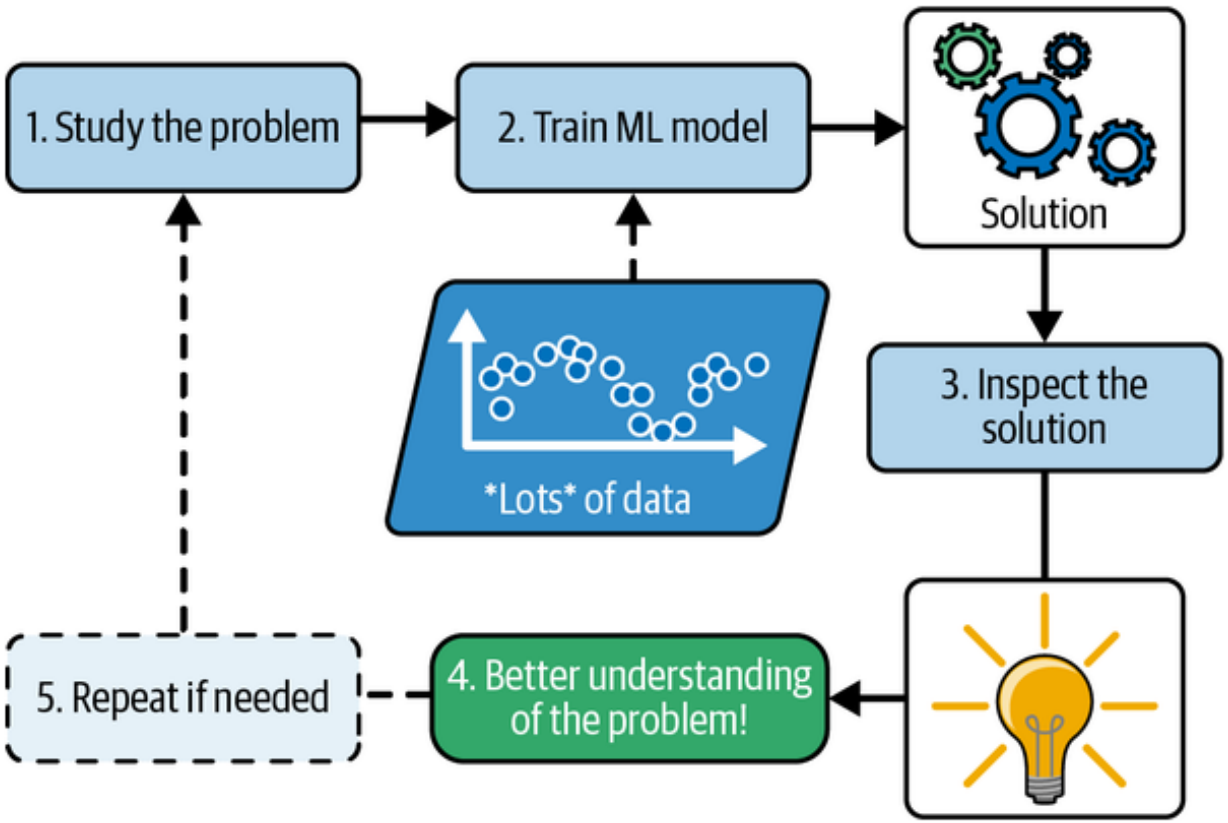
ML systems can be adjusted to new situations by retraining on new data (unless the data becomes ugly).



ML for Human Understanding

Spam filter: A trained system can be inspected for notorious spam features.

Some models allow direct inspection, such as decision trees or linear/logistic regression models.



Usage of Machine Learning

Machine learning suits various applications, especially where traditional methods fall short. Here are some areas where it excels:

- Solving complex problems where fine-tuning and rule-based solutions are inadequate.
- Tackling complex issues that resist traditional problem-solving approaches.
- Adapting to fluctuating environments through retraining on new data.
- Gaining insights from large and complex datasets.

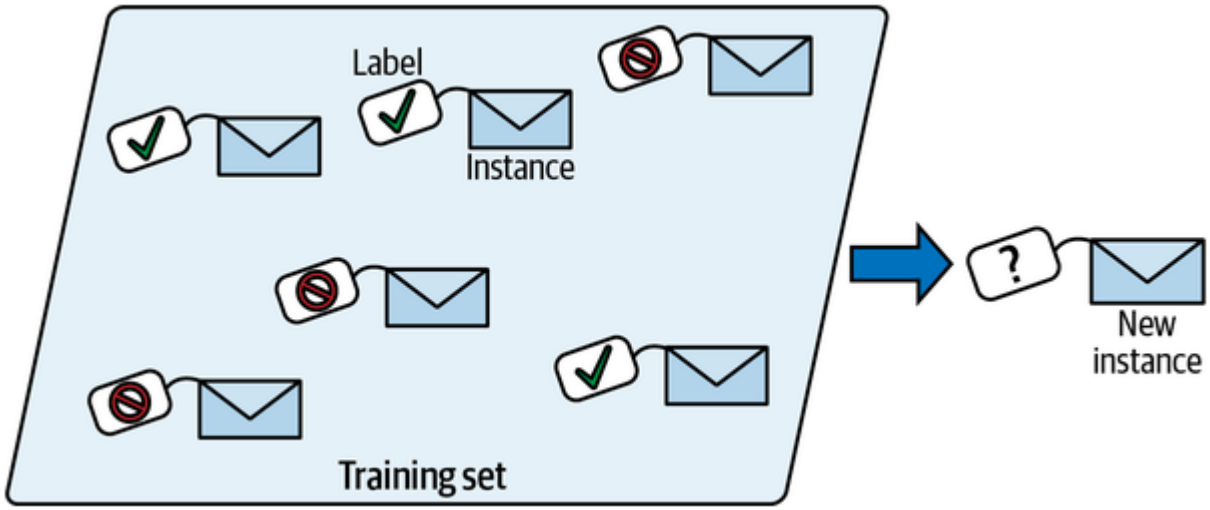
In summary, machine learning offers innovative solutions and adaptability for today's complex and ever-changing problems, (sometimes) providing insights beyond the reach of traditional approaches.

Types of Learning

There are main categories based on information available during the training:

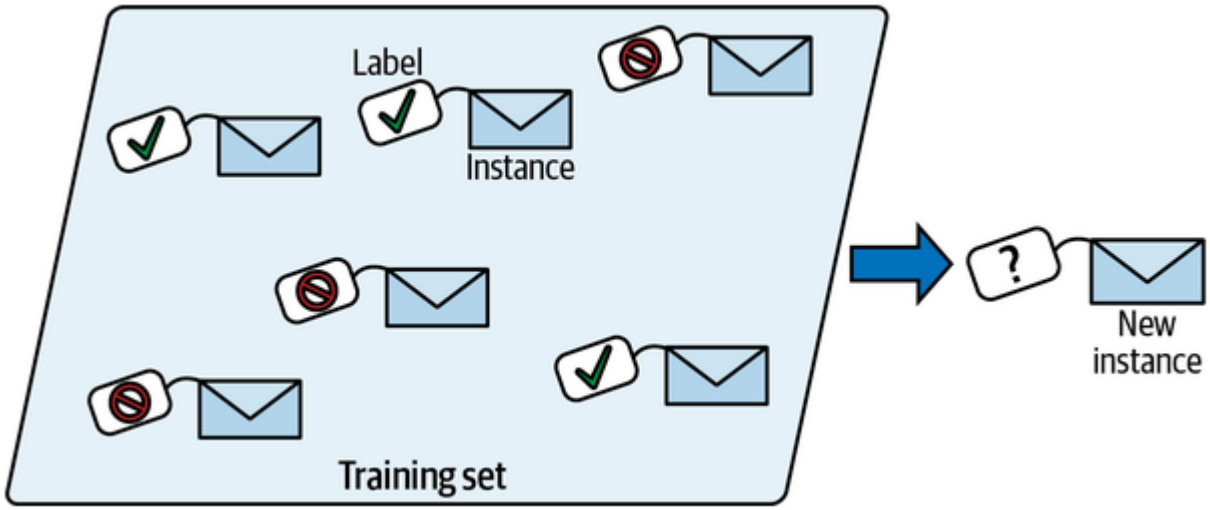
- Supervised learning
- Unsupervised learning
- Semi-supervised learning
- Self-supervised learning
- Reinforcement learning

Supervised Learning



Labels are available for all input data.

Supervised Learning



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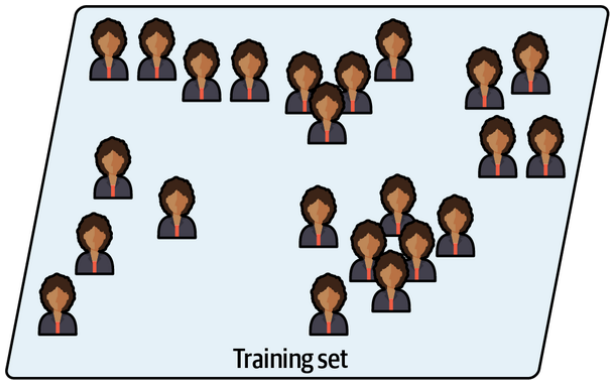
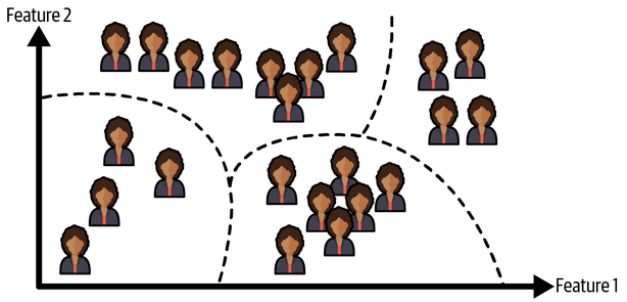
Typical supervised learning tasks are

- *Classification* where the aim is to classify inputs into (typically few) classes
  (e.g., the spam filter where the classes are spam/ham)
- *Regression* where a numerical value is output for a given input
  (e.g., housing prices)

Unsupervised Learning





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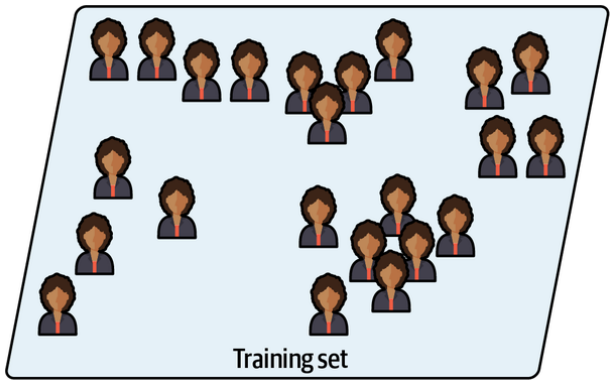

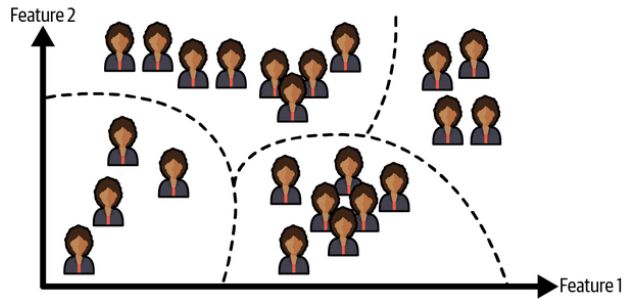

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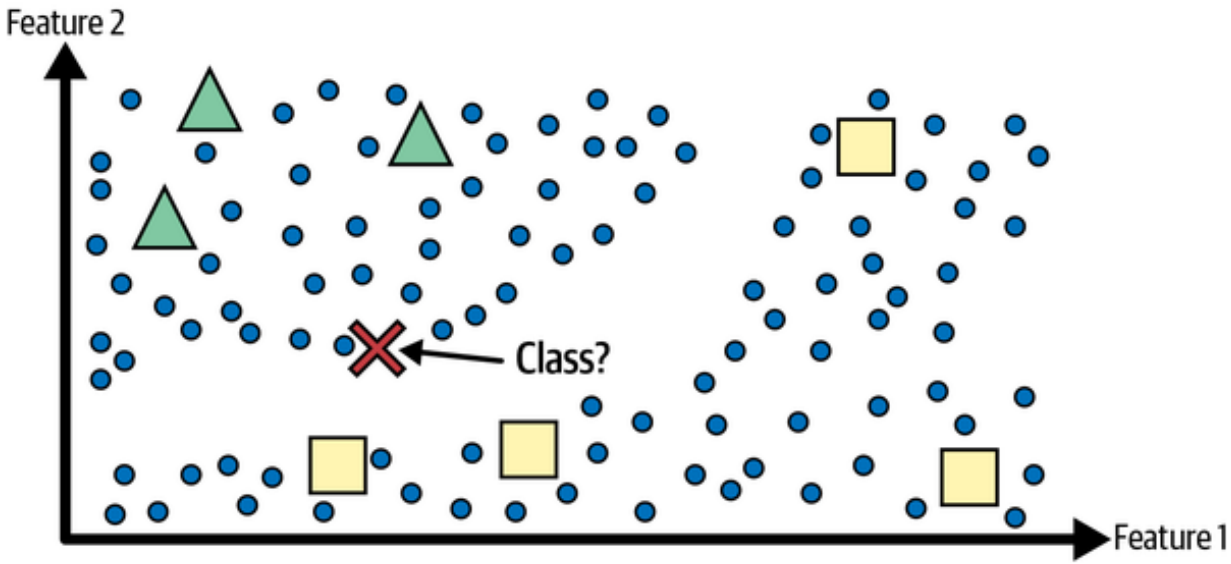
Typical unsupervised learning tasks are

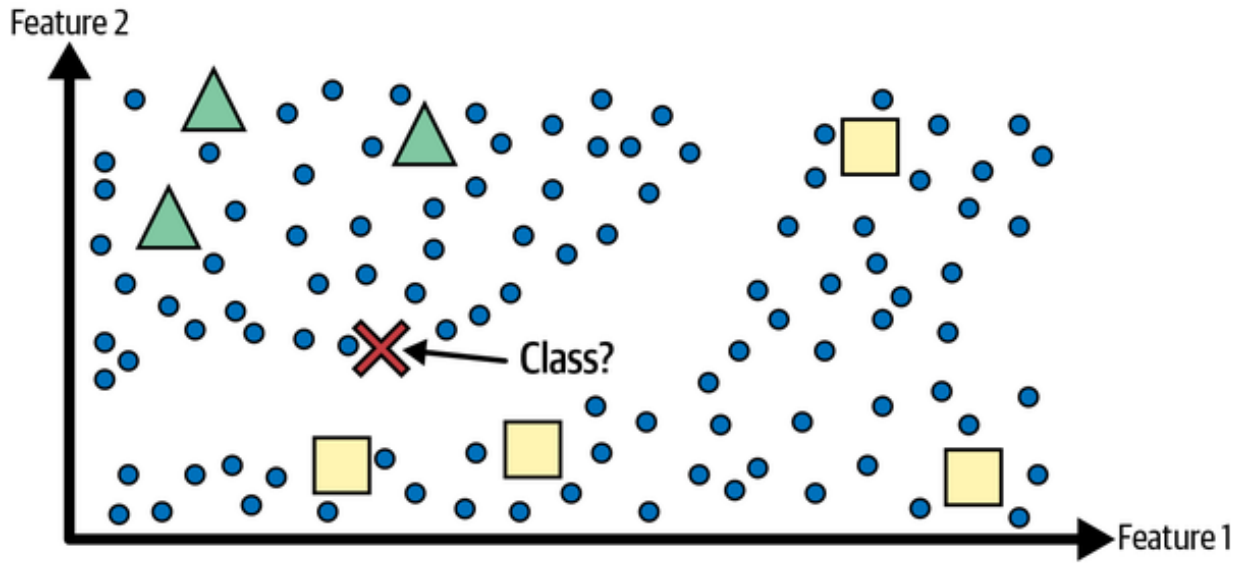
- *Clustering* where inputs are grouped according to their features
  (e.g., clients of a bank grouped according to their age, wealth, etc.)
- *Association* where interesting relations and rules are discovered among the features of inputs
  (e.g., market basket mining where associations between various types of goods are being learned from the behavior of customers)
- *Dimensionality reduction* reduce high-dimensional data to few dimensions (e.g., images to few image features)

Semi-Supervised Learning



Labels for some data.

Semi-Supervised Learning

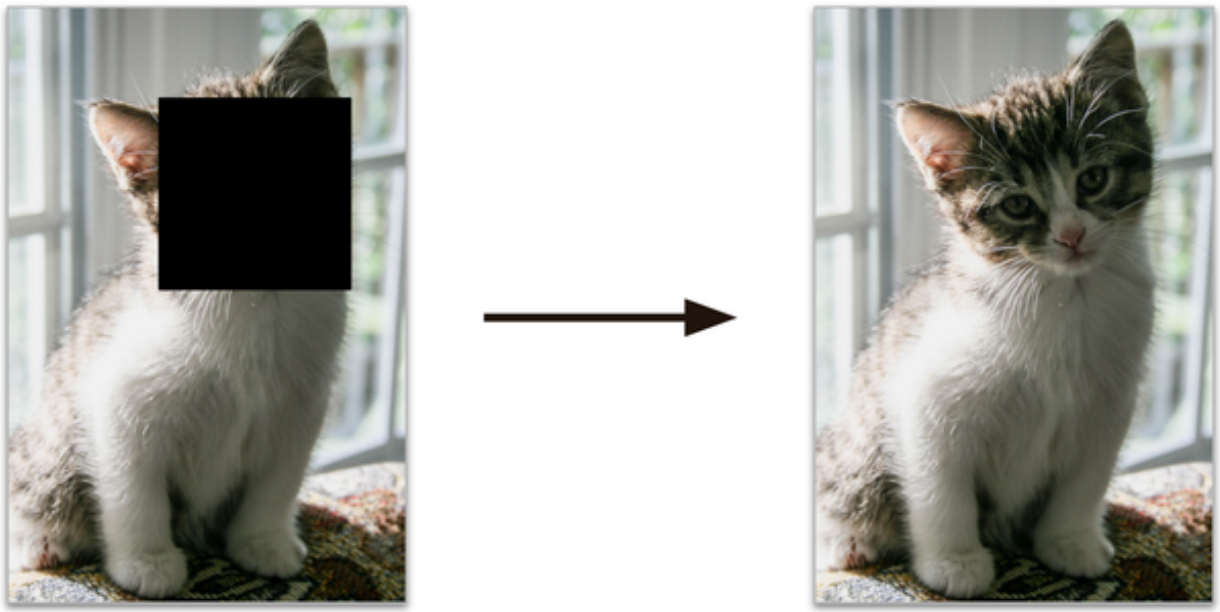


Labels for some data.

For example, Medical data, where elaborate diagnosis is available only for some patients.

Combines supervised and unsupervised learning: e.g., clusters all data and labels the unlabeled inputs with the most common labels in their clusters.

Self-Supervised Learning

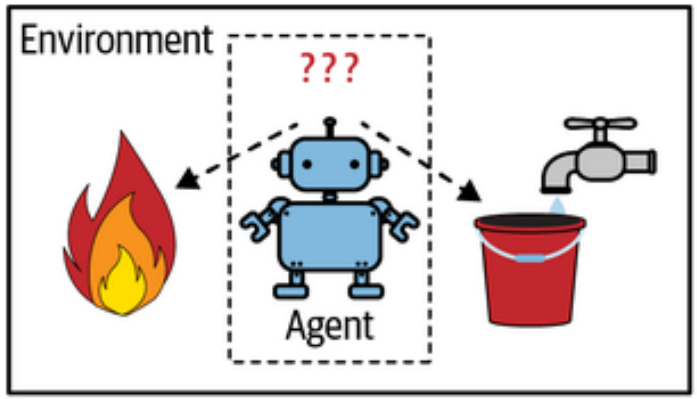


Generate labels from (unlabeled) inputs.

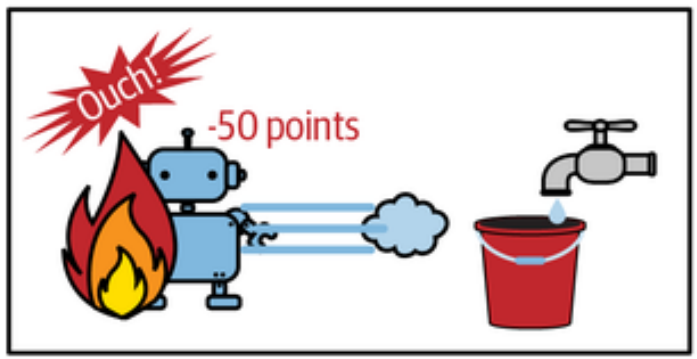
The goal is to learn typical features of the data.

It can be later modified to generate images, classify, etc.

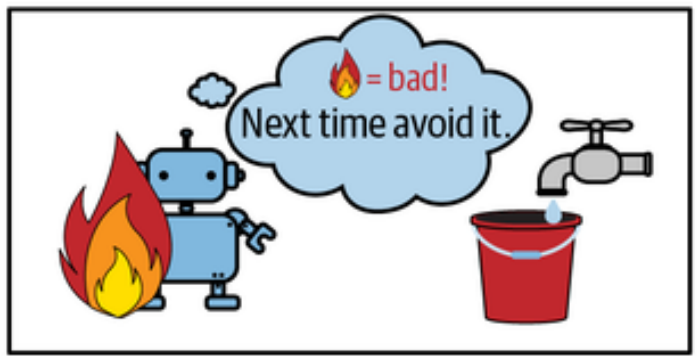
Reinforcement Learning



1. Observe
2. Select action using policy



3. Action!
4. Get reward or penalty



5. Update policy (learning step)
6. Iterate until an optimal policy is found

Learn from performing *actions* and getting feedback from *environment*.

ML Applications Highlights

- ChatGPT (and similar generative models)
  - The basis forms a generative language model, i.e., a text-generating model trained on texts in a self-supervised way
  - Currently extended to multimodal versions (text, image, sound)

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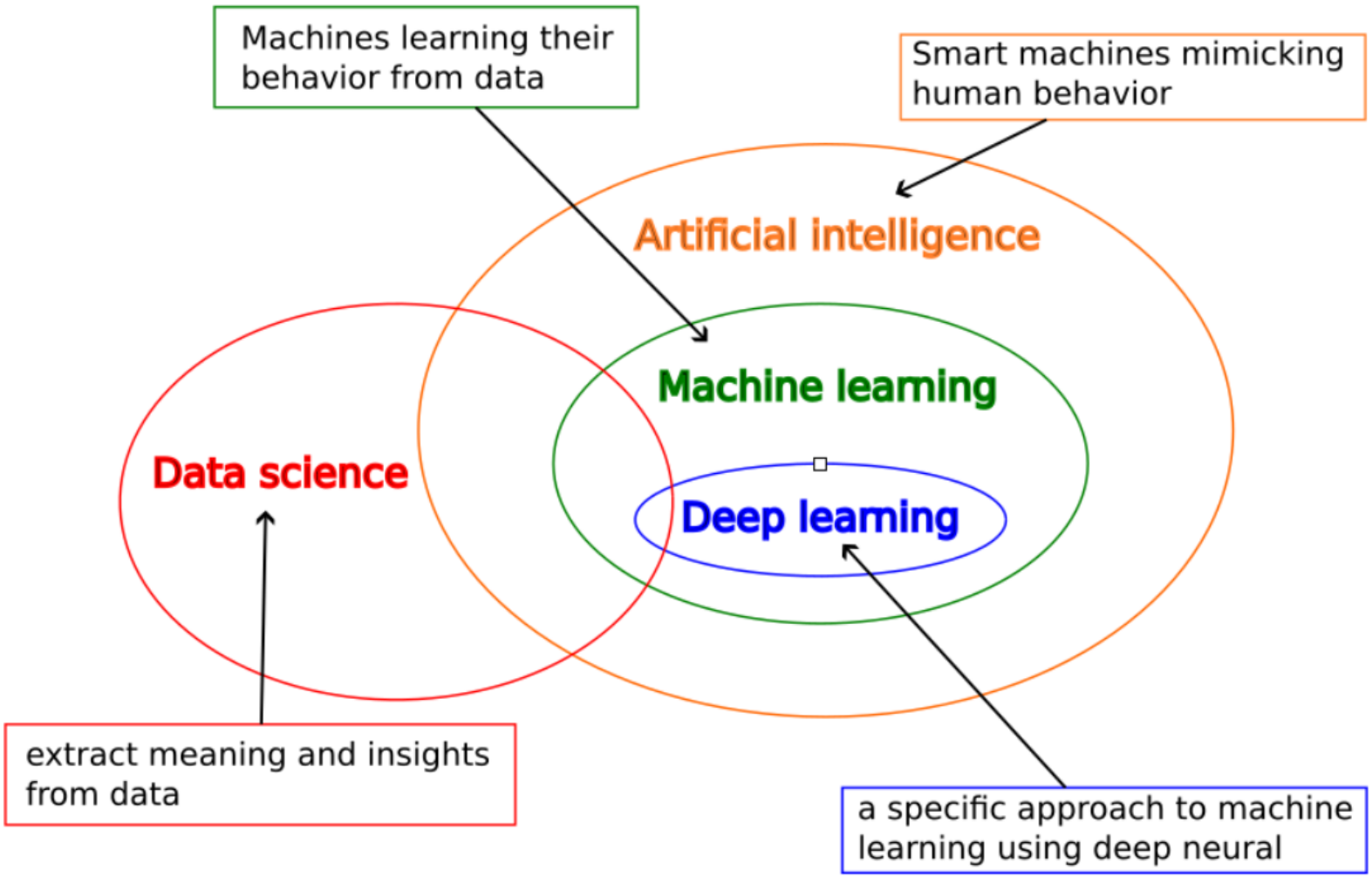
- Game playing: More fancy than useful, learning models beating humans in several difficult games.

ML in Context



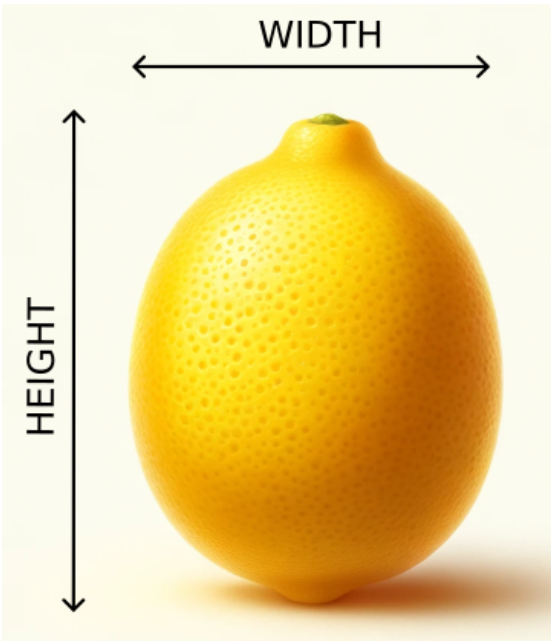
Supervised Learning

Example - Fruit Recognition

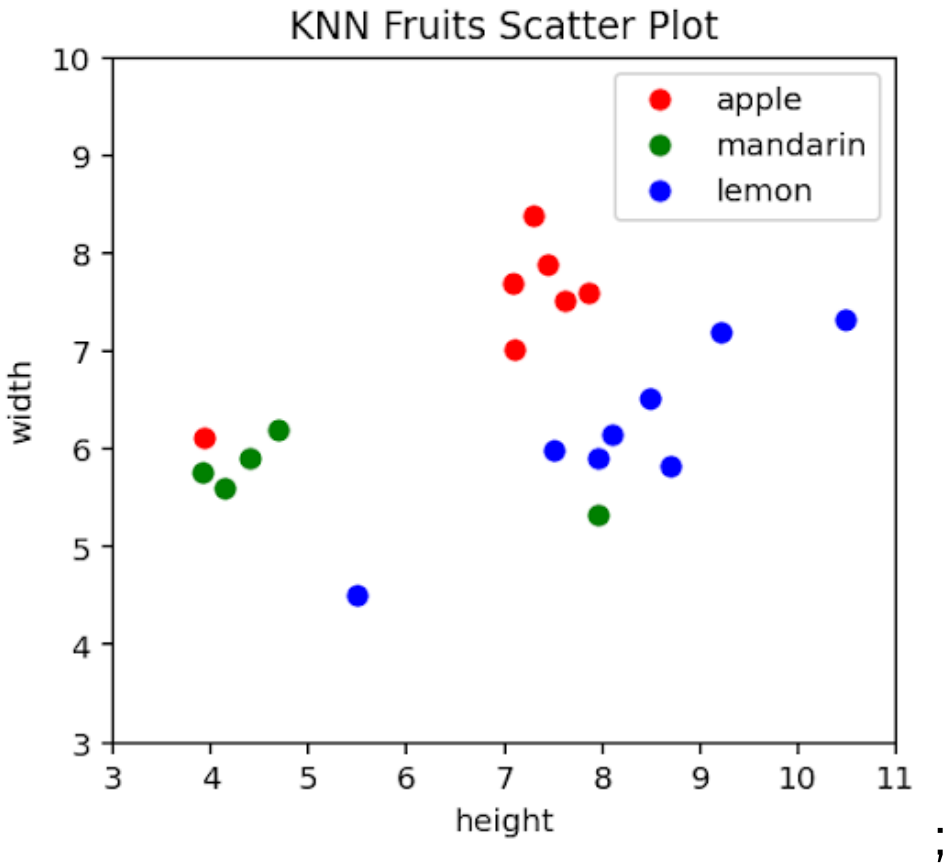
The goal: Create an automatic system for fruit recognition, concretely apple, lemon, and mandarin.

Inputs: Measures of *height* and *width* of each fruit.

Suppose we have a dataset of dimensions of several fruits labeled with the correct class.



Data



;

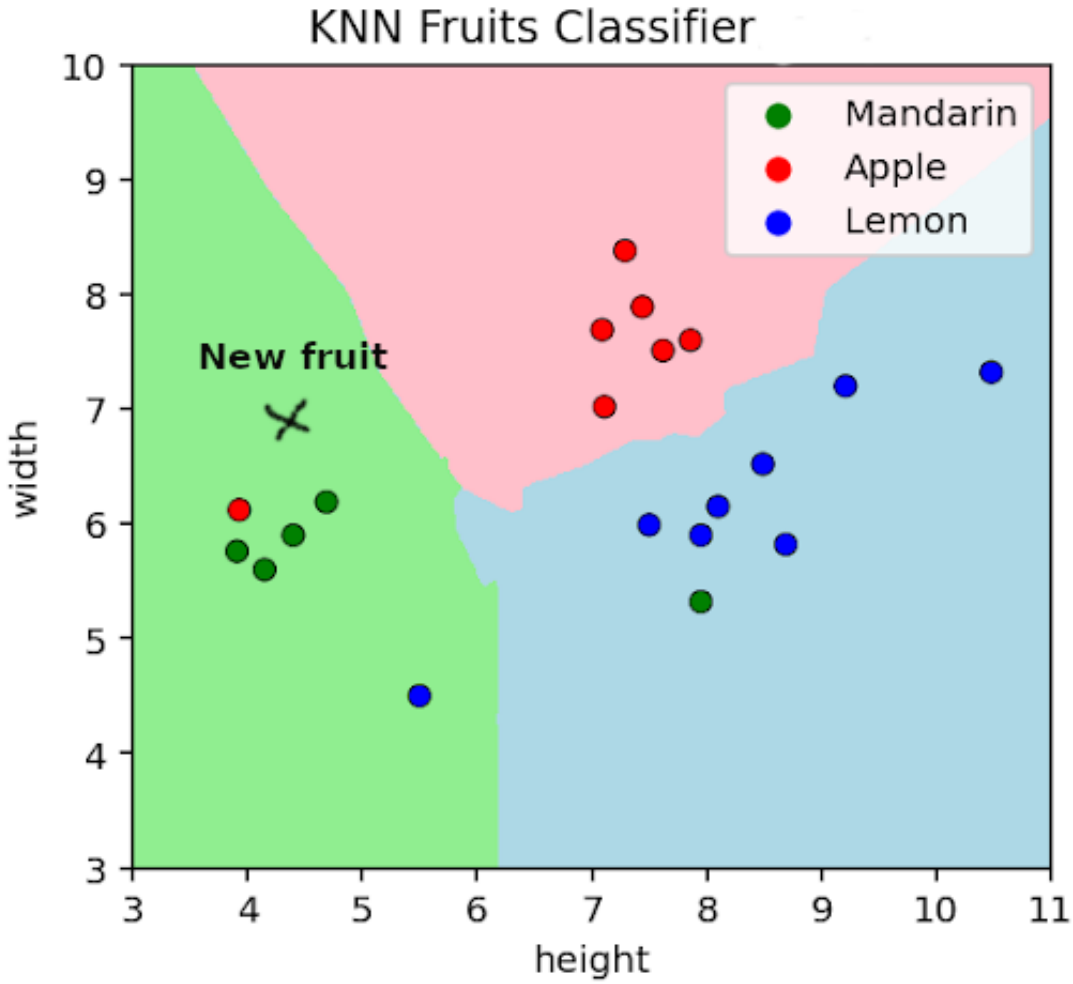
	height	width	fruit
0	3.91	5.76	Mandarin
1	7.09	7.69	Apple
2	10.48	7.32	Lemon
3	9.21	7.20	Lemon
4	7.95	5.90	Lemon
5	7.62	7.51	Apple
6	7.95	5.32	Mandarin
7	4.69	6.19	Mandarin
8	7.50	5.99	Lemon
9	7.11	7.02	Apple
10	4.15	5.60	Mandarin
11	7.29	8.38	Apple
12	8.49	6.52	Lemon
13	7.44	7.89	Apple
14	7.86	7.60	Apple
15	3.93	6.12	Apple
16	4.40	5.90	Mandarin
17	5.50	4.50	Lemon
18	8.10	6.15	Lemon
19	8.69	5.82	Lemon

Use similarity to solve the problem.

KNN Classification

Given a new fruit.
What is it?

Find five closest examples



Where is the machine learning?

KNN Classification

Given a new fruit.
What is it?

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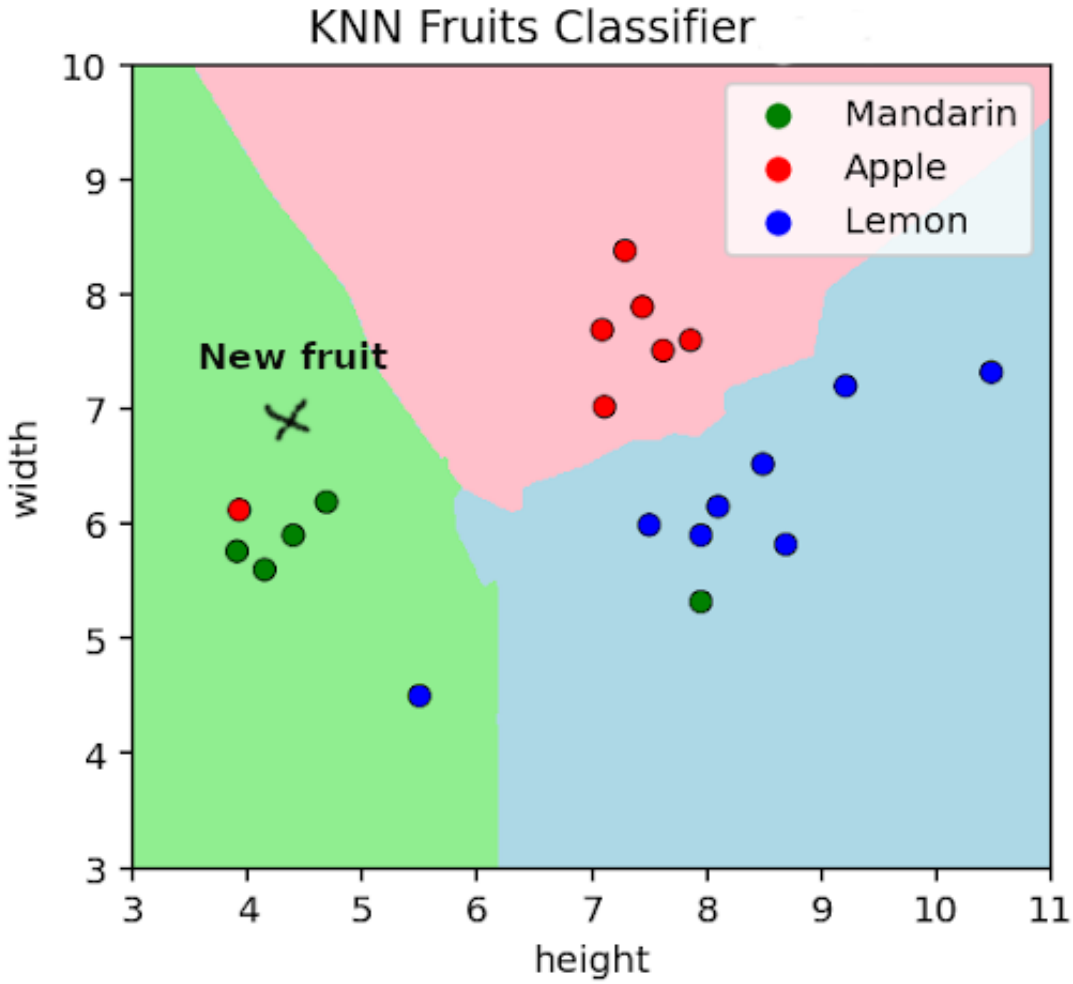
Among the five closest:

- $M = 4$ mandarins
- $A = 1$ apples
- $L = 0$ lemons



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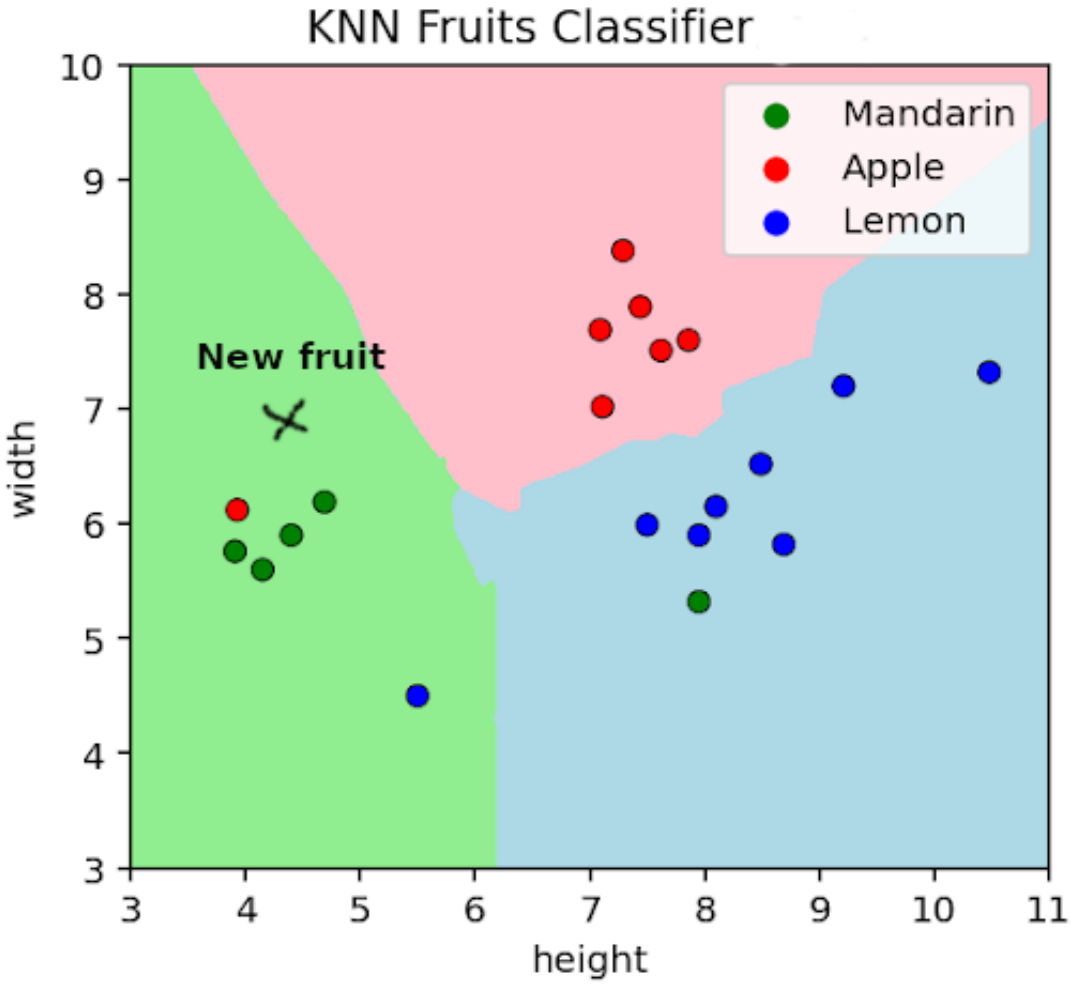
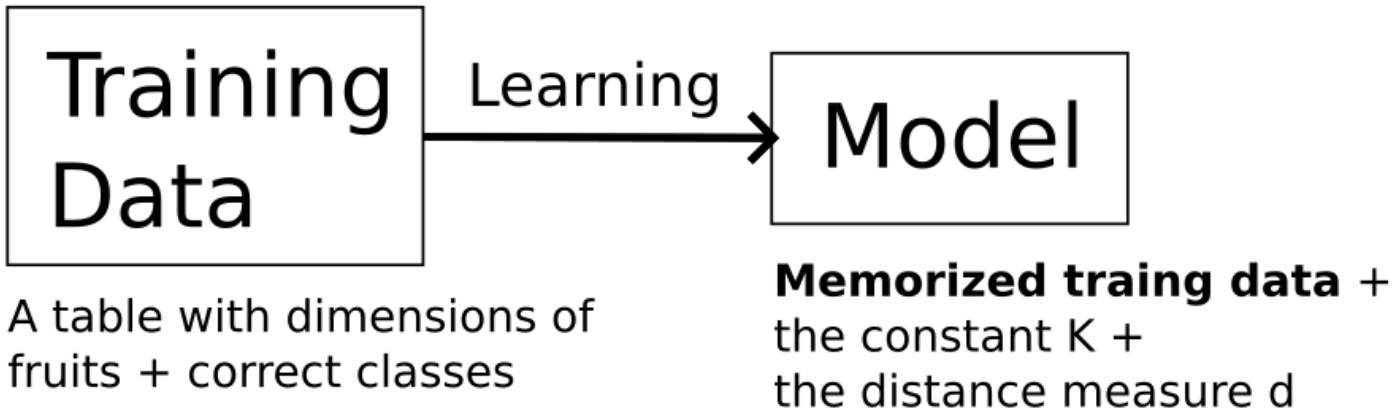
It is a **mandarin**!



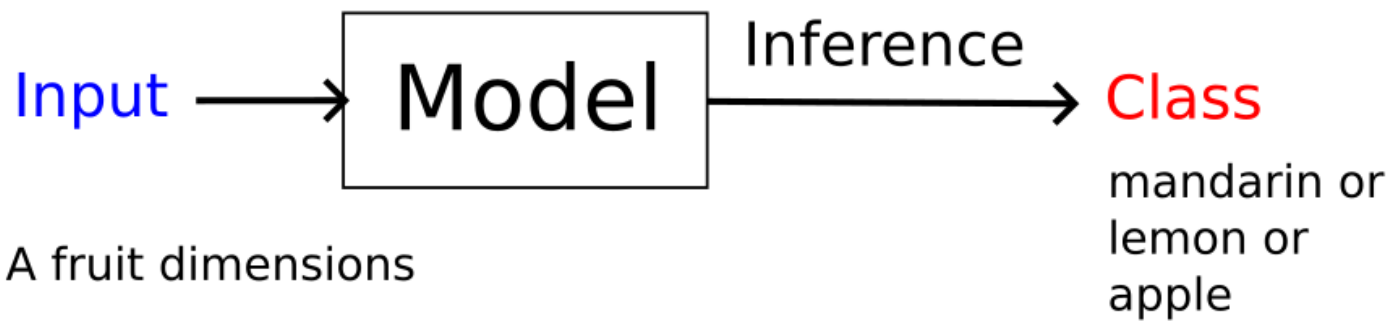
Where is the machine learning?

Learning in Fruit Classification with KNN

Learning:



Inference:



Fruit Classification Algorithm

Input: A fruit F with dimensions *height*, *width*

Output: *mandarin*, *lemon*, *apple*

1: Find K examples $\{E_1, ..., E_K\}$ in the dataset whose dimensions are closest to the dimensions of the fruit F

2: Count the number of examples of each class in $\{E_1, ..., E_K\}$

M mandarins in $\{E_1, ..., E_K\}$

L lemons in $\{E_1, ..., E_K\}$

A apples in $\{E_1, ..., E_K\}$

3: **if** $M \geq L$ and $M \geq A$ **then return** *mandarin*

4: **else if** $L \geq A$ **then return** *lemon*

5: **elsereturn** *apple*

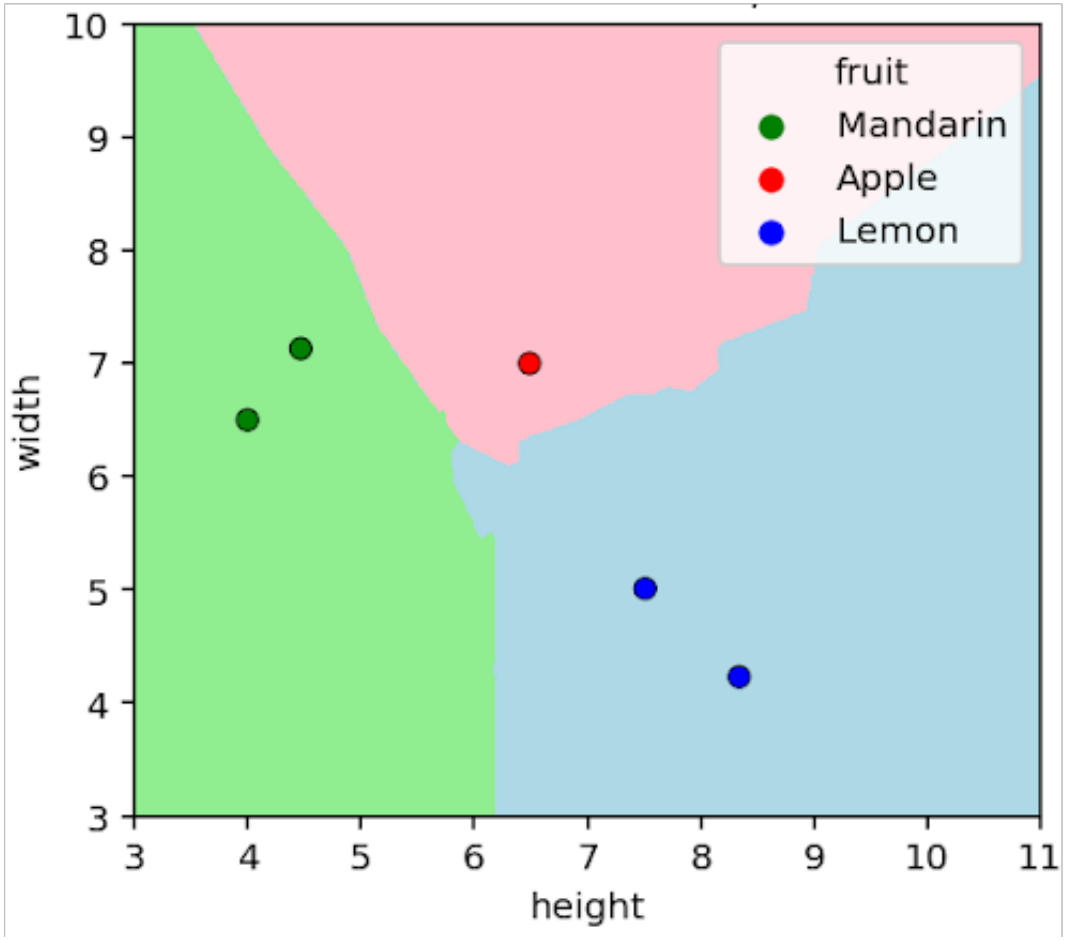
6: **end if**

Does it work?

Testing the Model for Fruit Classification

Consider a test set of new instances ($K = 5$, d is Euclidean):

height	width	fruit
4.0	6.5	Mandarin
4.47	7.13	Mandarin
6.49	7.0	Apple
7.51	5.01	Lemon
8.34	4.23	Lemon



Perfect classification of new data! Just deploy and sell!!

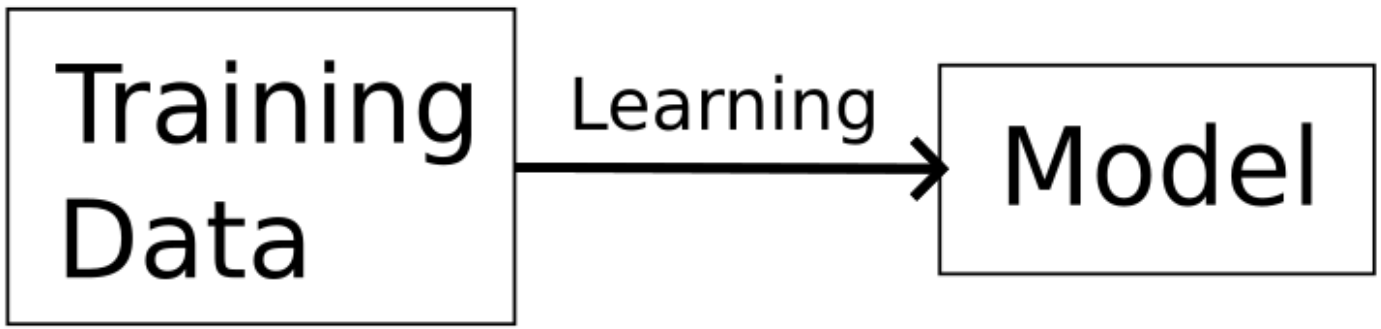
K Nearest Neighbors

... on ideal data

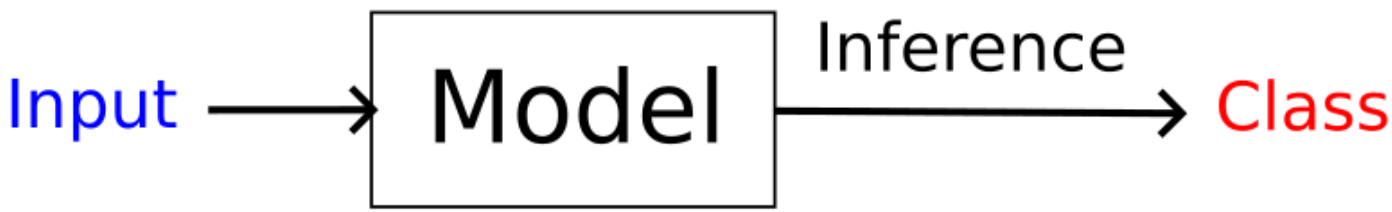
Learning and Inference

Two crucial components of machine learning are the following:

Learning:
Creating model



Inference:
Using model



Training Data

Assume table training data, i.e., of the form

$$\left.\begin{array}{cccc|c} x_{11} & x_{12} & \cdots & x_{1n} & c_1 \\ x_{21} & x_{22} & \cdots & x_{2n} & c_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{p1} & x_{p2} & \cdots & x_{pn} & c_p \end{array}\right.$$

height	width	fruit
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Formally, we define **training dataset**

$$\mathcal{T} = \{(\vec{x}_k, c_k) \mid k = 1, \ldots, p\}$$

Here each $\vec{x}_k \in \mathbb{R}^n$ is an input vector and $c_k \in C$ is the correct class.

$$\begin{aligned}\mathcal{T} = \{&(3.91, 5.76), M),\\ &(7.09, 7.69), A),\\ &\ldots\}\end{aligned}$$

KNN: Learning

Consider the training set:

$$\mathcal{T} = \{(\vec{x}_k, c_k) \mid k = 1, \ldots, p\}$$

and *memorize it* exactly as it is.

Store in a table.

Possibly use a clever representation allowing fast computation of nearest neighbors such as KDTrees (out of the scope of this lecture).

Also,

- determine the number of neighbors $K \in \mathbb{N}$,
- and the distance measure d.

Inference in KNN

Assume a KNN "trained" by memorizing $\mathcal{T} = \{(\vec{x}_k, c_k) \in \mathbb{R}^n \times C \mid k = 1, \ldots, p\}$, a constant $K \in \mathbb{N}$ and a distance measure d.

For d, consider Euclidean distance, but different norms may also be used to define different distance measures.

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Input: A vector $\vec{z} = (z_1, \ldots, z_n) \in \mathbb{R}^n$

Output: A class from C

1: Find K indices of examples $X = \{i_1, ..., i_K\} \subseteq \{1, \ldots, p\}$ with minimum distance to $\vec{z}$, i.e., satisfying

$$\max\{d(\vec{z}, \vec{x}_\ell) \mid \ell \in X\} \leq \min\{d(\vec{z}, \vec{x}_\ell) \mid \ell \in \{1, \ldots, p\} \setminus X\}$$

2: For every $c \in C$ count the number $\#c$ of elements ℓ in X such that $c_\ell = c$

3: Return some

$$c_{max} \in \arg\max_{c \in C} \#c$$

A class $c_{max} \in C$ which maximizes $\#c$.

The resulting model

What exactly constitutes the model? The *model* consists of

- The *trained parameters*: In this case the memorized training data.
- The *hyperparameters* set "from the outside": In this case, the number of neighbors K and the distance measure d.

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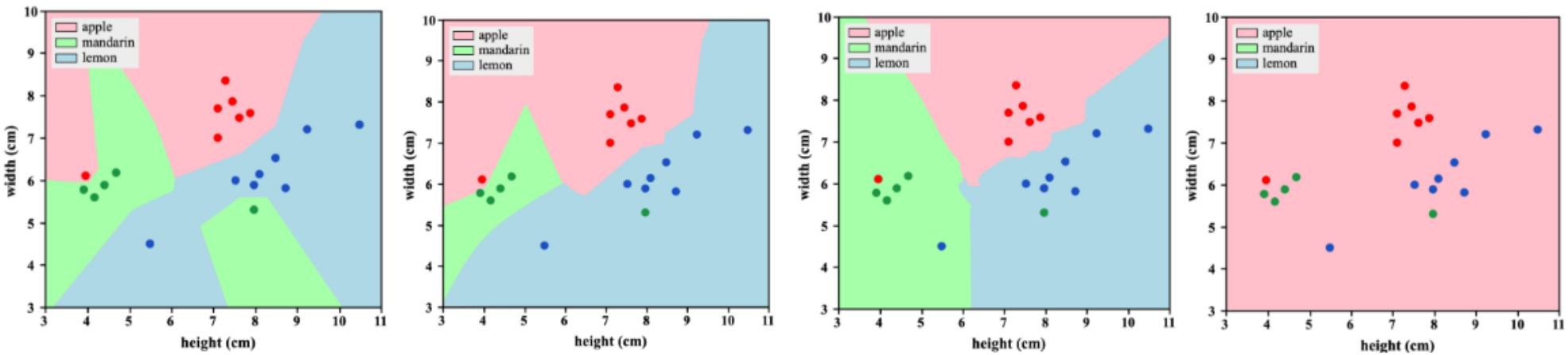
Note that different settings of K lead to different classifiers (for the same d):



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- Deal with the wrong model by testing and validation in as realistic conditions as possible.
- Deal with deployment - real-world application issues involving, e.g., implementation in embedded devices with limited resources.

Models Considered in This Course

Throughout this course, we will meet the following models:

- KNN (already did)
- Decision trees
- (Naive) Bayes classifier
- Clustering: K-means and hierarchical
- Linear and logistic regression
- Support Vector Machines (SVM)
- Kernel linear models
- Neural networks (light intro to feed-forward networks)
- Ensemble methods + random forests
- (maybe some reinforcement learning)

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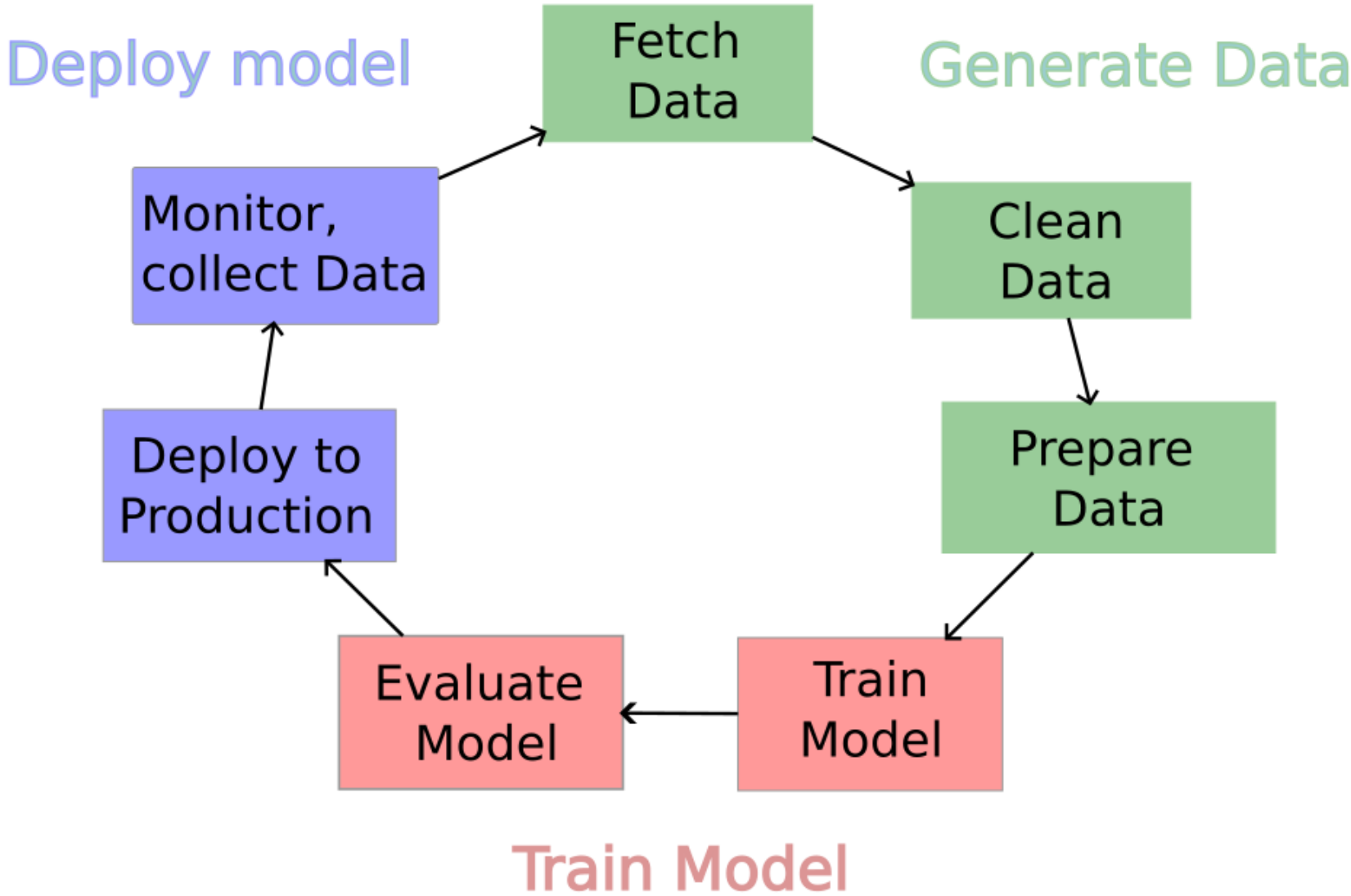
... but first, let us see the whole machine learning pipeline.

Machine Learning Pipeline



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- Integrate data from various sources.

  A serious diagnostic system must be trained/tested on data from many hospitals. You must blend the data from various sources (different formats, etc.).

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Tools such as ML Flow or Weights & Biases might be helpful.

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Data Separation

At this point, you should randomize the ordering of the data and select a test set to be used in model evaluation!

The test data are supposed to simulate the actual conditions, i.e., they should be "unseen".

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Data Exploration

Compute basic statistics to identify missing values, outliers, etc.

Clean Data

The cleaning usually comprises the following steps:

- Fix or remove incorrect or corrupted values.
- Identify outliers and decide what to do with them.

  Outliers may harm some training methods and are not "representative". However, sometimes, they naturally belong to the dataset, and expert insight is needed.
- Fix formatting.

  For example, the Date may be expressed in many ways, and a simple Yes/No answer.
- Resolve missing values (by either removing the whole examples or imputing)

  Many methods have been developed for missing values imputation. It is a susceptible issue because new values may strongly bias the model.
- Remove duplicates.

The above steps often affect the training and need expertise in the application domain.

Later in this course, we will discuss techniques for data cleaning.

ID	Age	Income	Gender	Customer_Satisfaction
1	38	46641.356413713	nan	Unsatisfied
2	42	49129.0615585107	female	Neutral
3	18	119965.049731014	Male	nan
4	18	66828.0762224329	nan	very unsatisfied
5	58	57422.2721106762	female	very unsatisfied
6	28	59502.8174855665	Other	Satisfied
7	18	42659.6675768587	Other	Neutral
8	18	54019.1173206374	Other	Satisfied
9	40	25429.1604541137	female	Unsatisfied
10	21	15595.5862129548	Other	Satisfied
11	18	58094.2328460069	Other	very unsatisfied
12	18	39097.3278583155	female	Very Satisfied
13	30		Other	Satisfied
14	50	30617.3914472273	Female	Very Satisfied
15	18		nan	Neutral
16	34	39902.4430953214	male	nan
17	49	68381.6997683133	Female	Very Satisfied
18	33	44796.0962271524	Other	Very Satisfied
19	47	39218.9560738814	Female	very unsatisfied
20		14544.9226784447	Other	Satisfied

Prepare Data

Unlike cleaning, which is application-dependent, data preparation/transformation is model-dependent. This usually subsumes:

- **Scaling**: Settings values of inputs to a similar range.

  Some models, especially those utilizing distance, are sensitive to large differences between input sizes.

- **Encoding**: Encode non-numeric data using real-valued vectors.

  Many models, especially those based on geometry, work only with numeric data. Non-numeric data such as Yes/No, Short/Medium/Long must be encoded appropriately.

- **Binning or Discretization** Convert continuous features into discrete bins to capture patterns in ranges.

Comment: Sometimes **Normalization**, that is changing the distribution of inputs to resemble the normal distribution, is mentioned. However, this step is typically not essential for machine learning itself. However, it is important to use statistical inference to test the significance of learned parameters.

Prepare Data

- **Feature selection** Throw out input features that are too "similar" to other features.

  For example, if the temperature is measured both in Celsius and in Kelvin, keep one of them. The relationship can, of course, be a more complex (non-linear) correlation.

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- **Dimensionality reduction** Transforming data from $\mathbb{R}^n$ to $\mathbb{R}^m$ where $m << n$.

  Growing dimension means growing difficulty of training for all models. Some models cease to work for high-dimensional data. The reduction typically searches for a few important characteristic features of inputs.

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- **Feature aggregation** Introducing new features using operations on the original ones.

  We will see kernel transformations later in this course, allowing simple models to solve complex problems.

Train Model

Now the dataset has been cleaned; we may train a model.

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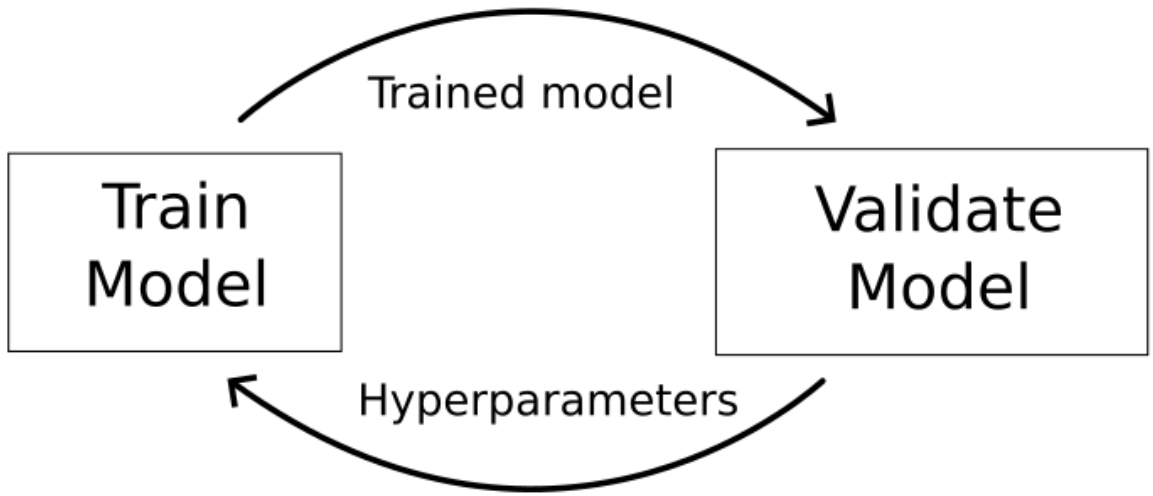
Before training, we should split the dataset into

- *training* dataset on which the model will learn
- *validation* dataset on which we fine-tune hyperparameters



The resulting model is obtained after several iterations of the above process.

Evaluate Model

Here, we use the test set that we separated during data fetching.

In some cases, a brand new test set can be generated.

patients are examined regularly, creating new records continuously.

In some cases, it is tough to obtain new data.

For example, new expensive and difficult measurements are needed to obtain new data.

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patients are examined regularly, creating new records continuously.

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For example, new expensive and difficult measurements are needed to obtain new data.

Critical issue: Make sure that you are truly testing

exactly the whole inference process.

Often, just a model is tested, and the testing and production inference engines are separated. This leads to truly nasty errors in the production!

We will discuss various generic metrics helpful in measuring the quality of the resulting model.

Deploy to Production

Deployment of machine learning models is a complex question, application dependent.

The recently emerging area of MLOps is concerned with the engineering side of the model deployment.

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The recently emerging area of MLOps is concerned with the engineering side of the model deployment.

From the technical point of view, the typical issues solved by ML Ops teams are

- how to extract/process data in real-time
- how much storage is required
- how to store/collect model (and data) artifacts/predictions
- how to set up APIs, tools, and software environments
- What the period of predictions (instantaneous or batch predictions) should be
- how to set up hardware requirements (or cloud requirements for on-cloud environments) by the computational resources required
- how to set up a pipeline for continuous training and parameter tuning

Deploy to Production

From the user's point of view:

- How to get a sensible and valuable user output?
  - AI researchers will be satisfied with tons of running text in terminals.
  - "Normal" people need a graphical interface with understandable output.
  - Experts working in other domains typically demand speed and clarity at the extreme.

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  - AI researchers will be satisfied with tons of running text in terminals.
  - "Normal" people need a graphical interface with understandable output.
  - Experts working in other domains typically demand speed and clarity at the extreme.
- How do you persuade users that the AI is working for them?
  - Especially if safety is at stake, you need to have outstanding arguments and explanations ready for end-users
  - In many areas, the devices need to be certified (medicine, automotive) for ML-based systems.

This complex subject will be only touched on in this course.

Monitor, collect Data

Deployed machine learning models must be constantly monitored.

Because of the influx of new data, ML models work in highly dynamic environments.

For example, an image-processing medical diagnostic model suddenly misdiagnosed a patient because a nurse marked the sample with a marker pen.

Every customer has a different infrastructure and may produce data slightly differently.

Data for retraining and improvement should be stored.

Also, many areas allow the *active learning* where users provide feedback for (continuous) retraining of the models.

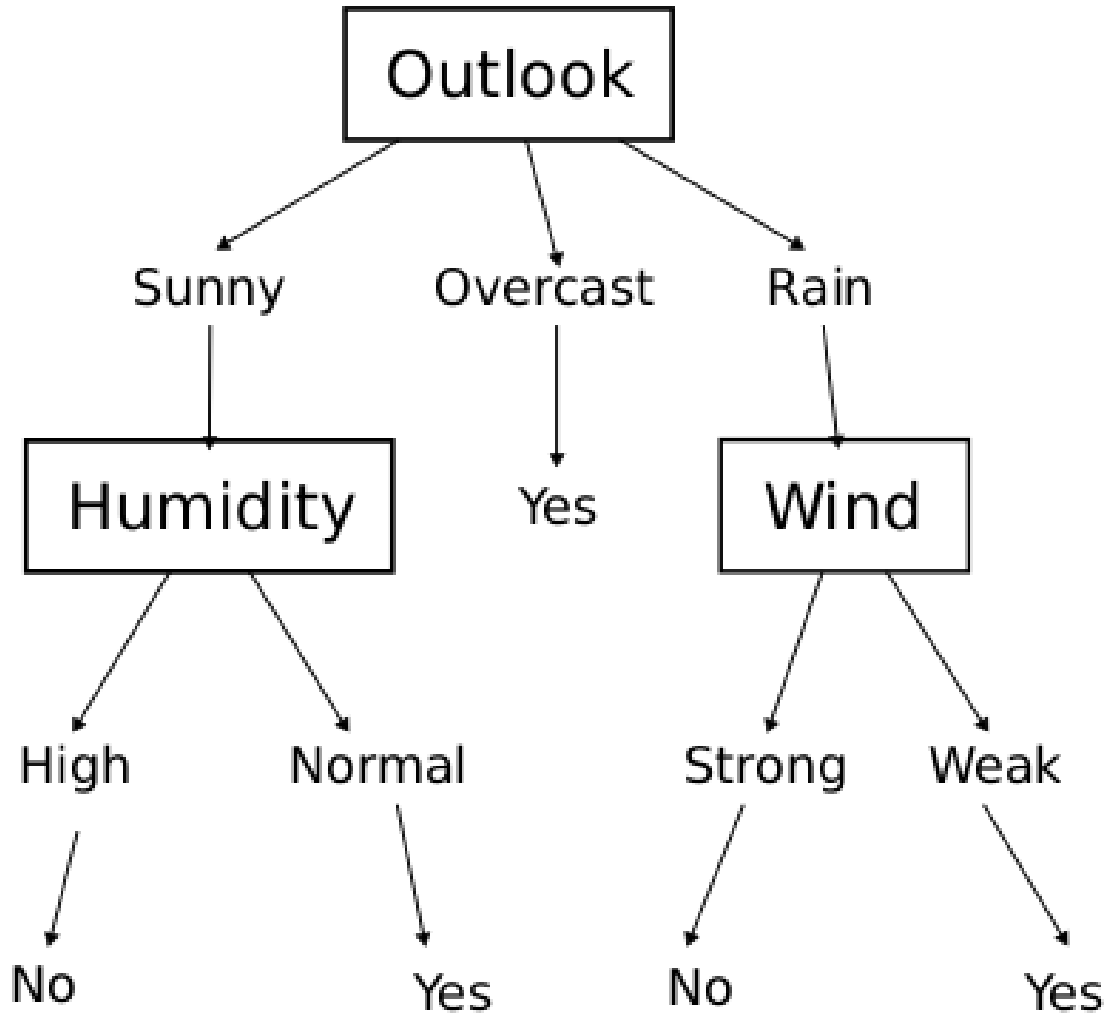
Decision Trees

Decision Trees

- One of the most widely used methods for machine learning.
- Intuitively simple, directly explainable.
- Basis for random forests (a powerful model).

- We will consider the ID3 algorithm.
- A peek at the C4.5 algorithm.
  (just an optimized version of ID3)

Consider the weather forecast for tennis playing. How would you decide whether to play today?



Now, how do we obtain such a tree based on experience/data?

Learning Decision Trees

We start with trees on discrete datasets. That is, consider data represented as follows:

- A finite set of *attributes* $\mathcal{A} = \{A_1, \ldots, A_n\}$.
- Each attribute $A \in \mathcal{A}$ has its *set of values* $D(A)$.

Examples are then vectors of values of all attributes:

$$\vec{x} = (x_1, \ldots, x_n) \in D(A_1) \times \cdots \times D(A_n)$$

Given $\vec{x}$ and an attribute A_k we denote by $A_k(\vec{x})$ the value x_k of the attribute A_k in $\vec{x}$.

Consider a set C of classes.

We consider a multiclass classification in general, i.e., C is an arbitrary finite set.

Example

The tennis problem:

- The attributes are:

$$A_1 = Outlook, A_2 = Temperature, A_3 = Humidity, A_4 = Wind$$

- The sets of values of the attributes:
  - $D(A_1) = \{Sunny, Overcast, Rain\}$
  - $D(A_2) = \{Hot, Mild, Cool\}$
  - $D(A_3) = \{High, Normal\}$
  - $D(A_4) = \{Strong, Weak\}$
- Consider

$$\vec{x} = (Overcast, Hot, Normal, Weak)$$
$$\in D(A_1) \times D(A_2) \times D(A_3) \times \mathcal{D}(A_4)$$

  Then

$$A_3(\vec{x}) = Humidity(\vec{x}) = Normal$$

$$A_4(\vec{x}) = Wind(\vec{x}) = Weak$$

- $C = \{Yes, No\}$

Decision Trees

Consider (directed, rooted) *trees* (V, E) where V is a set of nodes and $E \subseteq V \times V$ is a set of directed edges.

Denote by $V_{leaf} \subseteq V$ the set of all leaves of the tree and by V_{int} the set $V \setminus Z$ of internal nodes.

A *decision tree* is

- a tree (V, E) where
- each leaf $z \in V_{leaf}$ is assigned a class $C(z) \in C$,
- each internal node $h \in V_{int}$ is assigned an attribute $A(h) \in \mathcal{A}$,
- and there is a bijection between edges from h and values of the attribute $A(h)$. Given an edge $(h, h') \in E$ we write $D(h, h')$ to denote the value of the attribute $A(h)$ assigned to the edge.

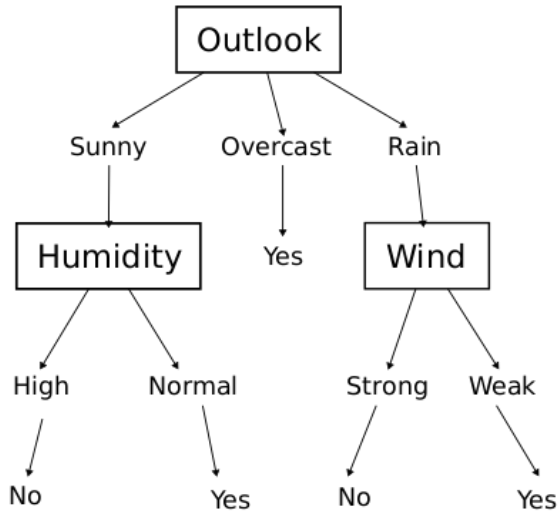
Inference: Given an input $\vec{x} \in D$, we traverse the tree from the root to a leaf, always choosing edges labeled with values of attributes from $\vec{x}$. The output is the class labeling the leaf.

Example

$V = \{O, H, W, z_1, z_2, z_3, z_4, z_5\}$

$V_{leaf} = \{z_1, z_2, z_3, z_4, z_5\}, V_{int} = \{O, H, W\}$

$E = \{(O, H), (O, W), (H, z_1), (H, z_2), (O, z_3), (W, z_4), (W, z_5)\}$



$A(O) = Outlook,\ A(H) = Humidity,\ A(W) = Wind$

$D(O, H) = Sunny,\ D(O, z_3) = Overcast,\ D(O, W) = Rain$
$D(H, z_1) = High,\ D(H, z_2) = Normal$
$D(W, z_4) = Strong,\ D(W, z_5) = Weak$

Inference: For $(Rain, Hot, High, Strong)$ we reach z_4, yielding No.

Training Dataset

Consider a *training dataset*

$$\mathcal{T} = \{(\vec{x}^{(k)}, c^{(k)}) \mid k = 1, \ldots, p\}$$

Here $\vec{x}^{(k)} \in D(A_1) \times \cdots \times D(A_k)$ and $c^{(k)} \in C$ for every k.

Index	Outlook	Temperature	Humidity	Wind	PlayTennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

$$\mathcal{T} = \{((Sunny, Hot, High, Weak), No),$$
$$((Sunny, Hot, High, Strong), No)$$
$$\ldots$$
$$((Rain, Mild, High, Strong), No)\}$$

Learning Decision Trees

The learning algorithm ID3 works as follows:

- Start with the whole training dataset $\mathcal{T}$.
- If there is just a single class in $\mathcal{T}$, create a single node decision tree that returns the class.
- Otherwise, identify an attribute $A \in \mathcal{A}$ which *best classifies* the examples in $\mathcal{T}$. For every $v \in D(A)$ we obtain

$$\mathcal{T}_v = \{\vec{x} \mid \vec{x} \in \mathcal{T}, A(\vec{x}) = v\}$$

  We aim to have each $\mathcal{T}_v$ as pure as possible, that is, ideally, to contain examples of just a single class.
- Finally,
  - create a root node h of a decision tree,
  - assign the attribute A to h,
  - for every $v \in D(A)$ introduce an edge (h, h') assigned v,
  - recursively construct a subtree using $\mathcal{T}_v$, attach its root to h'.

1: **procedure** ID3(dataset $\mathcal{T}$, attribute set $\mathcal{A}$)
2: Create a root node h for the tree
3: **if** all examples in $\mathcal{T}$ are of the same class c **then**
4: Return the single-node tree, where h is assigned c
5: **else if** Attributes set $\mathcal{A}$ is empty **then**
6: Return the single-node tree where h is assigned the most common class in $\mathcal{T}$
7: **else**
8: Choose attribute $A \in \mathcal{A}$ *best classifying* examples in $\mathcal{T}$
9: Set the decision attribute for h to A
10: **for** each value $v \in D(A)$ such that $\mathcal{T}_v \neq \emptyset$ **do**
11: Add a new edge (h, h') assigned v,
12: Attach the subtree ID3$(\mathcal{T}_v, \mathcal{A} \setminus \{A\})$ to h'
13: **end for**
14: **end if**
return *Root*
15: **end procedure**

For illustration, see the green board...

What is the Best Classifying Attribute?

There are several measures used in practice.

The most common are *information gain* and *Gini impurity*.

The information gain is based on the notion of *entropy*.

We need some notation:

- Given a training set $\mathcal{T}$ and a class $c \in C$ we denote by p_c the proportion of examples with class c in $\mathcal{T}$.
- We define the *entropy* of $\mathcal{T}$ by

$$Entropy(\mathcal{T}) = \sum_{c \in C} -p_c \log_2 p_c$$

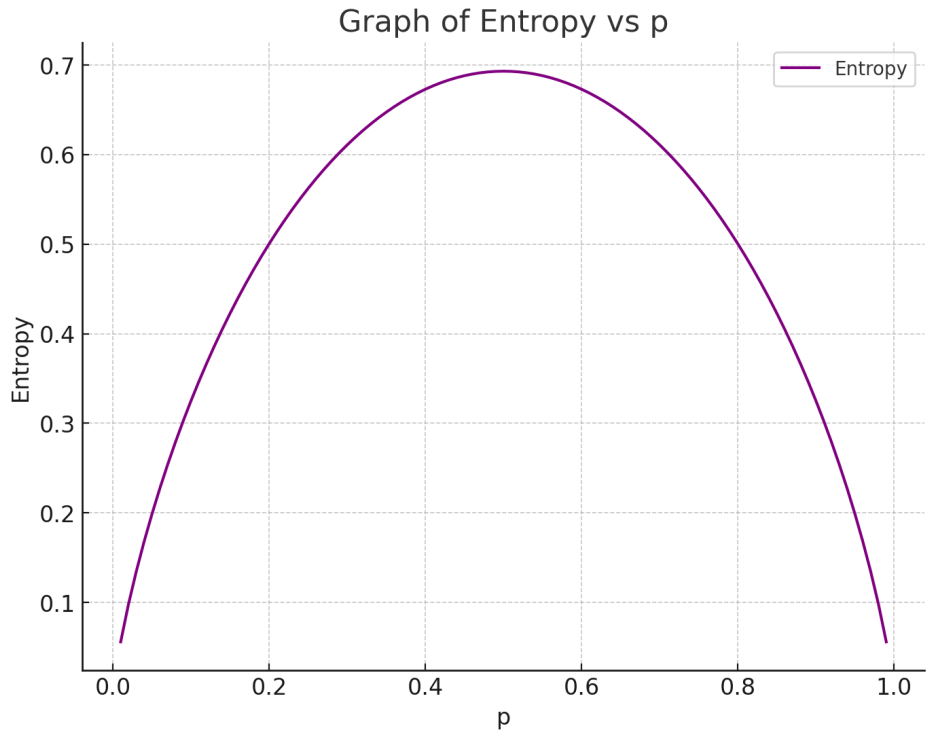
- The *information gain* of an attribute A is then defined by

$$Gain(\mathcal{T}, A) = Entropy(\mathcal{T}) - \sum_{v \in D(A)} \frac{|\mathcal{T}_v|}{|\mathcal{T}|} Entropy(\mathcal{T}_v)$$

Bleh?!?

Information Gain

- Consider $C = \{0, 1\}$ and p the proportion of examples of class 1. p measures the "uncertainty" of the class:



- $\sum_{v \in D(A)} \frac{|\mathcal{T}_v|}{|\mathcal{T}|} Entropy(\mathcal{T}_v)$ is weighted uncertainty of classes in each $\mathcal{T}_v$ (weighted by the relative size of $\mathcal{T}_v$).
- $Gain(\mathcal{T}, A)$ measures reduction in uncertainty of classes by dividing $\mathcal{T}$ according to A.

Gini Impurity

- We define *Gini index* of $\mathcal{T}$ by

$$Gini(\mathcal{T}) = 1 - \sum_{c \in C} p_c^2$$

- The information gain of an attribute A is then defined similarly to the gain in the entropy case

$$Gain(\mathcal{T}, A) = Gini(\mathcal{T}) - \sum_{v \in D(A)} \frac{|\mathcal{T}_v|}{|\mathcal{T}|} Gini(\mathcal{T}_v)$$

What is the intuition behind $Gini(\mathcal{T})$?

Assume we randomly independently choose objects from $\mathcal{T}$.

$1 - \sum_{c \in C} p_c^2$ is the probability of choosing two objects of different classes in two consecutive independent trials.

Indeed, p_c is the probability of choosing an object of class c, p_c^2 the probability of choosing objects of the class c twice, and $\sum_{c \in C} p_c^2$ the probability of choosing two objects of the same class.

Continuous-Valued Attributes

What if values of A_k come from a "continuous" variable?

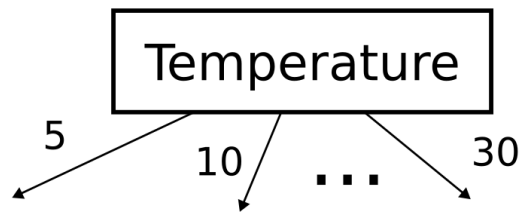
Such as temperature, size, time, etc.

Then consider an internal node $v \in V$ assigned an attribute A with outgoing edges $e_1, \ldots, e_i$.
Each of these edges e_j is assigned a value $v_j \in D(A)$, assume that the values satisfy

$$v_1 < v_2 < \cdots < v_i$$

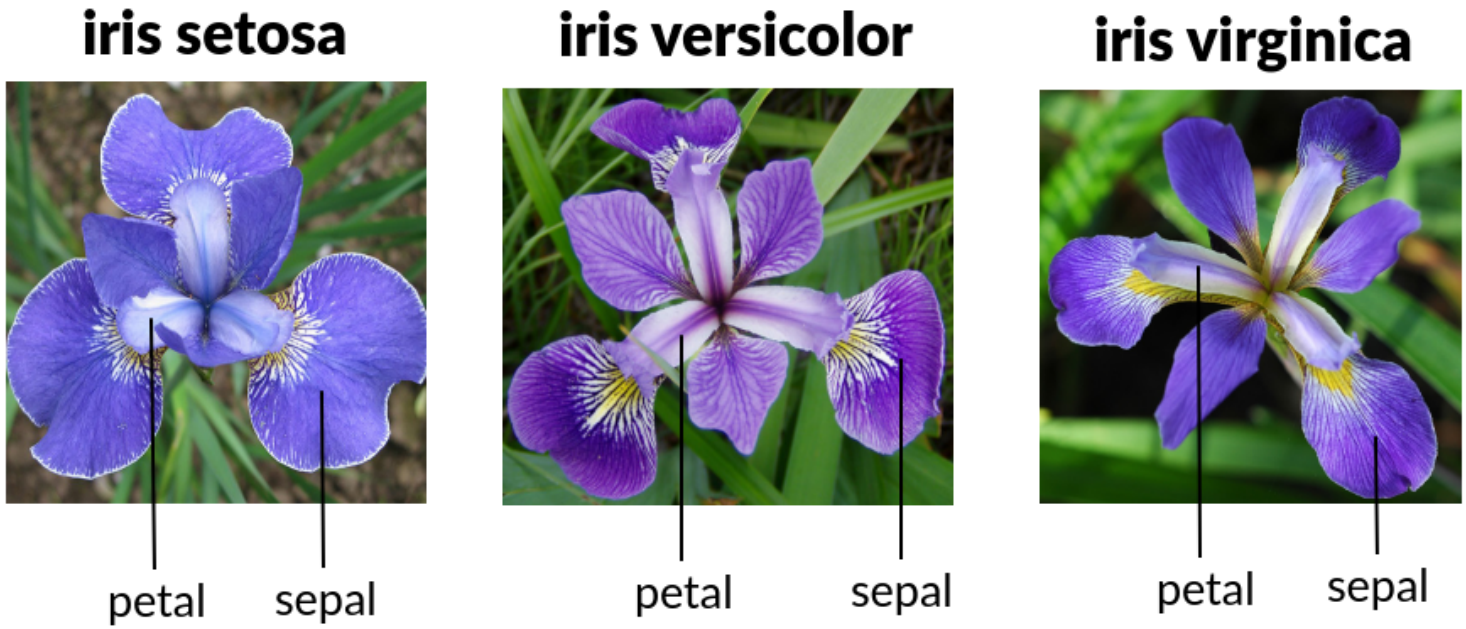
When considering an example $\vec{x}$ in the node v, we follow the edge

- e_1 if $A(\vec{x}) \leq v_1$
- e_2 if $v_1 < A(\vec{x}) \leq v_2$
- $\ldots$
- e_i if $v_i < A(\vec{x})$



- $\leq 5 \Rightarrow$ leftmost edge
- > 5 & $\leq 10 \Rightarrow$ second left
- $\ldots$

Iris Example



Attributes

Sepal.Length, Sepal.Width, Petal.Length, Petal.Width

Classes (Variety)

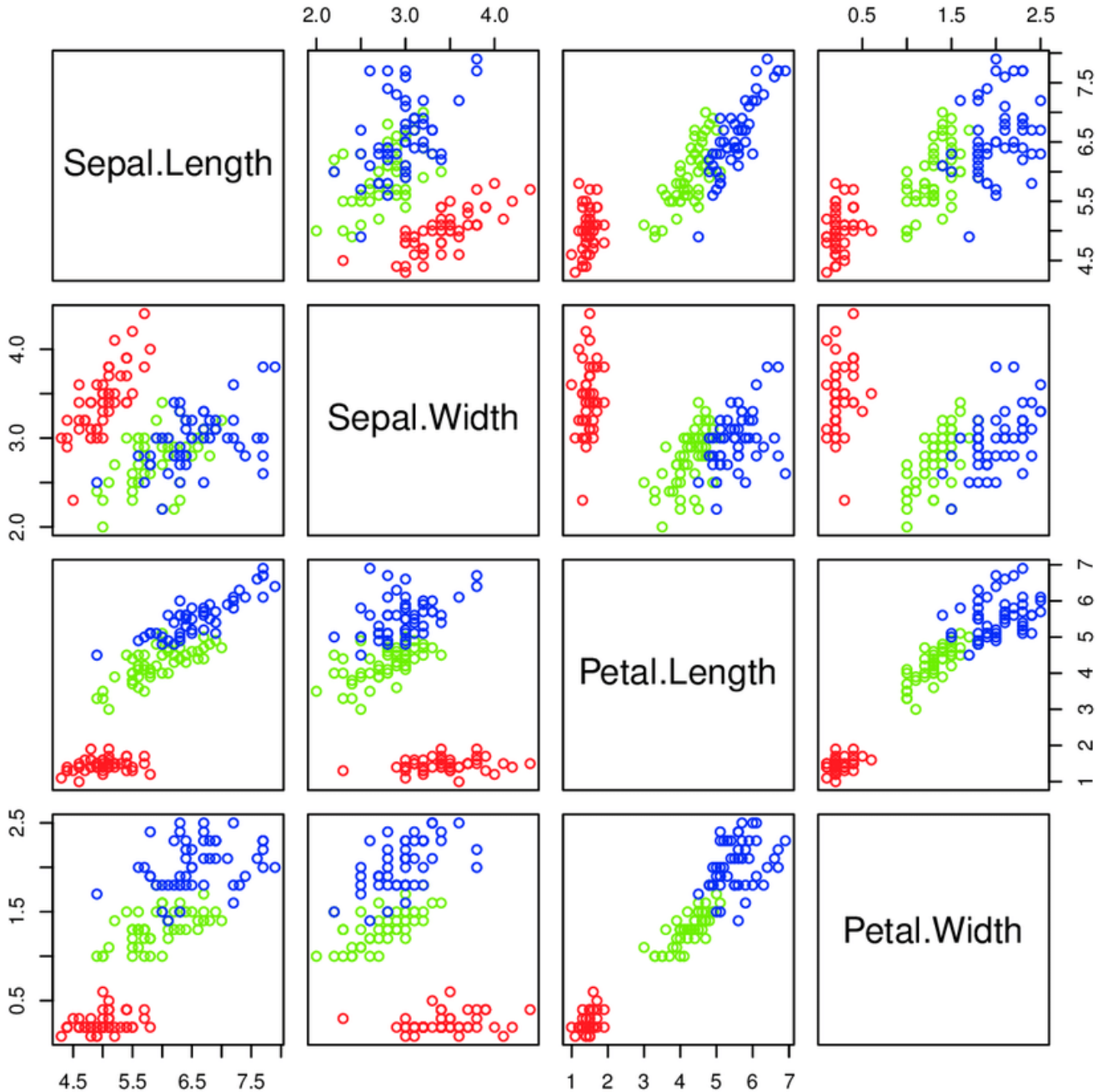
Setosa, Versicolor, Virginica

Iris Example

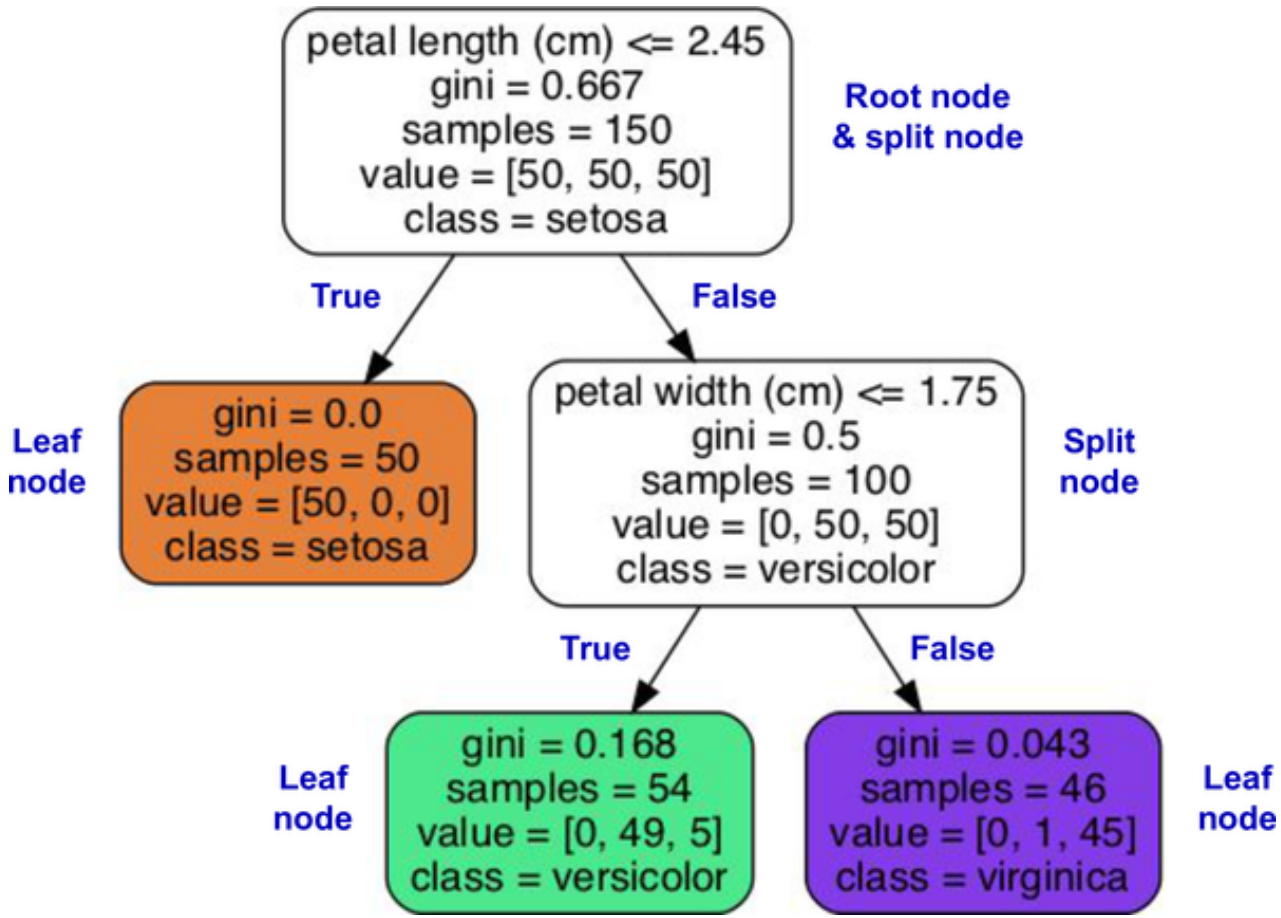
The dataset (150 examples):

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Variety
5.5	3.5	1.3	0.2	Setosa
6.8	2.8	4.8	1.4	Versicolor
6.7	3.1	4.7	1.5	Versicolor
6.9	3.1	5.1	2.3	Virginica
7.3	2.9	6.3	1.8	Virginica
5.4	3.7	1.5	0.2	Setosa
4.6	3.4	1.4	0.3	Setosa
6.2	2.8	4.8	1.8	Virginica
5.4	3.0	4.5	1.5	Versicolor
4.7	3.2	1.6	0.2	Setosa
6.7	3.3	5.7	2.1	Virginica
5.0	3.4	1.5	0.2	Setosa
5.0	3.0	1.6	0.2	Setosa
4.4	2.9	1.4	0.2	Setosa
6.0	3.4	4.5	1.6	Versicolor
5.1	3.5	1.4	0.2	Setosa
6.6	3.0	4.4	1.4	Versicolor
5.9	3.2	4.8	1.8	Versicolor
5.6	2.8	4.9	2.0	Virginica
...				

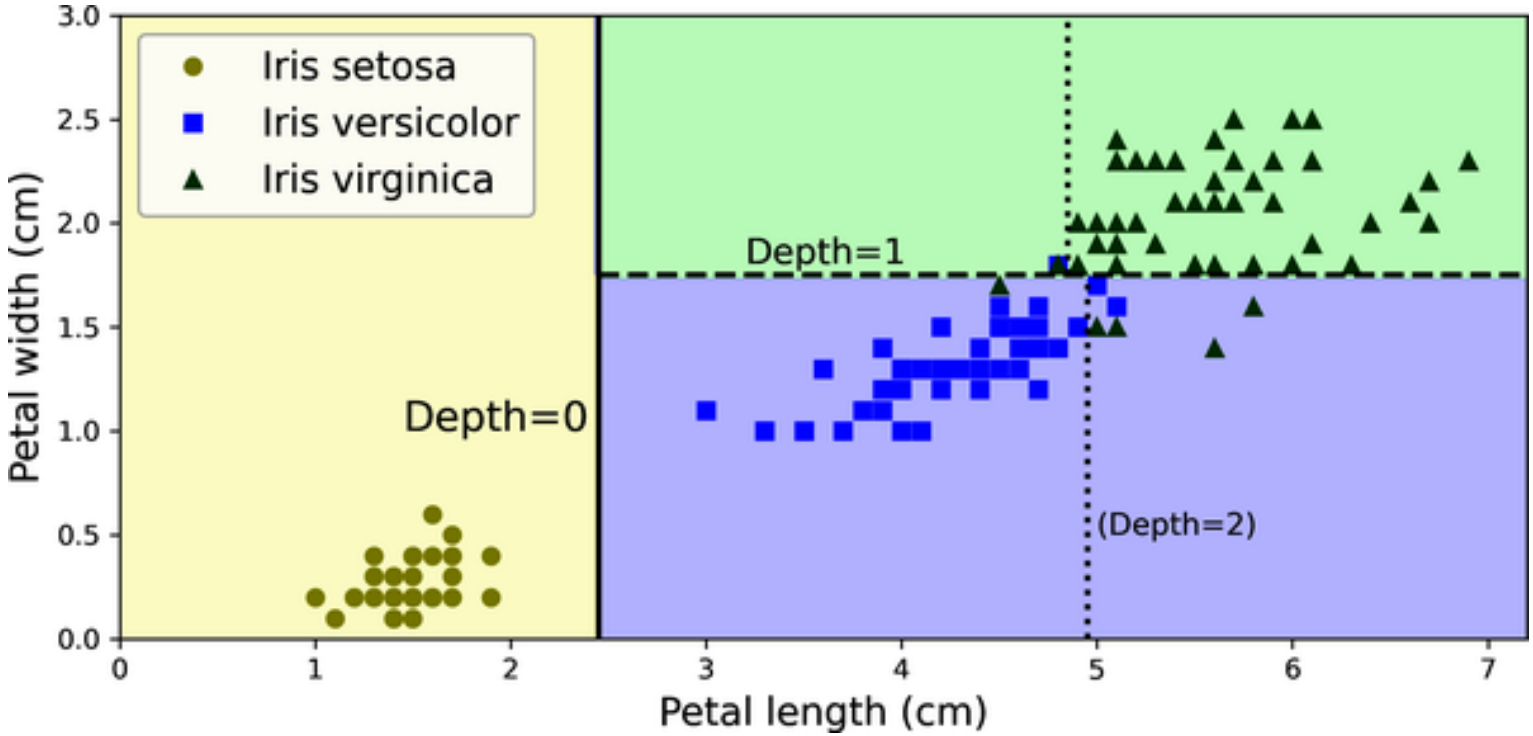
Iris Example



Iris Example - Decision Tree



Iris Example - Decision Tree Boudaries



If the leaves are split further, the Depth $= 2$ boundary would be added.

Data Preprocessing

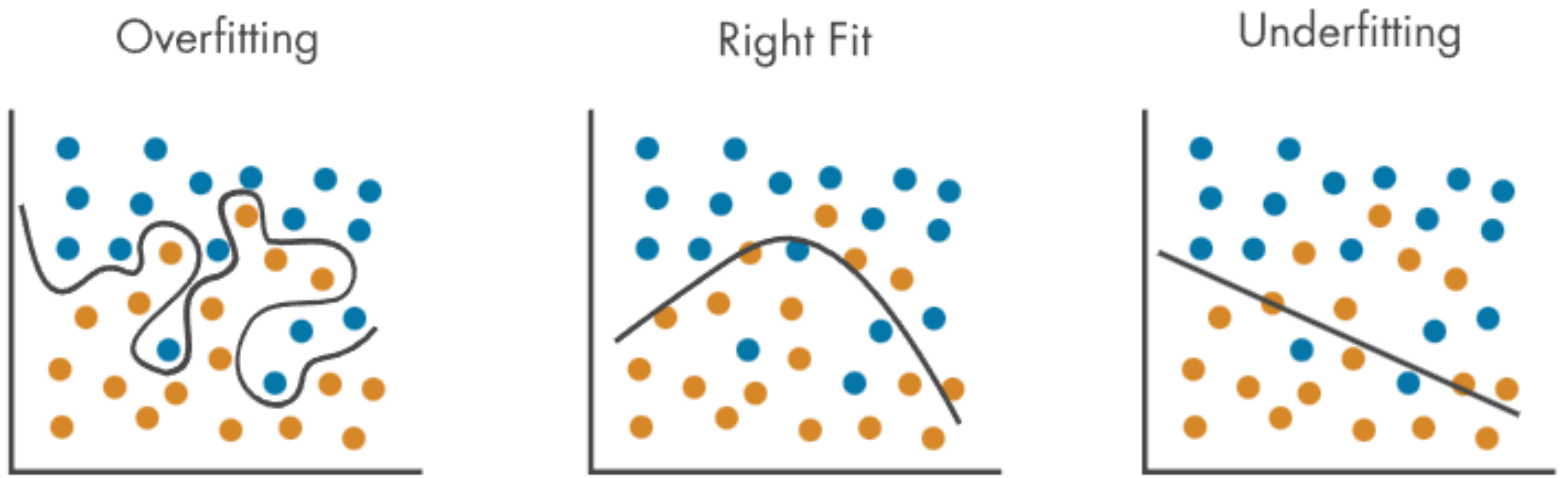
Little preprocessing is needed for decision trees.

Of course, ideally, clean up the data, but

- Missing values are not such a big issue
  (considering a concrete example, exclude the attributes with missing values)
- Outliers are not such a big issue either; the division of nodes is done based on relative counts, not concrete values.

Decision trees can cope with continuous and categorical values directly (i.e., no encoding necessary)

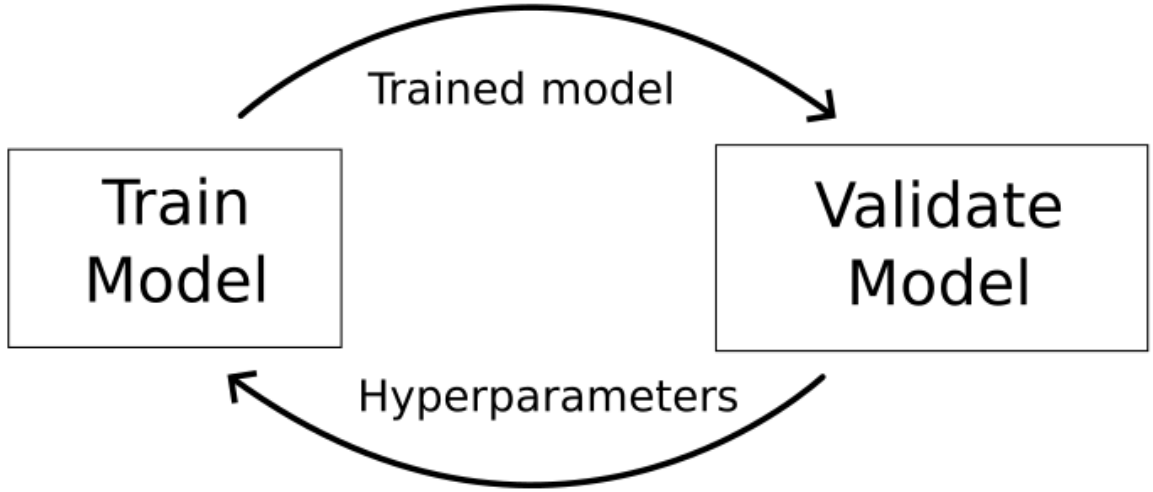
Intermezzo on Over/Under Fitting



Both overfitting and underfitting are best avoided. But how do I find out?

Hyperparameter Tuning for Decision Trees

Recall from the first lecture:



The validation should be done on a **validation set** separated from the training set.

We will discuss more sophisticated techniques later.

What hyperparameters to set? (see the next slide)

What to observe? In the case of decision trees, one should observe the difference between performance measures (e.g., classification accuracy) on the training and test sets.

The too-large difference implies an improperly fitting model.

Hyperparameter Tuning for Decision Trees

Usual hyperparameters:

- Maximum depth

  The deeper the tree, the more complex models you can create $\Rightarrow$ overfitting. Low depth may restrict expressivity.

- Minimum number of examples to split a node

  Higher values prevent a model from learning relations specific only for a few examples. Too high values may result in underfitting.

- Minimum samples required to be in a leaf

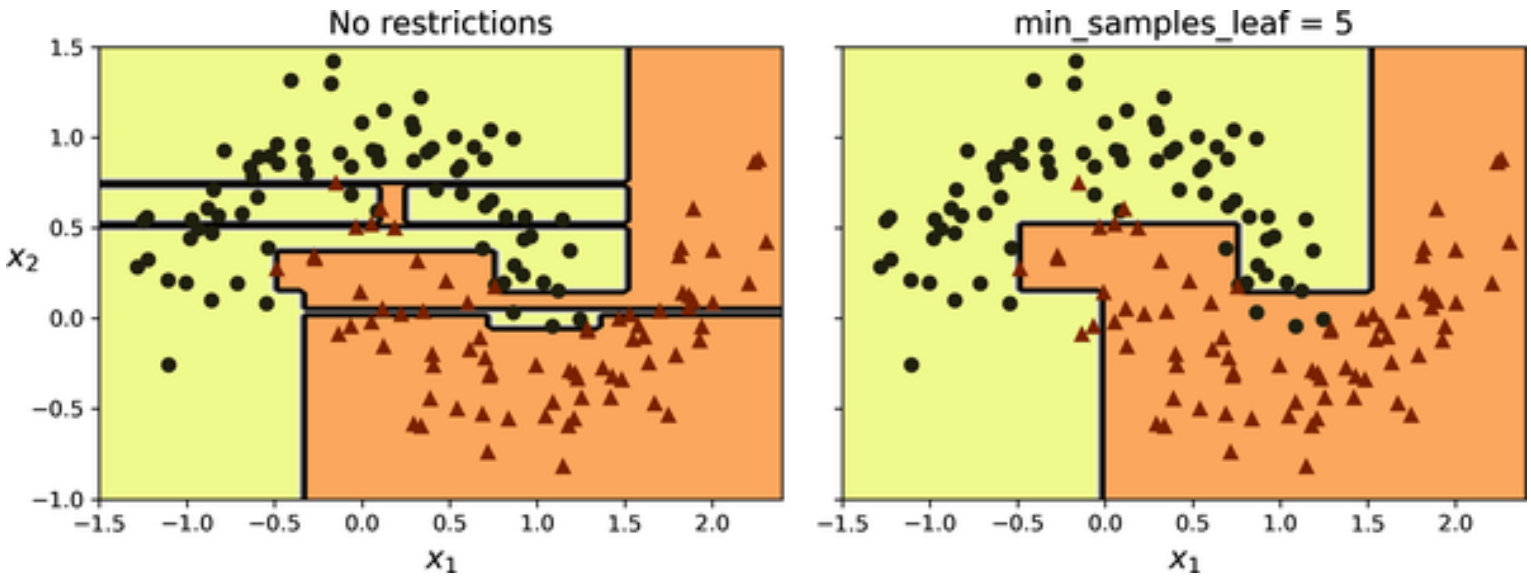
  Similar to the previous one. A higher number means we cannot have very specific branches concerned with particular combinations of features.

- Minimum impurity decrease

  Small impurity decrease means that the split does not contribute too much to the classification (their proportions after split are similar to proportion before split). However, keep in mind that it is *weighted average impurity* after the split.

- ...

Hyperparameters Tuning Example



See the overfitting on the left. The model on the right has been *regularized* by restricting the minimum number of samples in leaves.

Advantages of Decision Trees

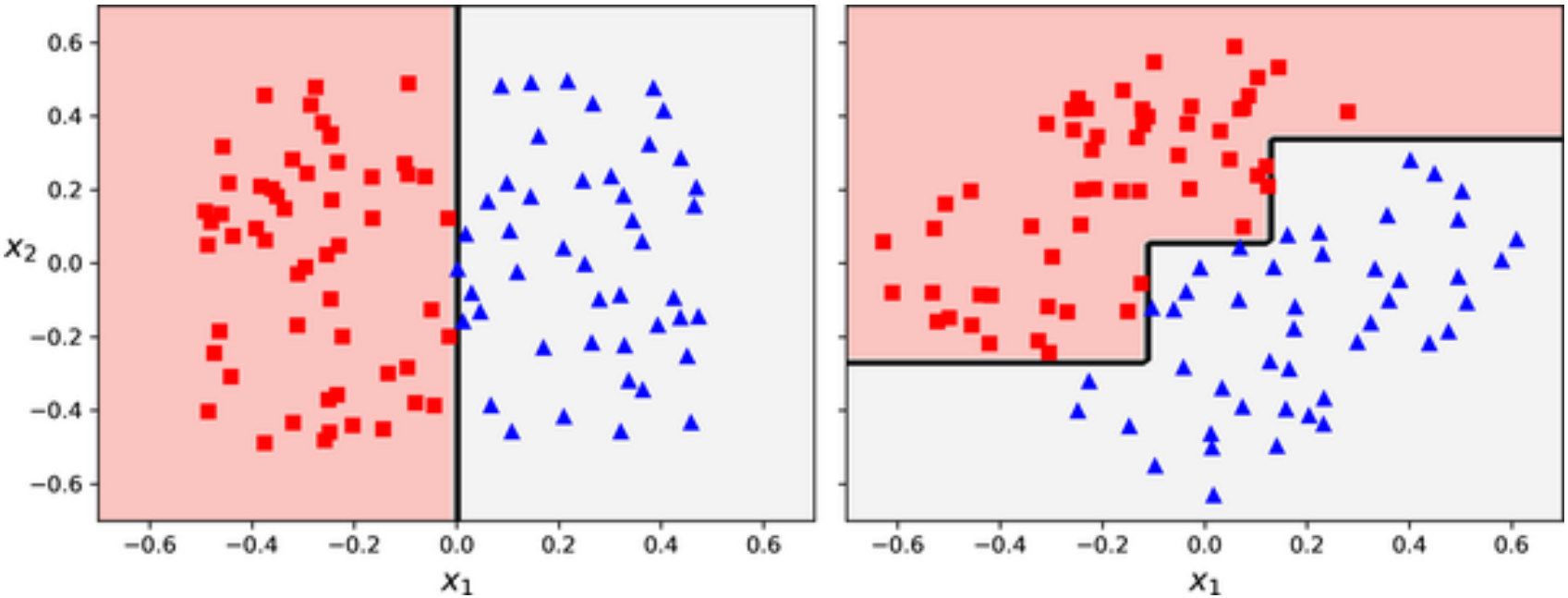
- Simple to understand and interpret; trees can be visualized.
- Requires little data preparation, unlike other techniques requiring normalization, dummy variables, or blank value removal.
- Cost of using the tree is logarithmic in the number of data points used to train it.
- Handles numerical and categorical data.
- Capable of handling multi-output problems.
- Uses a white box model, where conditions are easily explained by boolean logic.
- Allows for model validation using statistical tests, accounting for model reliability.
- Performs well even when the true model somewhat violates its assumptions.

Disadvantages of Decision Trees

- Overfitting: Trees can be over-complex and not generalize well, needing pruning or limits on tree depth.
- Instability: Small data variations can result in very different trees. This is mitigated in ensemble methods.
- Non-smooth predictions: Decision trees make piecewise constant approximations, which are not suitable for extrapolation.
- Learning optimal trees is NP-complete: Heuristic algorithms like greedy algorithms are used, which do not guarantee globally optimal trees. Ensemble methods can help.
- Difficulty expressing certain concepts, Such as XOR, parity, or multiplexer problems.
- Bias in trees: Decision trees can create biased trees if some classes dominate. Balancing the dataset is recommended.

Axis Sensitivity

Decision makes divisions along particular axes:

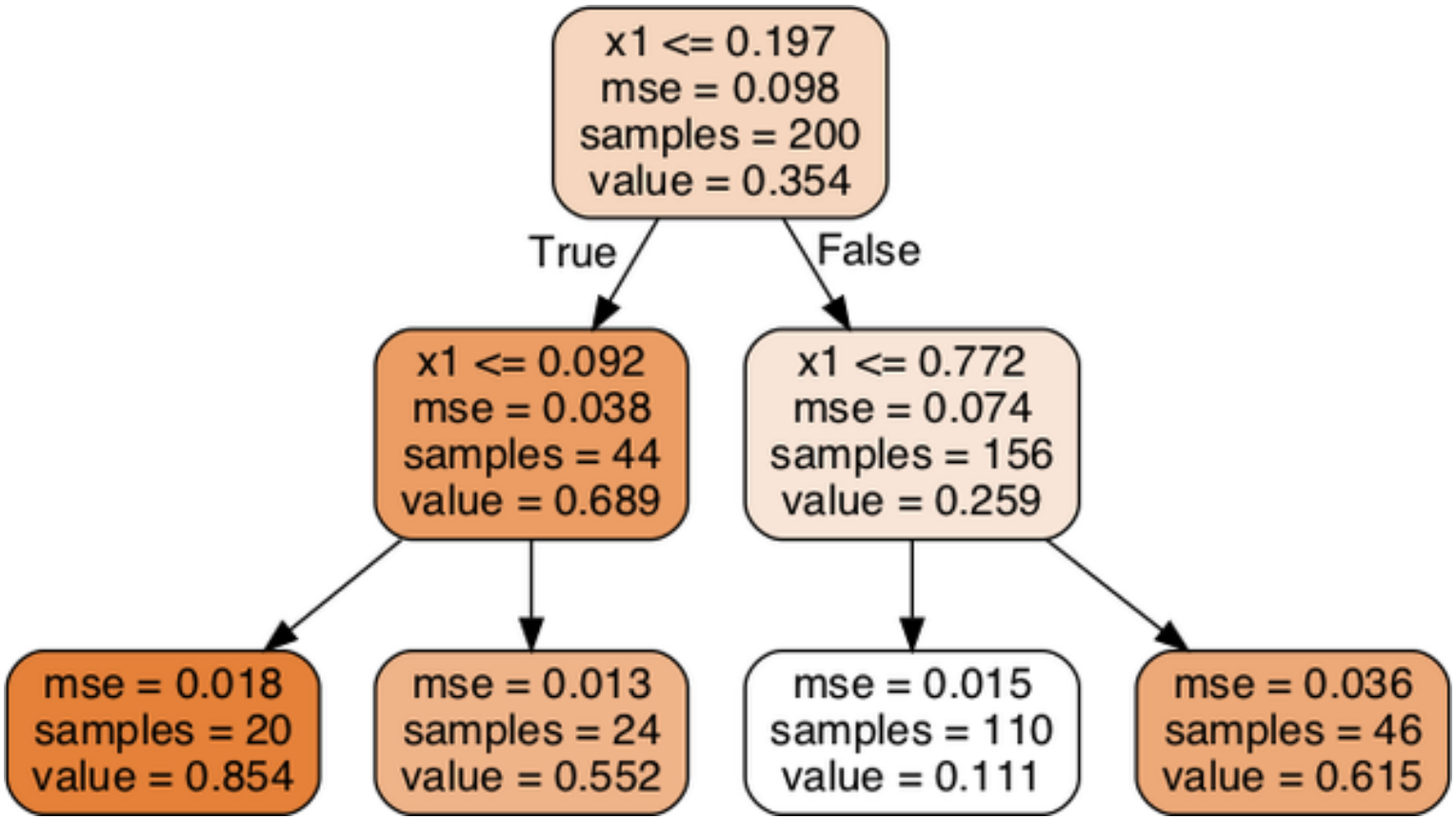


That is, rotated data may result in a completely different model.

That is why decision trees are often preceded by the *principal component analysis (PCA)* transformation, which aligns data along the axes of maximum data variance.

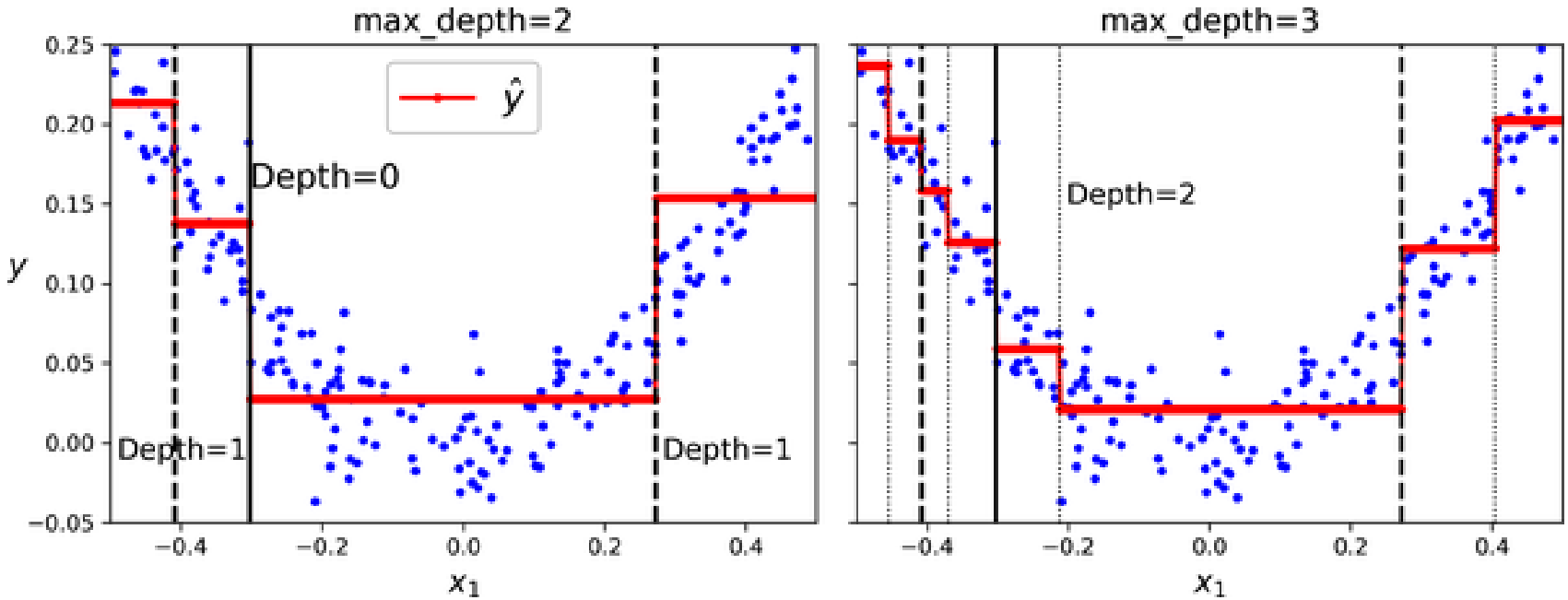
Comment on Regression Trees

Decision trees can also be used to approximate functions. Assign a function value to the leaves instead of classes.



Here "mse" is the mean-squared-error. We get to this notion later in connection with linear models and neural networks.

Comment on Regression Trees



Intuitively, for every subinterval of x_1 the value (the red line) is at the average y over the subinterval.

How are the subintervals being set? We will answer this question later once we master the mean-squared error.