# An Introduction to Supervised Machine Learning

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# Context

- An exponential increase of real-life applications of machine learning
- This is an introduction course. Next year you will follow more advanced courses (depending on your orientation)
- You need some basic knowledge regarding linear algebra, algorithms and complexity
- I ask questions very often, so please be interactive
- Feel free to stop me anytime. There is no stupid question!
- Speak up if you spot a typo or an error. You might get bonus points!!
- The evaluation will be decided later. Most likely it will be based on lecture questions and practical sessions
- The course is articulated around three parts: introduction, interpretable machine learning (myself), and neural networks (Arthur Bit Monnot)

# References


T. Hastie, R. Tibshirani, and J. H. Friedman, *The Elements of Statistical Learning: Data Mining, Inference, and Prediction, 2nd Edition.*
Springer Series in Statistics, Springer, 2009.

S. J. Russell and P. Norvig, *Artificial Intelligence - A Modern Approach, Third International Edition.*
Pearson Education, 2010.

C. Rudin, C. Chen, Z. Chen, H. Huang, L. Semenova, and C. Zhong, "Interpretable machine learning: Fundamental principles and 10 grand challenges," *CoRR*, vol. abs/2103.11251, 2021.

# Part 1: Introduction

# Chapter 1: Context

Figure 1: How to cycle? [1]

[1] Image from `https://en.wikipedia.org/wiki/Cycling`

Figure 2: How to teach a child animal recognition? [2]

[2] Image from `https://en.wikipedia.org/wiki/Global_biodiversity`

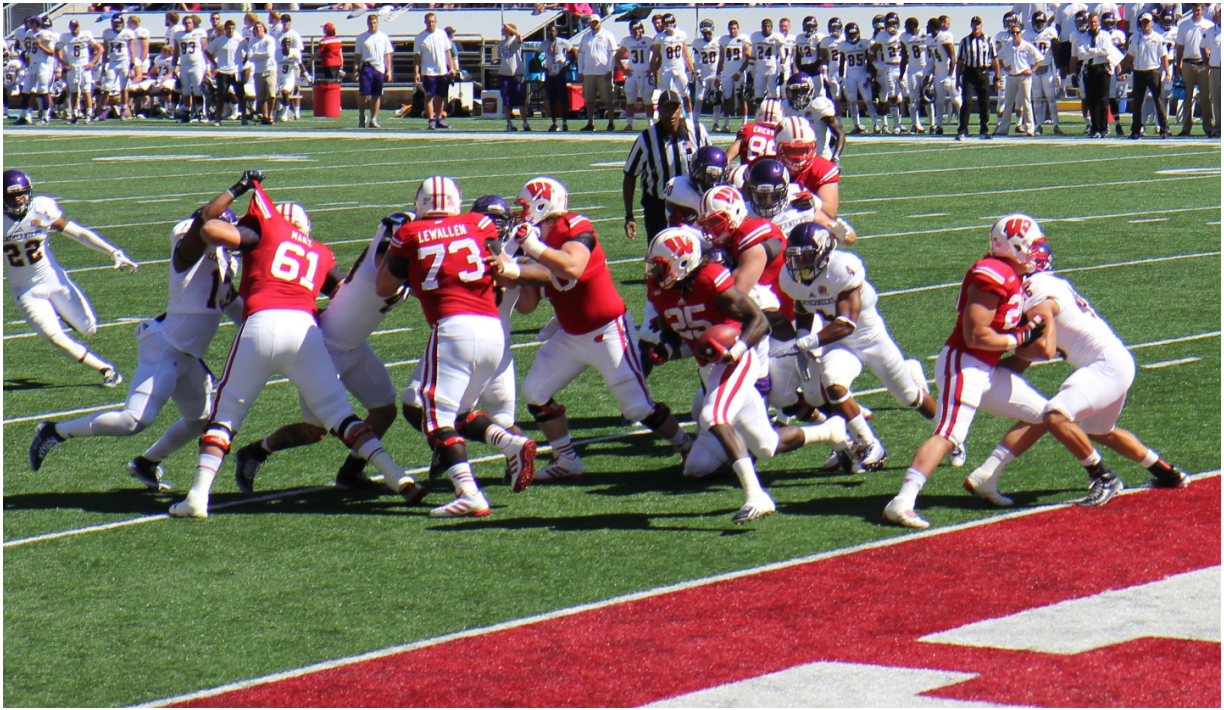



Figure 3: How to predict a player's performance? [3]

[3] Image from `https://en.wikipedia.org/wiki`

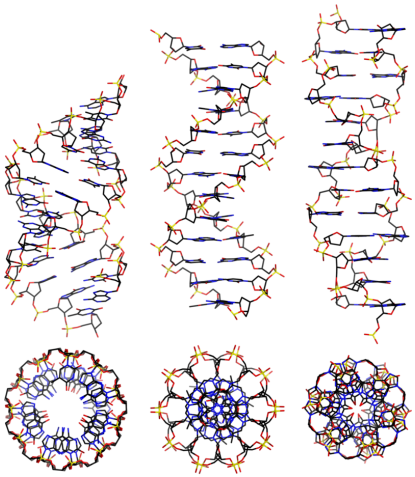


Figure 4: Analysis of evolutionary biology based on DNA patterns [4]

[4] Image from `https://en.wikipedia.org/wiki/DNA`

- Cycling: It needs a sequence of successful/unsuccessful trials!
- Animal recognition: It does not make sense to show the picture of every animal!

  $\Longrightarrow$ Show some pictures per animal and let the child learn
- Player performance: No straightforward formulae. Keep track of its latest performances and predict accordingly
- DNA clustering: Let the machine discover by itself the different patterns.
- That's pretty much the philosophy of machine learning: feed the computer some date, and let it learn by itself
- Note 1: Some computational problems are simply not solvable in a traditionally way and need machine learning
- Note 2: Machine learning is not always the solution! Consider for instance basic arithmetic operations

# Examples of Machine Learning Applications [1]

- Autonomous cars
- Flying drones
- Face recognition
- Computer vision
- Natural language processing
- Music/movie recommendation
- Dating apps
- Friends recommendation
- Weather prediction
- Trading
- ...

# The Big Picture

It depends on the problem at hand and on the nature of data!

1. **Labelled data**:
   - The task of animal recognition is to predict the animal in a given picture. The data (used to "train" the computer) is a set of pictures and each picture is associated to an animal. In this case, the **label** is a **category**
   - In trading, the task is to predict the price evolution of a given share and the data is simply historical evolution of the share. In this case the data is **labelled** with **real numbers**.
2. **Unlabelled data**: For instance, when using clustering to evaluate the density of a population. The data can simply be a set of coordinates with no labels.
3. **Continuously updated data**: The data is continuously updated according to previous experiences: For instance, a robot that tries to ride a bicycle learns how to bike by a sequence of trials

# Supervised/Unsupervised/Reinforcement Learning

- Supervised Learning (Labelled data): Predict a function that associates inputs to outputs based on historical data
  - Categorical labels (discrete values): Classification
  - Non-categorical labels (real numbers): Regression
- Unsupervised Learning: The task is to figure out patterns presented in the data (unlabelled data)
- Reinforcement learning: learning from a series of rewards /punishments
- But also, depending on the problem, data could be both labelled/non labelled, etc.. (semi-supervised learning)

Figure 5: How to teach a child animal recognition? [5]

Classification task

[5] Image from `https://en.wikipedia.org/wiki/Global_biodiversity`

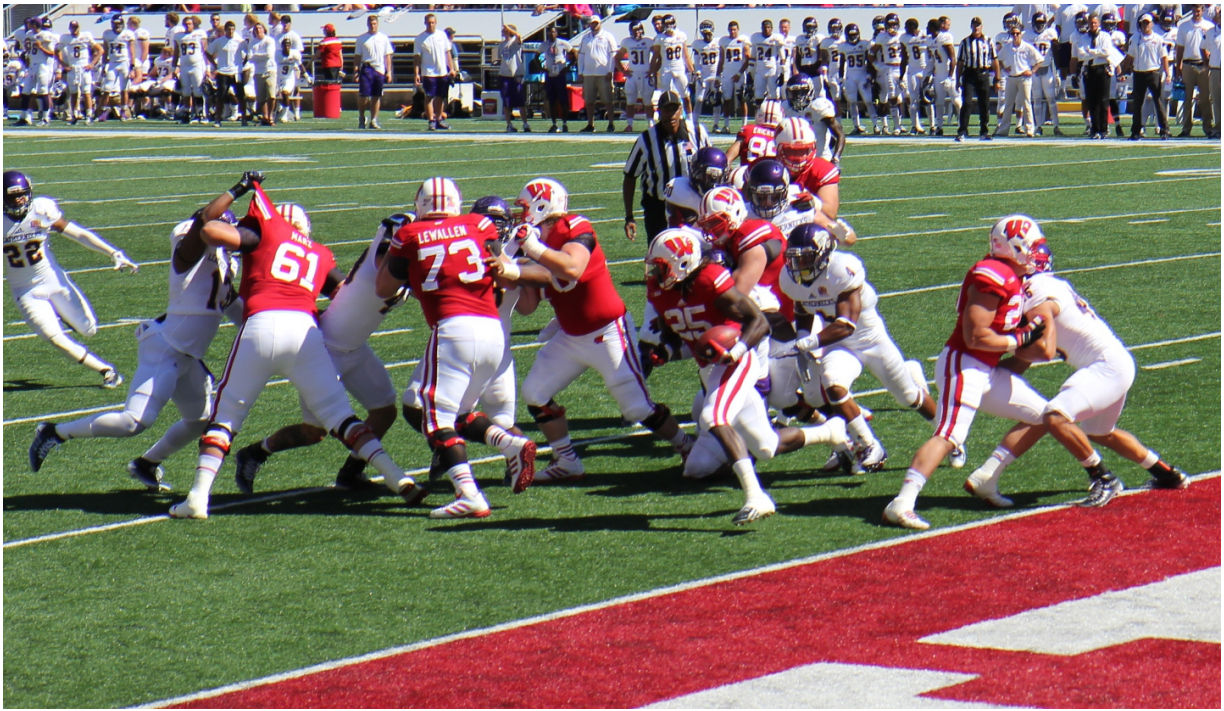



Figure 6: How to predict a player's performance? [6]

Regression task

[6] Image from `https://en.wikipedia.org/wiki`

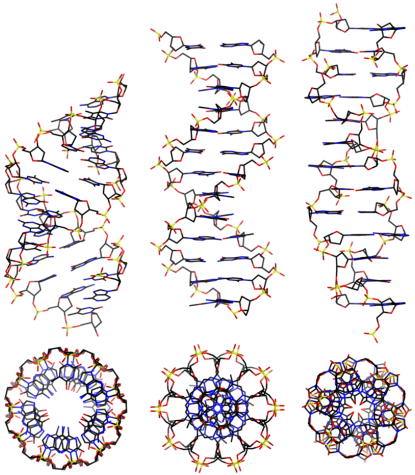


Figure 7: Analysis of evolutionary biology based on DNA patterns [7]

Unsupervised learning (clustering) task

[7] Image from `https://en.wikipedia.org/wiki/DNA`

Figure 8: How to cycle? [8]

Reinforcement learning

[8] Image from `https://en.wikipedia.org/wiki/Cycling`

# Chapter 2: Supervised Machine Learning

# Supervised Machine Learning: The Basics

- We focus in this course on Supervised ML
- Examples of applications
  - Tumor detection: The data is a collection of brain scans. Each scan is associated with a label indicating the type of tumor
    $\Longrightarrow$ Classification
  - Credit score: The data is a collection of clients profiles (age, salary, genre (?), job, ...) with a positive or negative feedback
    $\Longrightarrow$ Binary classification
  - Precipitation prediction: (loosely speaking) the data is a collection of sequential weather conditions and the purpose is to predict the Precipitation chance (real value)
    $\Longrightarrow$ Regression

# Problem Definition [2]

- Given a historical data (**training set**) in the form of input-output examples: $\{(x_1, y_1), \ldots (x_n, y_n)\}$ where $x_i$ is an input, $y_i$ is the output of $x_i$ drawn from an unknown function $f$
- Find a function $f_h$ (called a hypothesis or model) that approximates the true function $f$
- The approximation criterion can be defined in different ways. We can consider it as a function minimizing some error.

# Training Phase

- The function $f_h$ is constructed via a **training algorithm**
- The training algorithm depends on the hypothesis space
- Examples of hypothesis space (family of functions) include polynomial functions, trigonometry functions, decision trees, decision lists, neural networks, ...

# Testing Phase

- The evaluation of the constructed hypothesis (or model) is done via a set of unseen examples called **testing set**
- The testing set is usually taken randomly from the initial data. However, it shouldn't be part of the training set
- The common way is to split the initial data into a training and testing sets randomly

# Model Evaluation: Classification

- Training accuracy: percentage of training examples that are well predicted
- Testing accuracy: percentage of testing examples that are well predicted
- The concept of **generalisation** is precisely the quality of testing accuracy

# Classification Evaluation: The Confusion Matrix

- Accuracy alone hinders the way predictions are made. Model evaluation needs more refinement
- Consider binary classification (positive/negative classes) with 80% testing accuracy
- 80% seems good, however, a deeper investigation shows that most of negative examples are wrongly predicted! This shows a biases in the model (biased towards positive examples)
- The purpose of the confusion matrix is precisely to have a refined evaluation
- In the case on $m$ classes, the matrix is of dimension $m \times m$ where $M[i][j]$ is the number of examples of class $i$ that are predicted to be as the class $b$
- The model bias can be easily seen: For instance, one can answer statistical queries such as: is the error evenly distributed? to which class the model is likely to predict? ...

# The Confusion Matrix in the Case of Binary Classification

- A positive class and a negative class
- The confusion matrix is of dimension $2 \times 2$
- True Positive Rate (TP rate): the likelihood that a positive example is well classified
- False Positive Rate (FP rate): the likelihood that a positive example is wrongly classified
- True Negative Rate (TN rate): the likelihood that a negative example is well classified
- False Negative Rate (FN rate): the likelihood that a negative example is wrongly classified

# The Covid Example (1)

- Assume that we have a prediction model with 85% accuracy
- 100 individuals: 70 positives and 30 negatives
- The confusion matrix:

| | Positive | Negative |
|---|---|---|
| Positive | 65 | 5 |
| Negative | 10 | 20 |

- TP rate is $65/70 = 93\%$ ; FP rate is $5/70 = 7\%$
- TN rate is $20/30 = 66\%$ ; FN rate is $10/30 = 33\%$
- Positive individuals has 93% chance to be correctly predicted
- Negative individuals has 66% chance to be correctly predicted

# The Covid Example (2)

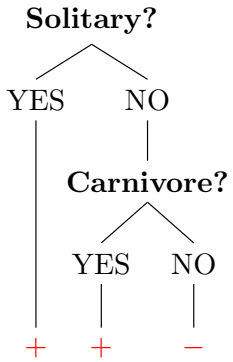
- The confusion matrix:

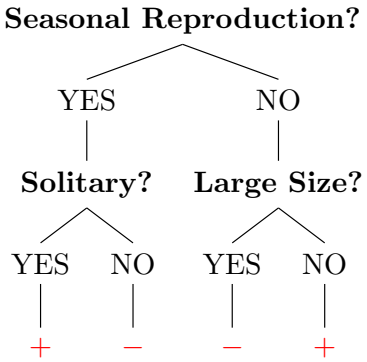
| | Positive | Negative |
|---|---|---|
| Positive | 65 | 5 |
| Negative | 10 | 20 |

  - TP rate is $65/70 = 93\%$ ; FP rate is $5/70 = 7\%$
  - TN rate is $20/30 = 66\%$ ; FN rate is $10/30 = 33\%$
  - Positive individuals has 93% chance to be correctly predicted
  - Negative individuals has 66% chance to be correctly predicted
- What is the probability for someone who tested positive to be truly positive? $= 65/(65 + 10) = 86\%$
- What is the probability for someone who tested negative to be truly negative? $= 20/(5 + 20) = 80\%$

# Toy Example: DTs to Predict The Likelihood of Animal Extinction

| Big Size | Carnivore | Seasonal Reproduction | Solitary | Extinct |
|---|---|---|---|---|
| 0 | 1 | 0 | 1 | yes |
| 1 | 0 | 0 | 1 | yes |
| 0 | 0 | 0 | 1 | no |
| 1 | 1 | 1 | 0 | no |
| 0 | 0 | 1 | 0 | yes |




- Tabular data
- Hypothesis space: Decision trees
- Left tree: accuracy 2/5
- Right tree: accuracy 2/5

# Model Evaluation: Regression

- In the case of classification, a simple way to define error is to count the number of examples wrongly predicted
- How about regression?
- Take the example of estimating the price of a house based on the surface and the distance to the city.
- Suppose that the real price of a house is 1 Million and the model predicted $999k$.
- Obviously it's not a correct prediction, however, it seems close enough! But how close?
- We need an error function that take into account a notion of distance between true values and predicted values

# Model Evaluation: Regression

- Two well known functions: Mean Absolute Error($MAE$) and Mean Square Error($MSE$) (or Root Mean Square Error($RMSE$))
- Consider a dataset with $n$ examples where $y$ is the vector of the true values and $\hat{y}$ is the vector of predicted values:

$$MAE = \frac{1}{n}\sum |y_i - \hat{y}_i|$$

$$MSE = \frac{1}{n}\sum (y_i - \hat{y}_i)^2$$

$$RMSE = \sqrt{MSE}$$

# Beyond Traditional Evaluations: Crucial Predictions

- Take the example of tumor detection
- Predicting the non-presence of a tumor for a patient that has a tumor is a serious problem
- How to deal with such situation?
- For instance, one can add a weight on the mis-classification error as follows: the cost of mis-classifying a patient with a tumor is 5 times the cost of mis-classifying a patient without a tumor
- In this case the objective function is slightly different from the standard accuracy (weighted sum)

# Computational Hardness

Out of these three questions, which one is the hardest and which one is the easiest (computationally)?

1. Build a perfect decision tree (a tree that classifies every example correctly) 100% accuracy ?
2. Build the best decision tree within a height $h$ ?
3. Build a perfect decision tree with a minimum height ?

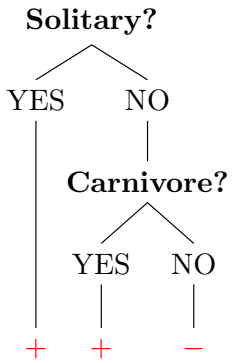
- Question 1 is the easiest: we can always develop children to classify every example
- Let $k$ be the number of features; $f(n)$ be the complexity of Question 2 and $g(n)$ be the complexity of Question 3
- $g(n) = O(k \times f(n))$: We can solve Question 3 by solving Question 2 iteratively by increasing/decreasing the height
- Different objective functions can be defined (i.e., the training problem itsetf can have different definitions)
- The definition of the objective function with the hypothesis space has an impact on the complexity of training

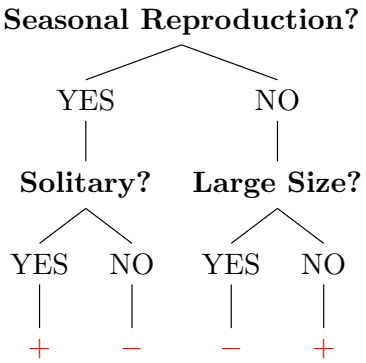
## To summarize

- Supervised Learning: The data is labelled
- Each example is defined by a sequence of values (of the different attributes/features) with an output
- Training vs. Testing sets (disjoints)
- **Generalisation:** when the model generalizes well on unseen data
- Regression: Supervised Learning with real values
- Classification: Supervised Learning with discrete values (classes)
- Regression evaluation: accuracy in terms of minimum error (Mean Absolute Error, Root Mean Square Error)
- Classification evaluation: accuracy in terms of examples well classified but also the confusion matrix (it can show some bias)
- Depending on the problem at hand, the objective function can have have different forms
- The way the optimisation problem is defined impacts its computational complexity

# Questions & Exercises

| Big Size | Carnivore | Seasonal Reproduction | Solitary | Extinct |
|---|---|---|---|---|
| 0 | 1 | 0 | 1 | yes |
| 1 | 0 | 0 | 1 | yes |
| 0 | 0 | 0 | 1 | no |
| 1 | 1 | 1 | 0 | no |
| 0 | 0 | 1 | 0 | yes |

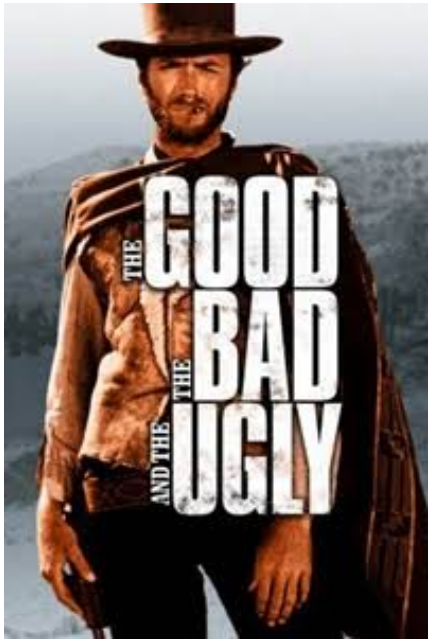


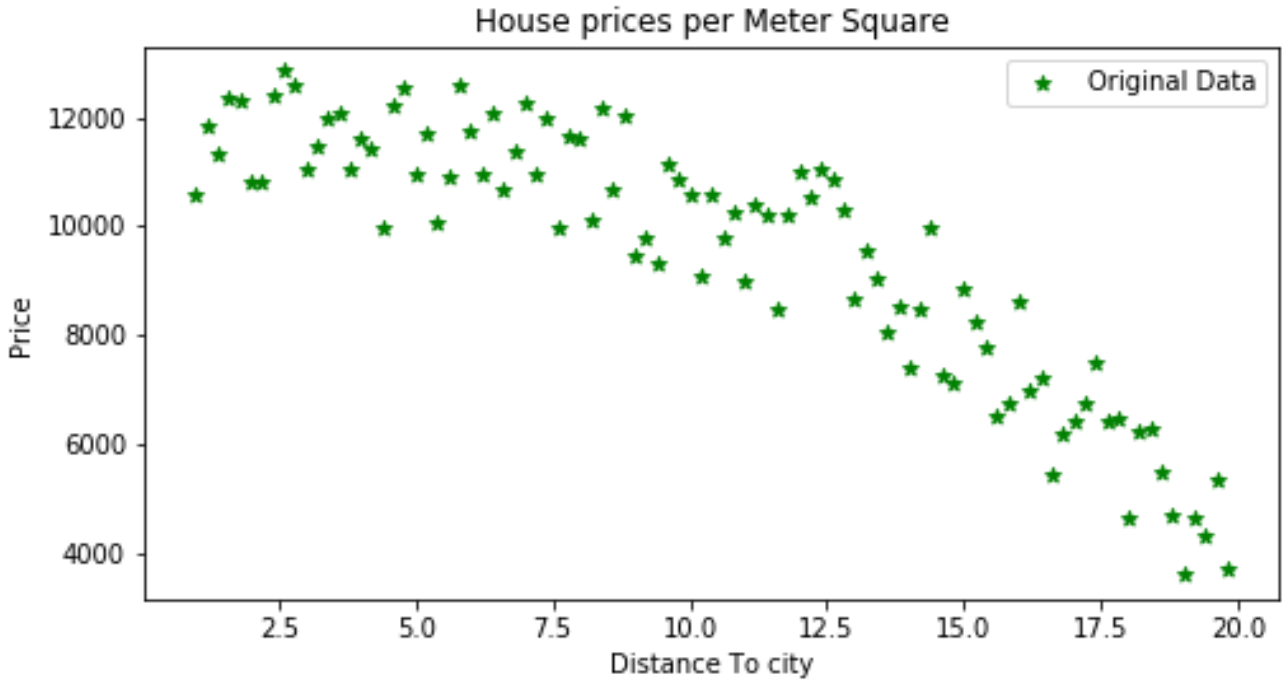

- Find a perfect tree
- Find a perfect tree with a minimum weight
- Find a best tree with height 2

# Chapter 3: Deeper Evaluations

# Overfitting, Underfitting, and Goodfitting

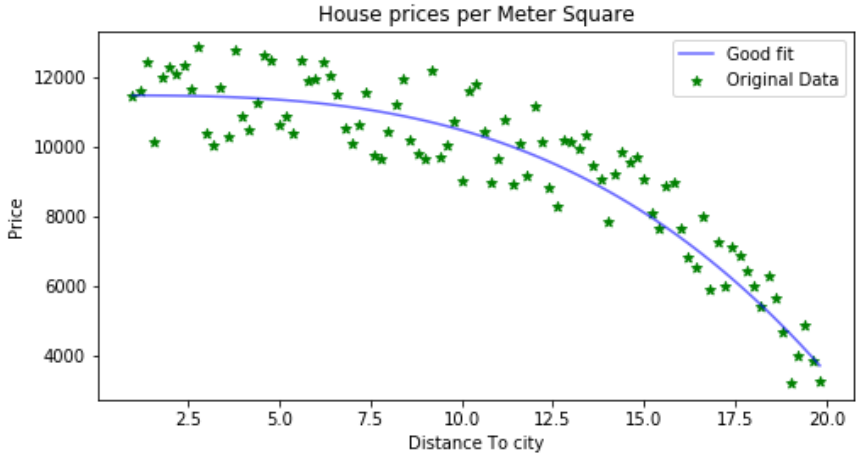


# The Housing Prices Example



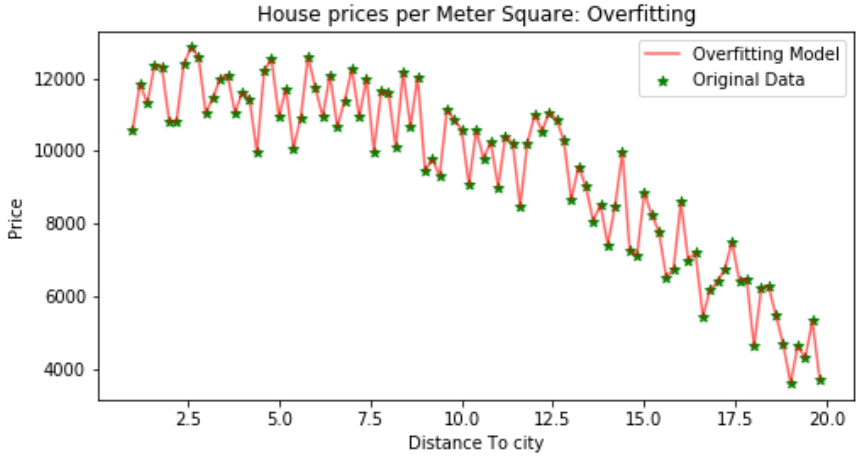

This data includes some **noise**. That is, points that are not correctly collected (which is often the case in real applications)

# The Housing Prices Example: The Good



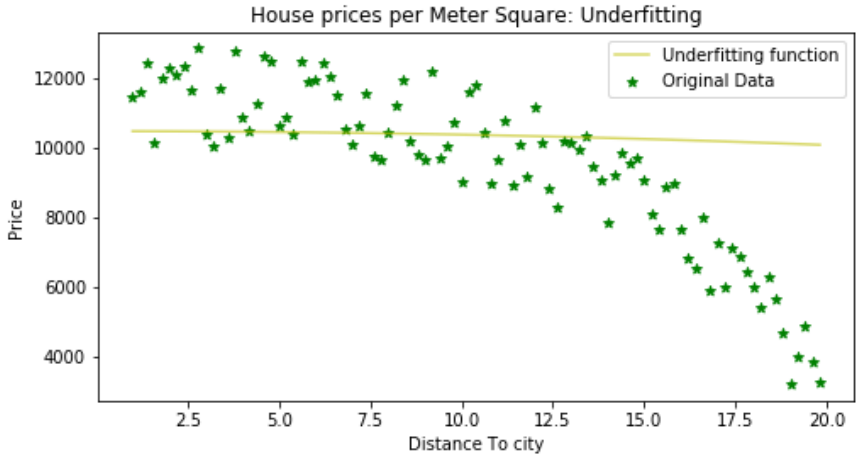

We can make an analogy to a smart student who has a good understanding of a lecture

# The Housing Prices Example: The Bad (Overfitting)



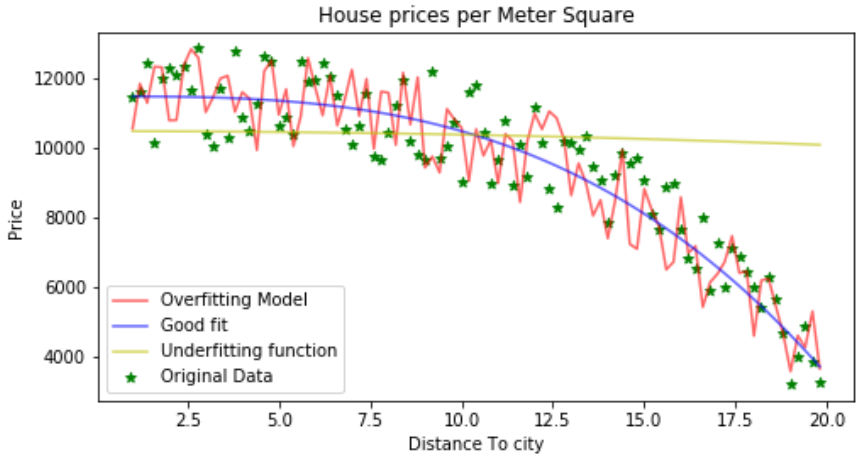

We can make an analogy to the student who "learns" the lecture mechanically without a real understanding.

# The Housing Prices Example: The Ugly (Underfitting)




We can make an analogy to a lazy student who barely remember the lecture without any understanding

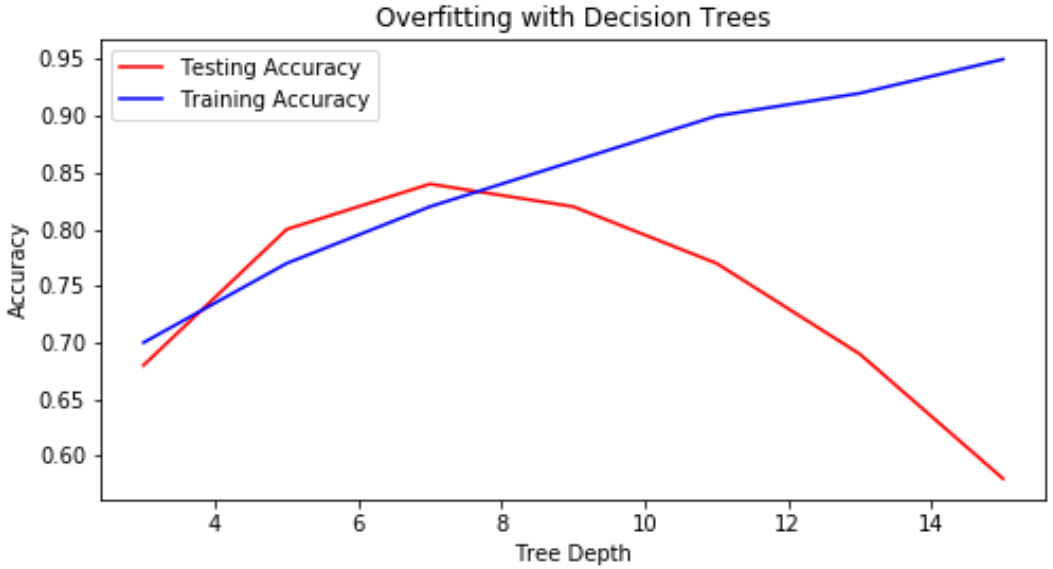
# The Housing Prices Example: All Together



# Overfitting, Underfitting, and a Good Fit

- Overfitting happens when the model tries to squeeze everything in including noise without an "intuitive understanding of the data"
- Underfitting happens when the model performs badly on the training and testing data (no real learning).
- A good fit happens when the model approximates well the true distribution without being disturbed by noise (good generalisation)

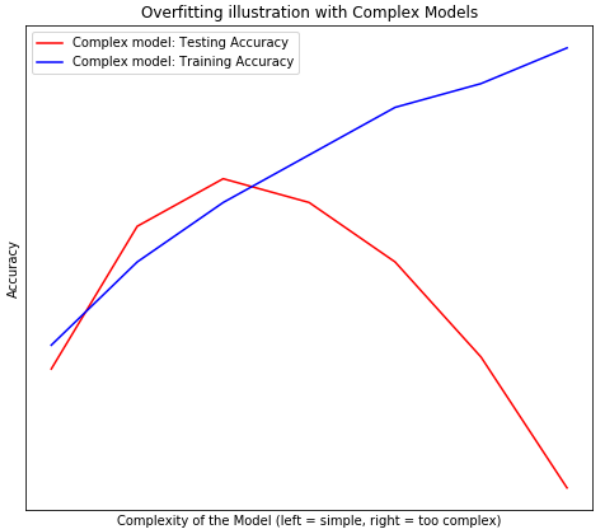
# Overfitting with Decision Trees as an Example



# Overfitting with Decision Trees as an Example

- The longer the tree, the better the training accuracy gets, however, this is not necessarily the case for the testing accuracy
- Testing accuracy increases at the beginning until a certain value (depth = 7), the it decreases afterwards
- This happens because with longer trees, the model can classify correctly more examples in the training set, however, this includes noise.

# Overfitting Based on the Complexity of the Model




- When the model is too simple, there is a risque of underfitting
- When the model is too complex, there is a risque of overfitting
- We need a Model that is somehow in between
- ML libraries offer parameters for regulation to avoid overfitting/underfitting

# Training Algorithms Evaluation

- Suppose that we have a number of training algorithms for a given hypothesis space
- How to choose the best?
- Generalisation should be evaluated a number of random splits
- Also the confusion matrices can be used for evaluation
- A common way is to use the $k-$fold cross validation:
  1. Split the data into $k$ folds
  2. Perform the training $k$ times. At each iteration, a different fold is chosen as a testing set and the rest is used for training
  3. Typical values for $k$ are 5 and 10

# Overcome Overfitting

- How to avoid overfitting?
- The testing set is inaccessible at the moment of training
- We can sacrifice a part of the training set as a 'validation set' to evaluate the generalisation of the model.
- Basically, the training set has a subset for training and a subset for validation (evaluation)
- A common way is to use $k-$cross validation on the training set to overcome overfitting
- Also, we can restrict the hypothesis space with simple models

# Complexity/Quality Tradeoff

- Training algorithms have resources costs: memory and runtime (we will see later how to train decision trees/linear functions)
- For instance, training quadratic functions is much harder (computationally) than training linear functions
- However, may be a quadratic function is a better fit for the data at hand
- There is a trade-off between the quality of predictions and the model complexity
- For example training a tree with depth 5 is much faster than training a tree of depth 9, but in terms of training quality, trees of depth 9 are better. However, trees with depth 9 might overfit
- Most ML libraries offer the possibility to control the complexity with a regularization parameter

# Ockham's Razor Principle

- In the previous example, we have two different trees with the same accuracy
- Which tree to choose?
- Hard to answer without specific requirements
- Ockham's Razor Principle[9]: pick the simplest!
- Simplicity is also hard to define
- In decision trees, simplicity could be the depth, the number of features, a combination of both, etc
- When using polynomials (as a hypothesis space), lower degrees seems to be simpler
- In other cases it is very hard to define simplicity

[9] Philosopher `https://en.wikipedia.org/wiki/William_of_Ockham`

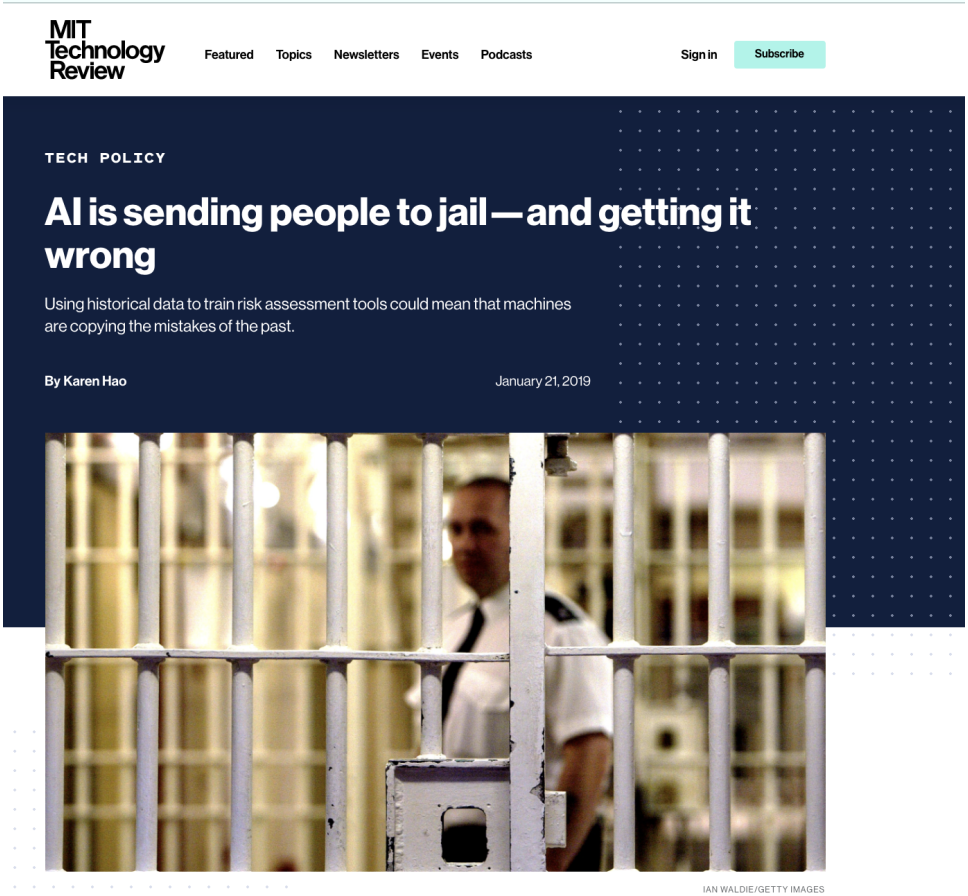
# Complexity/Quality/Overfitting Tradeoff

The bottom line

- There are fine lines between:
  - overfitting/underfitting
  - hard/easy training algorithms
  - complex/simple models
- Complex models can be computationally hard, however have better flexibility (some parameters can be turned off) and might have better quality
- Complex models might overfit
- Simple models might underfit
- Ideally, we look for a hypothesis that is 'easy' to compute and simple enough to be a good fit

# Chapter 4: Interpretable Models

# The COMPAS Tool



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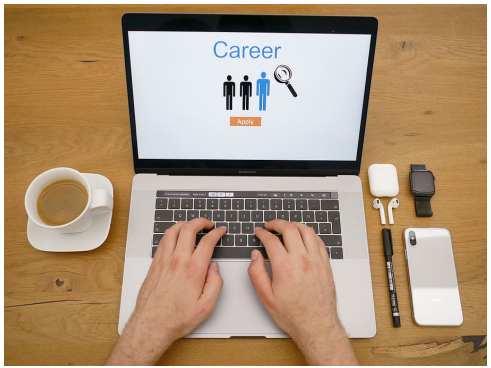
# Increasing Number of Real Life and Social AI Applications





# AI: Increasing Number of Real Life Applications Of Machine Learning

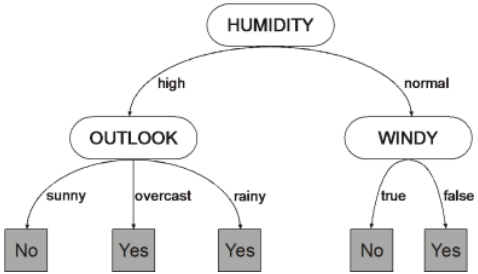
- The diverse applications of AI raised many ethical issues and questions
  - Job applications: AI that parses CVs for software engineers and recommends to hire mostly men
  - Credit scoring: AI that gives a credit score (for bank loans and credit applications) that recommends people from a particular geographical region, specific gender, social class, etc
  - Compass tool: (2016) used by judges in the US to predict which criminals are likely to re-offend is found to be biased by the ethnicity (African-American/Caucasian).

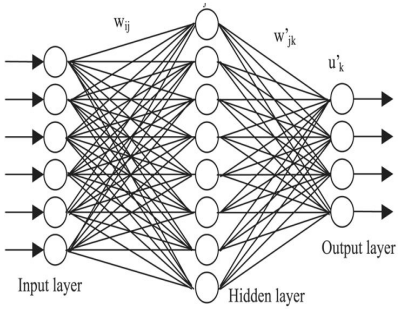
# COMPASS data and Rule-based Predictions

| Sex | Age | Priors | Juvenile Felonies | Juvenile Crimes | Ethnicity |
|---|---|---|---|---|---|
| Male | 15 | 1 | 0 | 1 | Caucasian |
| Male | 15 | 1 | 0 | 1 | African-American |
| Female | 33 | 1 | 0 | 1 | African-American |
| Female | 27 | 0 | 1 | 0 | Caucasian |
| Male | 41 | 0 | 1 | 0 | Caucasian |
| ... | ... | ... | ... | ... | ... |

The problem is to predict recidivism. That is, the tendency of a convicted criminal to re-offend.

# Black-Box vs Interpretable Models



# Definitions [3]

- **Black-box model** : A formula that is either too complicated for any human to understand, or proprietary, so that one cannot understand its inner workings
- **Interpretable model** obeys a domain-specific set of constraints to allow it (or its predictions, or the data) to be more easily understood by humans. These constraints can differ dramatically depending on the domain.

# Why Interpretable Models?

- Transparent
- Trustworthy
- Inherently Explainable
- Well adapted for troubleshooting and diagnosis
- **Mandatory criteria in high-stake decision making**

- We consider in this course tabular data (but extensions to other types is possible)
- Models:Decision trees, decision lists, decision rules, and linear functionns ...

# Decision rules & Decision Sets

- They are defined as If-Condition-Then-Prediction rules
- **Decision sets**: no specific order is given between the rules. Ties are broken by majority votes
- **Decision rules**: rules are ordered by priority

## Example of Rule List found by FairCORELS

- Data : `https://www.kaggle.com/danofer/compass`
- FairCORELS: `https://github.com/ferryjul/fairCORELS`

```
if [priors:>3] then [recidivism]
else if [age:21-22 && gender:Male] then [recidivism]
else if [age:18-20] then [recidivism]
else if [age:23-25 && priors:2-3] then [recidivism]
else [no recidivism]
```

*Rule list 5.* Example of an unconstrained rule list found by `FairCORELS` on COMPAS dataset, with Accuracy $= 0.681$, $\text{UNF}_{\text{EOdds}} = 0.217$ and $\text{UNF}_{\text{CUAE}} = 0.046$