An Introduction to Supervised Machine Learning

Mohamed Siala
https://siala.github.io/

INSA-Toulouse & LAAS-CNRS

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- The course is articulated around three parts: introduction, interpretable machine learning (myself), and neural networks (Arthur Bit Monnot)

References

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Course Syllabus

1. Part 1: Introduction
   - Context
   - Supervised Machine Learning
   - Deeper Evaluations
2. Interpretability
   - Motivation
   - Interpretable Models
   - Interpretability vs. Explanability

Part 1: Introduction

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

Figure 1: How to cycle? [1]

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

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

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

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

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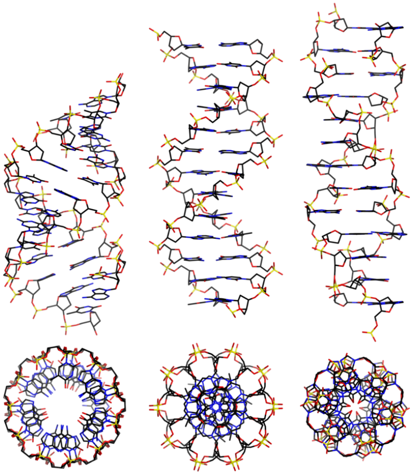

Figure 4: Analysis of evolutionary biology based on DNA patterns [4]

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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
- ...

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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

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- 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)

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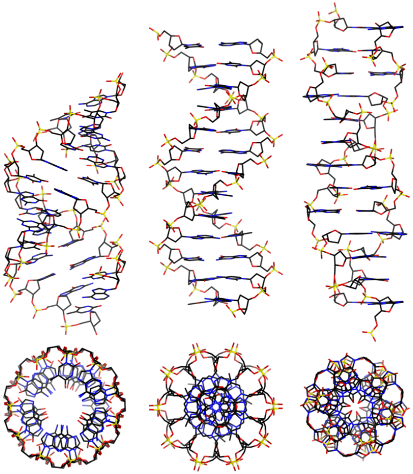

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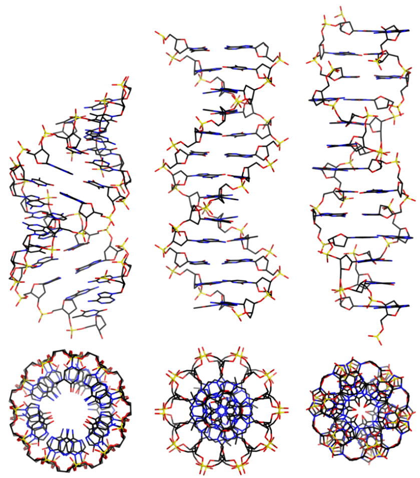

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Unsupervised learning (clustering) task

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    $\Longrightarrow$ Regression

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- 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.

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- Examples of hypothesis space (family of functions) include polynomial functions, trigonometry functions, decision trees, decision lists, neural networks, ...

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- 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? ...

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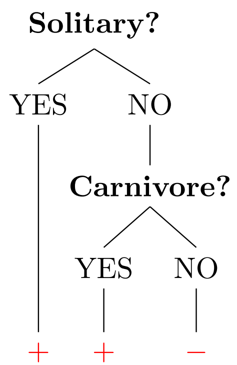

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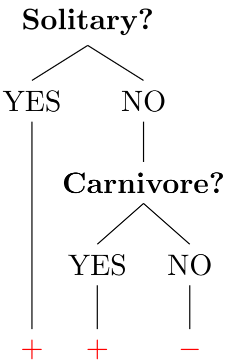

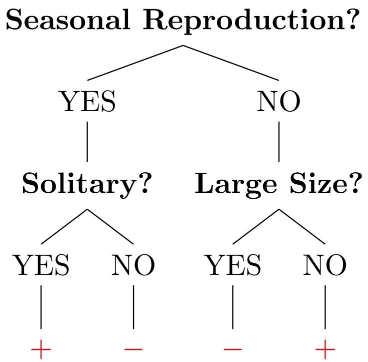

Toy Example: DTs to Predict The Likelihood of Animal Extinction

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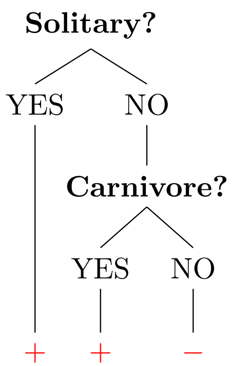
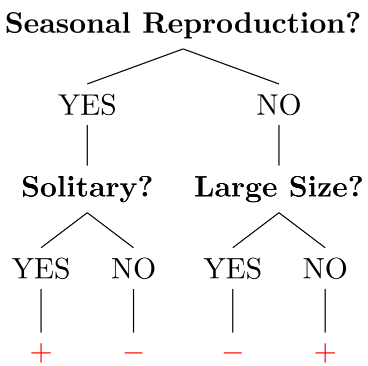
1	0	0	1	yes
0	0	0	1	no
1	1	1	0	no
0	0	1	0	yes





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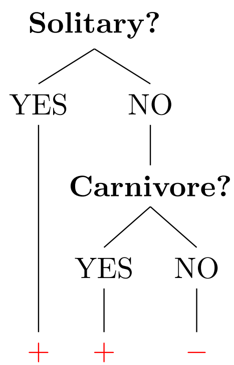

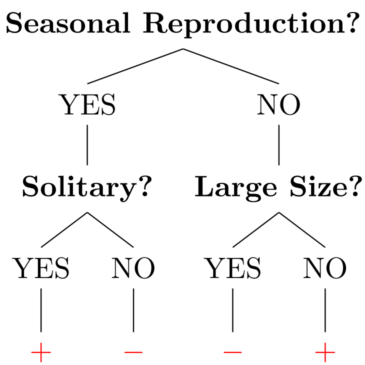

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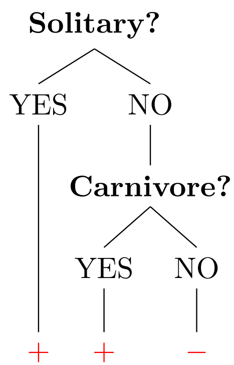

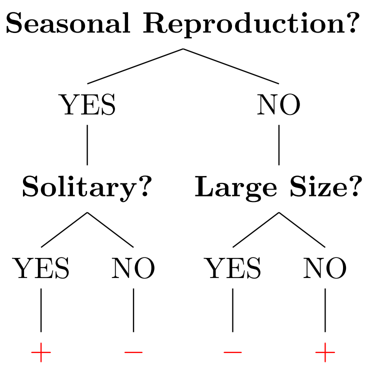

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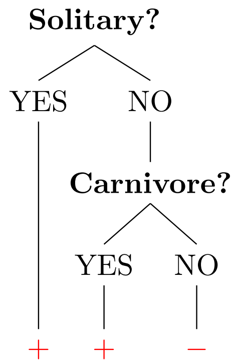

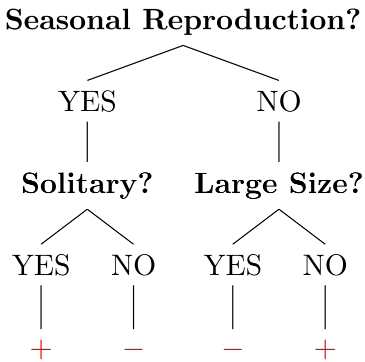

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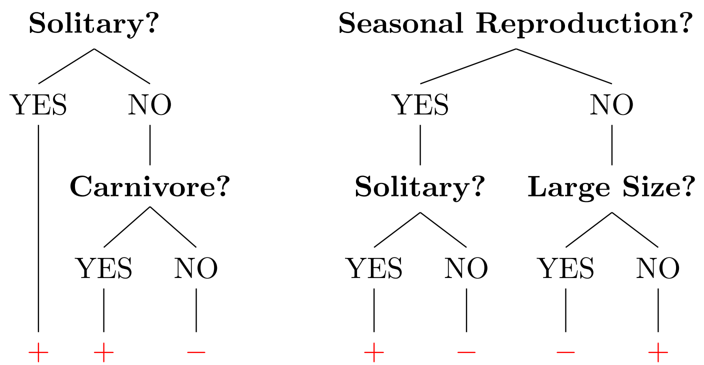

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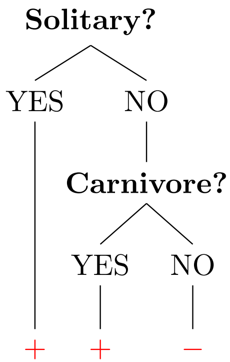

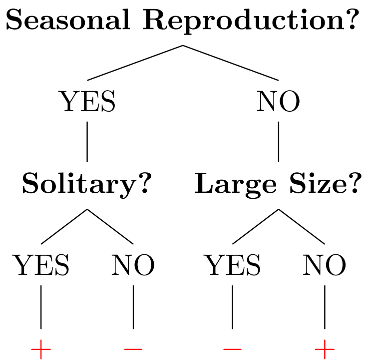

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- We need an error function that take into account a notion of distance between true values and predicted values

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- Consider a dataset with n examples where y is the vector of the true values and $\hat{y}$ is the vector of predicted values:

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

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

$$RMSE = \sqrt{MSE}$$

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- 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 ?
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- Let k be the number of features; $f(n)$ be the complexity of Question 2 and $g(n)$ be the complexity of Question 3
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- 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

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- The way the optimisation problem is defined impacts its computational complexity

Questions & Exercises

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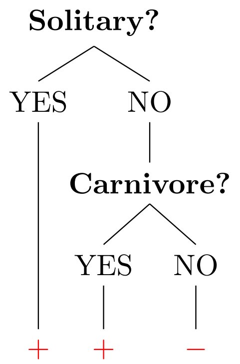

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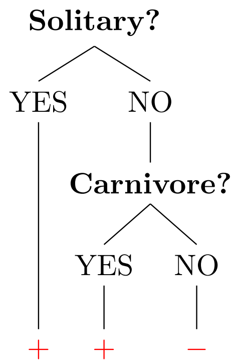

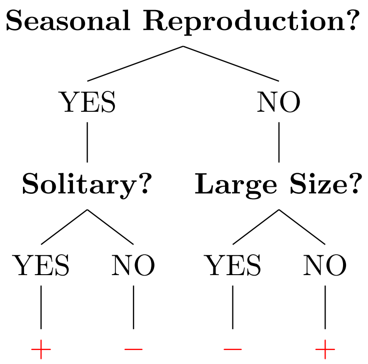

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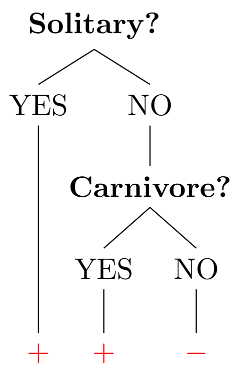

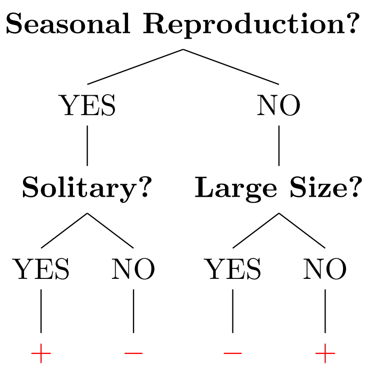

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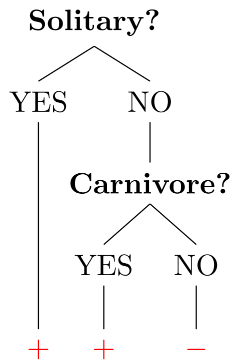

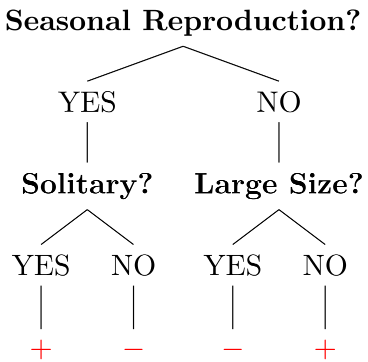

- Find a perfect tree

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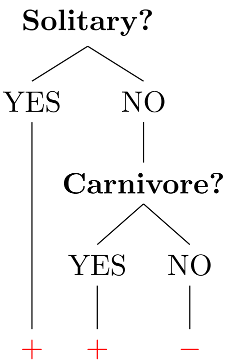

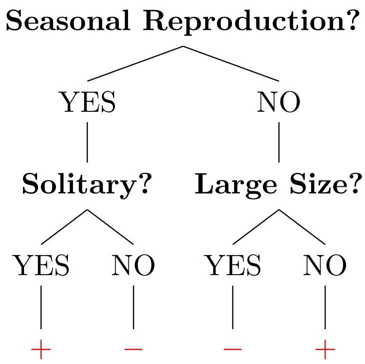

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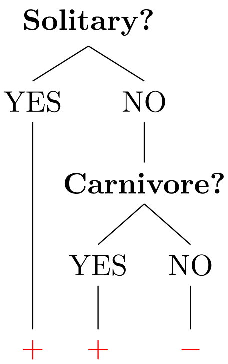

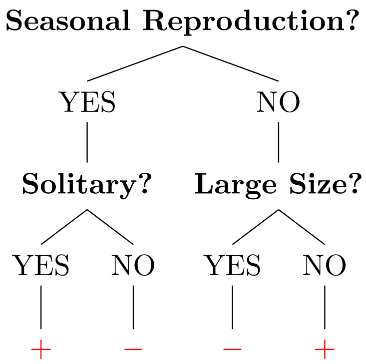

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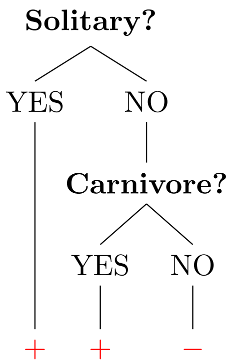

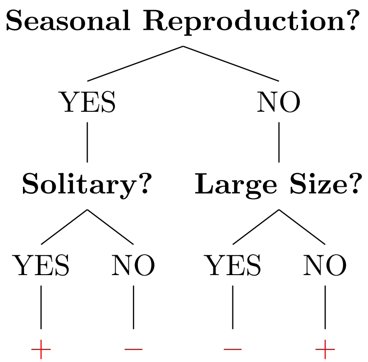

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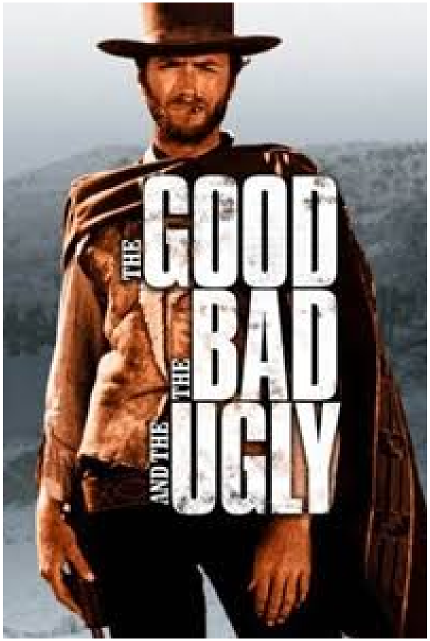
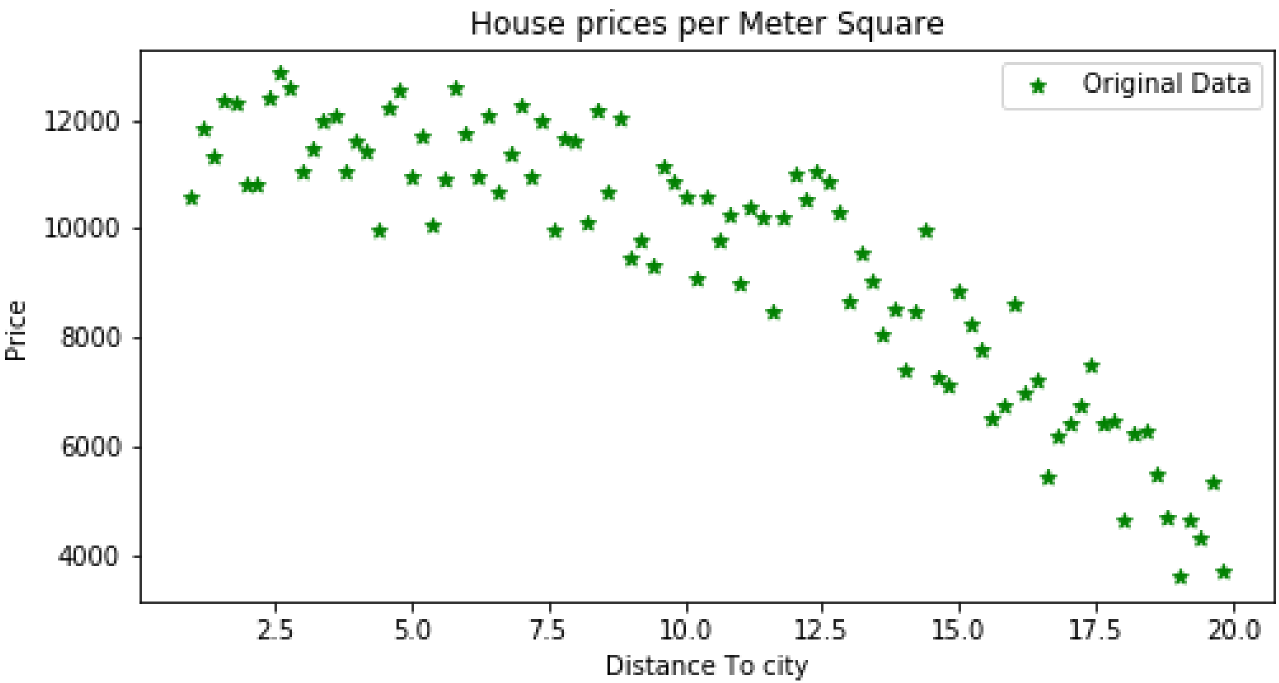
Deeper Evaluations

Overfitting, Underfitting, and Goodfitting

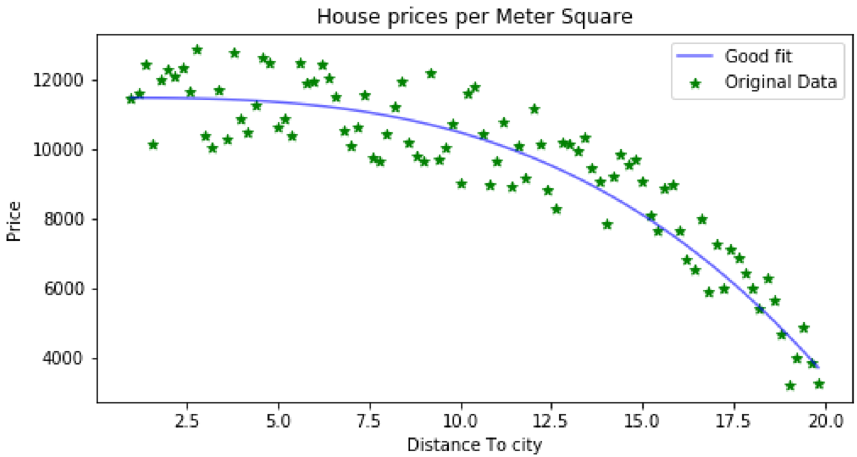


The Housing Prices Example



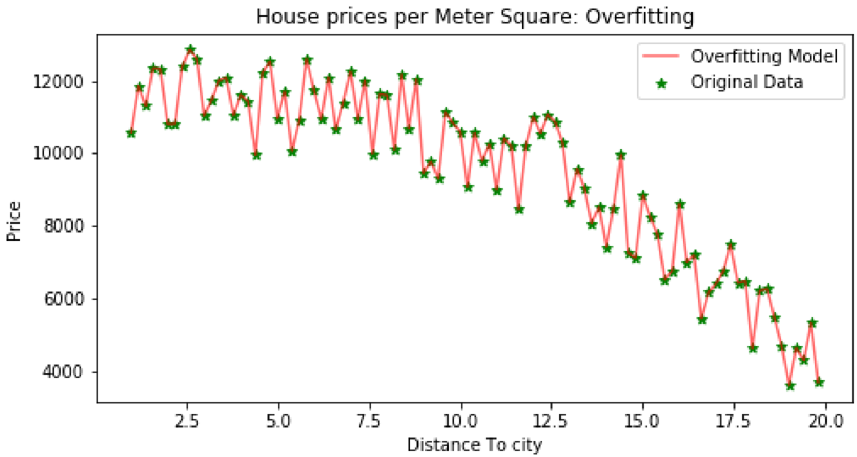
This data includes some **noise**. That is, points that are not correctly collected (which is often the case in real applications)

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)



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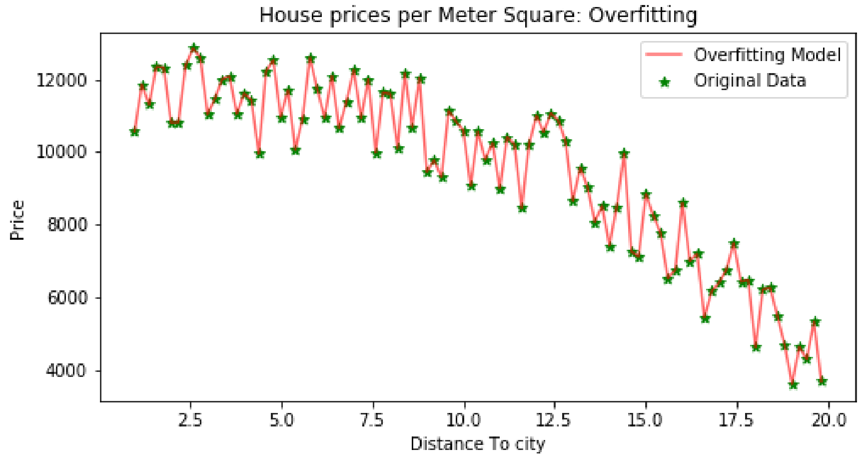

We can make an analogy to the student who "learns" the lecture mechanically without a real understanding.

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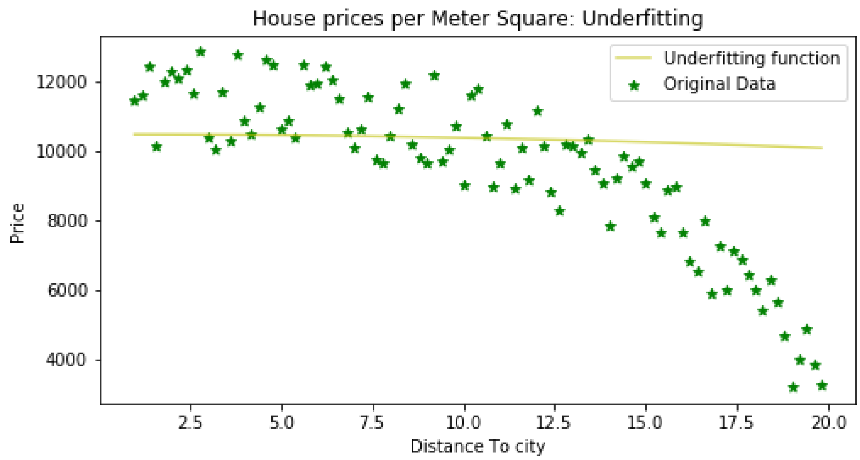

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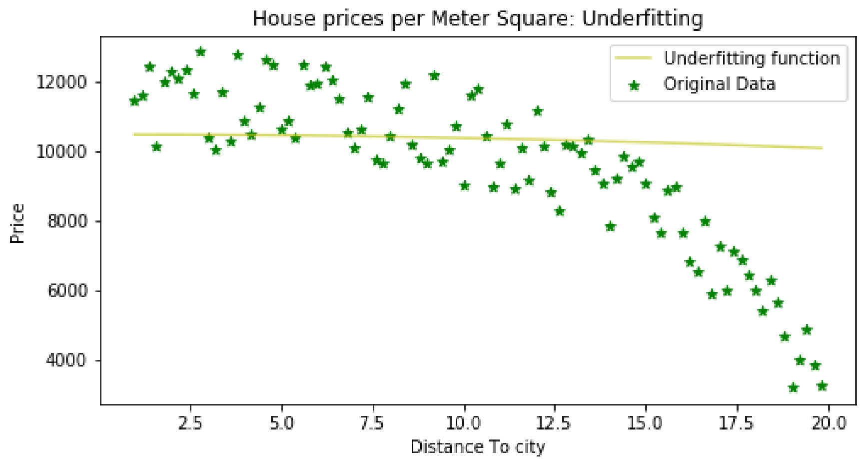
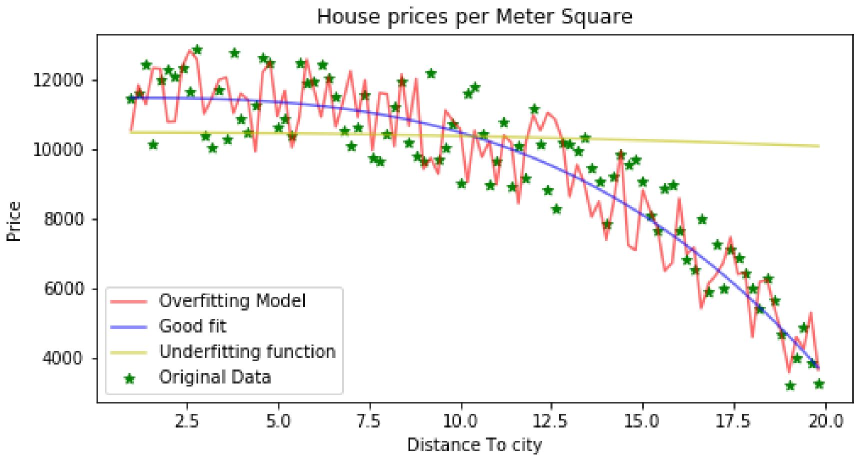


We can make an analogy to a lazy student who barely remember the lecture without any understanding

The Housing Prices Example: All Together



Overfitting, Underfitting, and a Good Fit

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- 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

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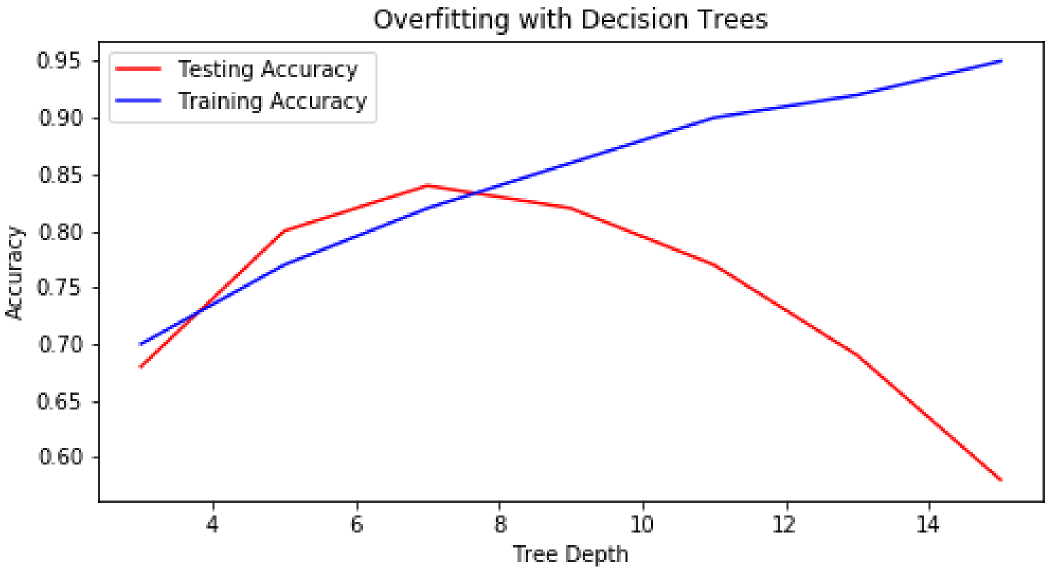

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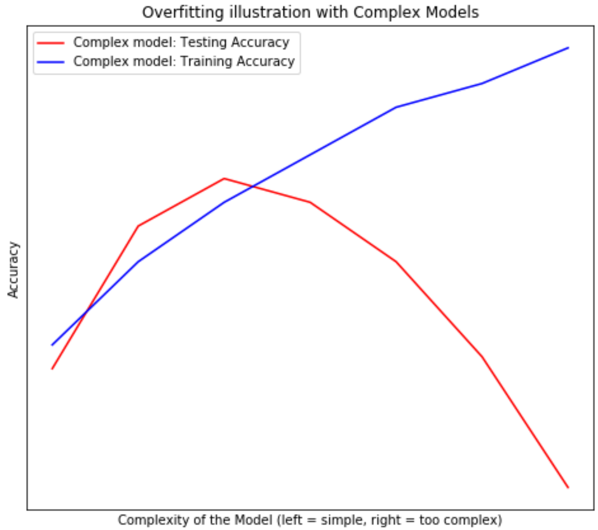
- Testing accuracy increases at the beginning until a certain value (depth $= 7$), the it decreases afterwards
- This happens because with longer trees, the model can classify correctly more examples in the training set, however, this includes noise.

Overfitting Based on the Complexity of the Model

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

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- 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?

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

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- Most ML libraries offer the possibility to control the complexity with a regularization parameter

Ockham's Razor Principle

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

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- When using polynomials (as a hypothesis space), lower degrees seems to be simpler
- In other cases it is very hard to define simplicity

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Complexity/Quality/Overfitting Tradeoff

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  - 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

Part 2: Interpretability

Motivation

The COMPAS Tool

MIT Technology Review

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TECH POLICY

AI is sending people to jail—and getting it wrong

Using historical data to train risk assessment tools could mean that machines are copying the mistakes of the past.

By Karen Hao January 21, 2019

IAN WALDIE/GETTY IMAGES

Increasing Number of Real Life and Social AI Applications

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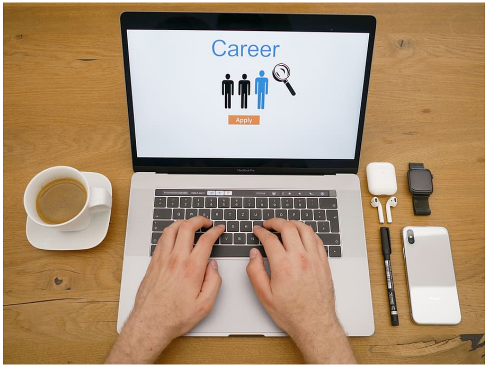

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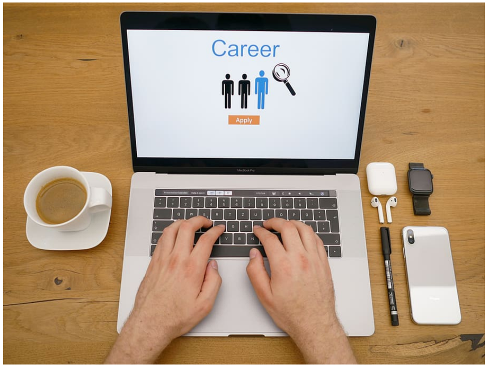

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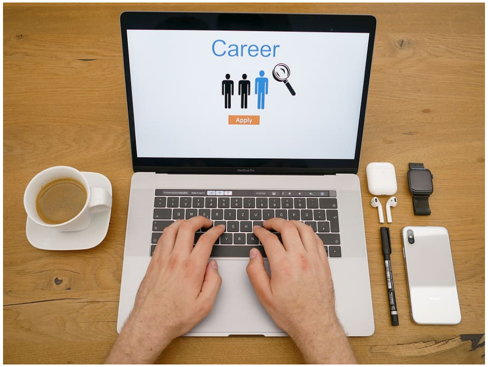

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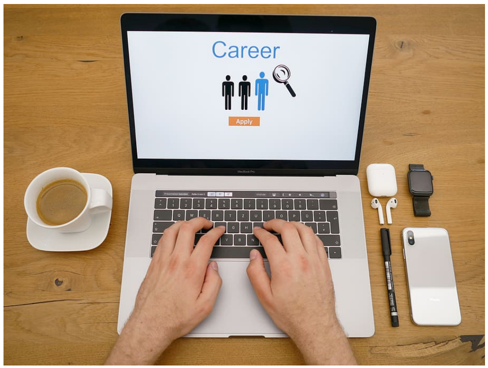

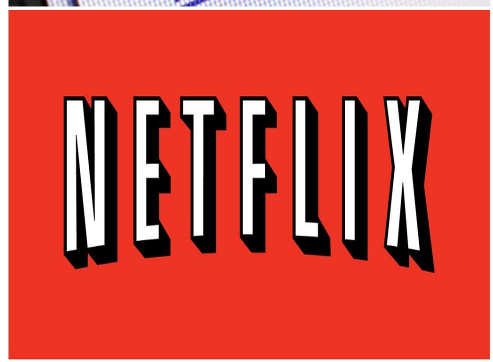

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  - Job applications: AI that parses CVs for software engineers and recommends to hire mostly men
  - Credit scoring: AI that gives a credit score (for bank loans and credit applications) that recommends people from a particular geographical region, 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

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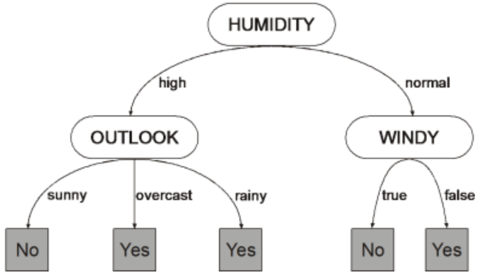

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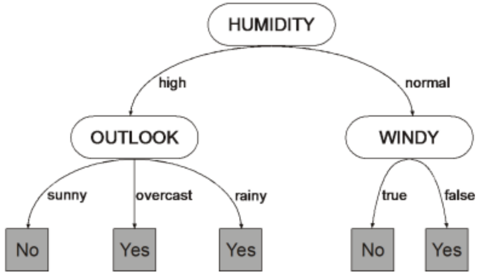

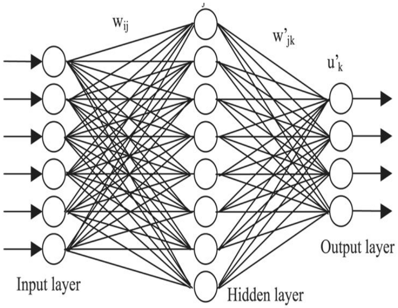

Definitions [3]

- **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?

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- **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

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Example of Rule List found by FairCORELS

- Data : `https://www.kaggle.com/danofer/compass`
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```
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 $= 0.681$, $\mathrm{UNF}_{\mathrm{EOdds}} = 0.217$ and $\mathrm{UNF}_{\mathrm{CUAE}} = 0.046$

Interpretable Models

Case Study: Decision Trees

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- Without loss of generality, we use the term 'positive' for the class 1 and 'negative' for the class 0
- The data is a collection of examples $\{e_1, \dots, e_n\}$

Toy Example: The Likelihood of Animal Extinction

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Big Size	Carnivore	Seasonal Reproduction	Solitary	Extinct
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- Data= $\{e_1, e_2, \ldots e_7\}$

Definition of Decision Tree (in the case of binary classification)

- A decision tree is a binary tree where each leaf node corresponds to a binary value (positive/negative class) and each internal node j is associated to a feature $feature(j) \in \mathbb{F}$
- Let DT be a decision tree. Denote by $feature(j)$ the feature associated to node j in DT. We name the children of an internal node j as right and left. We also use $(j, r(j))$ ($(j, l(j))$ respectively) to denote the arc from a node j to its right (respectively left) child .

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- This definition can be extended to multiple classification and regression (by adapting the leaf values)

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- We are looking for a partial Boolean function g over the set of possible partial Boolean functions $\mathbb{S}$ defined over k features that meet the criteria of the decision tree. In this case $\mathbb{S}$ is the search space
- The size of the search space is $|\mathbb{S}|$
- With k features, there are 2^k possible Boolean function (outputs of the associated truth table). This is because a truth table is determined by the binary string corresponding to the output and because there are 2^k possible strings
- Out of $z = 2^k$ Boolean function we are looking for a partial Boolean function that meet the requirements.

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- This is a gigantic number!

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- Most of the approaches are greedy (heuristic) approaches
- Greedy algorithms follow a top-down approach: at each step, choose the best feature (to split the data) then recursively apply the same for the children until a certain stopping criterion

Building a decision Tree

- Decision trees can be represented as follows $(f, right, left)$ where f is a feature and $right$ (respectively $left$) are either decision trees or binary values (an outcome)
- We use the following oracles (functions):
  - $SelectBestFeature(data)$: select the best splitting feature according to some criterion
  - $UpdateInformation(Tree, Node)$: update information related to a given stopping requirement
  - $SelectClass(\mathbb{E})$: returns a class according to a selection criterion
  - $Explore(\mathbb{E}, info)$) a Boolean that indicates if the algorithm should develop more the tree
- The following is a high level greedy algorithm:

Building a decision Tree: A Greedy Algorithm

Algorithm 1 GREEDY

Require: $\mathbb{F} = \{f_1, \ldots f_k\}$, $\mathbb{E} = \{e_1, \ldots e_n\}$, a parent node *parent*, and an information $info$ regarding the stopping conditions

Result: A decision tree

if $Explore(\mathbb{E}, info))$ **then**

Building a decision Tree: A Greedy Algorithm

Algorithm 2 GREEDY

Require: $\mathbb{F} = \{f_1, \dots f_k\}$, $\mathbb{E} = \{e_1, \dots e_n\}$, a parent node *parent*, and an information $info$ regarding the stopping conditions

Result: A decision tree

if $Explore(\mathbb{E}, info))$ **then**

$f_j \leftarrow SelectBestFeature(data)$

Building a decision Tree: A Greedy Algorithm

Algorithm 3 GREEDY

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if $Explore(\mathbb{E}, info))$ **then**

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$L \leftarrow \{x \in E | f_j = 0\}$; $R \leftarrow \{x \in E | f_j = 1\}$;

Building a decision Tree: A Greedy Algorithm

Algorithm 4 GREEDY

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Result: A decision tree

if $Explore(\mathbb{E}, info))$ **then**

$f_j \leftarrow SelectBestFeature(data)$

$L \leftarrow \{x \in E | f_j = 0\}$; $R \leftarrow \{x \in E | f_j = 1\}$;

$LeftInfo \leftarrow UpdateInformation(L, parent)$;

Building a decision Tree: A Greedy Algorithm

Algorithm 5 GREEDY

Require: $\mathbb{F} = \{f_1, \ldots f_k\}$, $\mathbb{E} = \{e_1, \ldots e_n\}$, a parent node *parent*, and an information $info$ regarding the stopping conditions

Result: A decision tree

if $Explore(\mathbb{E}, info))$ **then**

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Building a decision Tree: A Greedy Algorithm

Algorithm 6 GREEDY

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Result: A decision tree

if $Explore(\mathbb{E}, info))$ **then**

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$L \leftarrow \{x \in E | f_j = 0\}$; $R \leftarrow \{x \in E | f_j = 1\}$;

$LeftInfo \leftarrow UpdateInformation(L, parent)$;

$RightInfo \leftarrow UpdateInformation(R, parent)$;

$LeftTree \leftarrow GREEDY(\mathbb{F} \setminus f_j, L, f_j, LeftInformation)$;

Building a decision Tree: A Greedy Algorithm

Algorithm 7 GREEDY

Require: $\mathbb{F} = \{f_1, \ldots f_k\}$, $\mathbb{E} = \{e_1, \ldots e_n\}$, a parent node *parent*, and an information $info$ regarding the stopping conditions

Result: A decision tree

if $Explore(\mathbb{E}, info))$ **then**

$f_j \leftarrow SelectBestFeature(data)$

$L \leftarrow \{x \in E | f_j = 0\}$; $R \leftarrow \{x \in E | f_j = 1\}$;

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Building a decision Tree: A Greedy Algorithm

Algorithm 8 GREEDY

Require: $\mathbb{F} = \{f_1, \ldots f_k\}$, $\mathbb{E} = \{e_1, \ldots e_n\}$, a parent node *parent*, and an information $info$ regarding the stopping conditions

Result: A decision tree

if $Explore(\mathbb{E}, info))$ **then**

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$LeftInfo \leftarrow UpdateInformation(L, parent)$;

$RightInfo \leftarrow UpdateInformation(R, parent)$;

$LeftTree \leftarrow GREEDY(\mathbb{F} \setminus f_j, L, f_j, LeftInformation)$;

$RightTree \leftarrow GREEDY(\mathbb{F} \setminus f_j, R, f_j, RightInformation)$;

return $(f_j, LeftTree, RightTree)$

else

return $SelectClass(\mathbb{E})$

end if;

Information Gain

- There are several ways to choose a 'good' feature
- The Information Gain is one of the most used criterion
- It uses the notion of Entropy that evaluates data uncertainty (initially proposed in the context of information theory by Shanon and Weaver)

Entropy

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- In the other extreme, a coin with heads on both sides has no uncertainty because of the constant outcome (always heads)
- In this case, $Entropy = 0$

Entropy

Let Y be a discrete random variable taking values y_j, the entropy of Y is defined as follows:

$$H(Y) = \sum_j P(y_j) \times log_2(1/P(y_j))$$

where $P(y_j)$ is the probability of the value y_j
Example: For a fair coin:

$$H(Y) = 0.5 \times log_2(2) + 0.5 \times log_2(2) = 1$$

For a coin with 90% with heads chance:

$$H(V) = 0.9 \times log_2(10/9) + 0.1 \times log_2(10) = 0.46$$

Entropy in the case of binary decision trees

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- Back to binary classification with a set E of n examples containing a positive examples and b negative examples. Consider the classification outcome as a random variable. We denote the entropy of this Boolean random variable as $H(data)$
- For a feature f_j, we define $n_1 = |E_1|$ where $E_1 = E \setminus \{x|x_j = 1\}$ and $n_0 = |E_0|$ where $E_0 = E \setminus \{x|x_j = 0\}$. We also denote by a_1 (respectively a_0) the number of positive examples in E_1 (respectively E_0) and by b_1 (respectively b_0) the number of negative examples in E_1 (respectively E_0)

Entropy in the case of binary decision trees

The expected entropy after splitting the data with the f_j is

$$Remaining(f_j) = n_1/n \times H(E_1) + n_0/n \times H(E_0)$$

We are looking for a feature that has a low level of uncertainty when splitting the data. A good splitter f_j is a feature with a minimum value of $Remaining(f_j)$ (this measures how much uncertainty is removed from the data).
This is equivalent to maximizing the *information gain (IG)*:

$$IG(f_j) = 1 - Remaining(f_j)$$

Exercise: The Likelihood of Animal Extinction

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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
0	1	1	0	yes
1	1	1	0	no

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- Build a decision tree with the previous approach where the the height is at most 3, and the classification follows a majority rule

Back to Greedy Algorithms

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- *Gini Index (GI)* reflects the purity of the data. The values range from 0 to 1 where 0 represents a pure data (with one class), 1 represents a random distribution, and 0.5 represents a completely equal distribution. The chosen split is to the one that minimzes the GI
- Both algorithms are efficient in practice, however without guarantee of optimality
- A trend is observed recently to build optimal DTs (for instance [6, 7])

Pruning as a post processing

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- The post processing might include other operations such as removing redundant sub-trees and useless splits

Ensemble Learning, Random Forest, and Boosted Trees

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- Bagging is a technique that learns several models by randomly selecting a subset of the data for each model. The predictions are made based on majority vote (in case of binary classification). In the case of bagging with decision trees, the model is called random forest.
- Boosting is a technique that learns several models in a sequence where each model relies on the mistakes of the previous ones to improve the quality of the learning. Usually, when boosting a model, each example is weighted by how many times it is badly classified in order to give it an advantage.

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- The linear model is a line on a two dimensional plane
- Let $E = \{(x_1, y1), \dots (x_n, y_n)\}$. The optimisation problem (considered here) is to find a function $h_{a,b} = a \times x + b$ that minimizes the following loss function (Sum of Square Error):

$$Loss_{h_{a,b}} = \sum_i (y_i - h_{a,b}(x_i))^2$$

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- There are two unique solutions:

$$a = \frac{n \times (\sum x_i \times y_j) - \sum x_i \times \sum y_i}{n \times \sum x_i^2 - (\sum x_i)^2}$$

$$b = \frac{\sum y_i - a \times \sum x_i}{n}$$

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- The gradient descent method can be seen as a local a search approach

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- The algorithm stops when a certain stopping criterion is met
- Note that local search suffer from local minimums
- A common way to handle this issue is to restart search from time to time

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- Stop until a certain criterion is met
- The slope $\frac{\partial p}{\partial p_i}$ is usually amplified by a regulator α that is called a step size

Interpretability vs. Explanability

The Debate & The 1 Million Dollars Reward

nature machine intelligence

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Perspective | Published: 13 May 2019

Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead

Cynthia Rudin

Nature Machine Intelligence **1**, 206–215 (2019) | Cite this article

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A preprint version of the article is available at arXiv.

https://www.youtube.com/watch?v=4oXFEDoEcAk

Back to Interpretable Models: Examples

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- Rule lists

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- Decision trees, Linear Models, but also:
- Rule lists
- Decision list
- Binary Decision Diagram (very useful to handle redundancy with decision trees)
- ...

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- Rule lists: an ordered list of if-then-else rules with a default prediction.

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  1. **If 'Carnivore' then Extinct**
  2. **Else If 'Solitary' and not 'Big Size' then Not Extinct**
  3. **Else Extinct**

Back to Interpretable Models: Decision Lists

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- Decision Lists: a set of if-then-else rules without any specific order. The prediction is made following a majority rule or a random choice if needed (e.g., if an example satisfies two different rules).
- For example: **{If 'Carnivore' then Extinct; If 'Solitary' and not 'Big Size' then Not Extinct ; If 'Seasonal Reproduction' then Extinct }**
- Consider an example that is 'Carnivore', follows a 'Seasonal Reproduction', 'Solitary', and does not have a 'Big Size'. Two rules classify the example positively (Extinct) and one rule classifies it negatively (Not Extinct). In this case the majority vote is used and the prediction is positive (Extinct).

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- **Mandatory criteria in high-stake decision making**

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- Very complex (and philosophical) notion (see for instance the interview with Richard Feynman on the 'Why' question `https://www.youtube.com/watch?v=36GT2zI8lVA`)
- To explain predictions one need a clear context to define explanations (user defined)
- In machine learning, we usually use a subset of the example that are 'responsible' for the prediction. That is, changing their values would change the prediction
- Explainability can be applied to black box models as a post processing step

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- It gets worse! Since different explanations can be used, one might pick a particular explanation to hide model biases (this is observed with many commercial tools!)
- Imagine a credit score black box model where a client might have several explanations regarding the refusal. The company might pick an explanation that doesn't show certain bias (such as predictions based on the gender)

Back to Interpretability

- Interpretability guarantees the transparency of the explanations
- No post-processing (in the sense of probing the model) is necessary for explanations. It is enough to look at the model
- However sometimes the explanations are not optimal (in the size of set inclusion). In this case, a user might ask for minimal explanations. This task can be done as a post-processing step
- Unfortunately, interpretable models (so far) are not adapted to all applications (for instance in tumor detection and computer vision). Such applications depend heavily on recent advances of black box models

Think about it..

Geoffrey Hinton
@geoffreyhinton

Suppose you have cancer and you have to choose between a black box AI surgeon that cannot explain how it works but has a 90% cure rate and a human surgeon with an 80% cure rate. Do you want the AI surgeon to be illegal?

8:37 PM · Feb 20, 2020 · Twitter Web App