# Machine Learning with Python MTH786U/P 2023/24 

## Week 12: Decision Trees

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## How can we deal with data like this one?

| Shadow | Garlic | Complexion Accent | Vampire |  |
| :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No |
| Yes | Yes | Ruddy | None | No |
| $?$ | No | Ruddy | None | Yes |
| No | No | Average | Heavy | Yes |
| $?$ | No | Average | Odd | Yes |
| Yes | No | Pale | Heavy | No |
| Yes | No | Average | Heavy | No |
| $?$ | Yes | Ruddy | Odd | No |

## Issues

All data is categorical

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Some features might not matter

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Some features might be important only is some cases

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Some features might not matter
Some features might be important only is some cases

Cost associated to different "measurements" to assess different features might not be the same

## Identification trees

Identification trees offer a solution to these problems

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## Identification trees

What are the characteristics of a good identification tree?

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Classify the data well with a small number of "tests" (called stumps)

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The longer the tree the higher the probability of overfitting

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Classify the data well with a small number of "tests" (called stumps)

The longer the tree the higher the probability of overfitting

How do we select the number and order of tests to do?!

## Identification trees

Let see how each test perform at the first level

## Identification trees

Let see how each test perform at the first level


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If they have a shadow they appear not to be vampires.

## Identification trees

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Let see how each test perform at the first level


## Identification trees

Which is the best to use?


| Accent |  |  |
| :---: | :---: | :---: |
| None |  | Odd |
| 1 Y | 1 Y | 1 Y |
| 2 N | 2 N | 1 N |

We should look for tests that divide the sample in homogenous samples

## Identification trees

Which is the best to use?


Idea: let us use a "score" of each test the number of samples that are split in homogenous classes

## Identification trees

Which is the best to use?


## Identification trees

Which is the best to use?


Number of samples that are classified in a homogenous class

## Identification trees

Which is the best to use?


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We can then select it as the root of the tree

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Identification trees


## Identification trees



We can apply the same method to the branch that is not homogenous

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| $?$ | No | Ruddy | None | Yes |
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## Identification trees



|  | Remaining |  |  | data |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| Shadow | Garlic | Complexio <br> n | Accent | Vampire |  |
| $?$ |  | Pale | None | No |  |
| $?$ | Yes | No | Ruddy | None | Yes |
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## Identification trees



Remaining data

| Shadow | Garlic | Complexio <br> n | Accent | Vampire |
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## Identification trees

What is the score of each second test?

Shadow

## Identification trees



## Identification trees

In real application it is rare to find perfectly homogenous classes

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What can we do? We need a less strict scoring system

## Identification trees

In real application it is rare to find perfectly homogenous classes

What can we do? We need a less strict scoring system

Idea: perfect homogenous branches are great, but we can a measure of disorder more in general

## Quantifying disorder

We can use metrics from information theory

$$
D(\text { set })=-\frac{P}{T} \log _{2}\left(\frac{P}{T}\right)-\frac{N}{T} \log _{2}\left(\frac{N}{T}\right)
$$

## Quantifying disorder

We can use metrics from information theory

$$
D(\text { set })=-\frac{P}{T} \log _{2}\left(\frac{P}{T}\right)-\frac{N}{T} \log _{2}\left(\frac{N}{T}\right)
$$

Where D is the disorder, P are the positive samples, N the negative samples, and T the total number of samples $T=P+N$

## Quantifying disorder

How does $D$ looks like as function of $P / T$ ?

$$
D(\text { set })=-\frac{P}{T} \log _{2}\left(\frac{P}{T}\right)-\frac{N}{T} \log _{2}\left(\frac{N}{T}\right)
$$



## Quantifying disorder

How does $D$ looks like as function of $P / T$ ?

$$
D(s e t)=-\frac{P}{T} \log _{2}\left(\frac{P}{T}\right)-\frac{N}{T} \log _{2}\left(\frac{N}{T}\right)
$$

If $P=N$ ?


## Quantifying disorder

How does $D$ looks like as function of $P / T$ ?

$$
\begin{aligned}
& D(\text { set })=-\frac{P}{T} \log _{2}\left(\frac{P}{T}\right)-\frac{N}{T} \log _{2}\left(\frac{N}{T}\right) \\
& \text { If } \mathrm{P}=\mathrm{N} \text { ? } \\
& \qquad D(\text { set })=-\frac{1}{2} \log _{2}\left(\frac{1}{2}\right)-\frac{1}{2} \log _{2}\left(\frac{1}{2}\right)
\end{aligned}
$$



## Quantifying disorder

How does $D$ looks like as function of $P / T$ ?

$$
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& \text { If } \mathrm{P}=\mathrm{N} \text { ? } \\
& \qquad \begin{aligned}
D(\text { set }) & =-\frac{1}{2} \log _{2}\left(\frac{1}{2}\right)-\frac{1}{2} \log _{2}\left(\frac{1}{2}\right) \\
& =\frac{1}{2}+\frac{1}{2}=1
\end{aligned}
\end{aligned}
$$



## Quantifying disorder

How does $D$ looks like as function of $P / T$ ?

$$
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$$

If $\mathrm{P}=\mathrm{N}$ ?

$$
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& \text { If } \mathrm{P}=0 ? \quad D(\text { set })=0 \\
& \text { If } \mathrm{P}=\mathrm{T} ? \quad D(\text { set })=0
\end{aligned}
$$



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So the quality of a test can we written as

$$
Q=\sum_{s} D(s)
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Q=\sum_{s} D(s) \frac{N_{s}}{N_{t}}
$$

## Quantifying disorder

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$$
Q=\sum_{s} D(s)
$$

It is however better to have a normalized quantity according to the number of samples

$$
Q=\sum_{s} D(s) \frac{N_{s}}{N_{t}}
$$

Where we have $N_{s}$ as the number of samples in the set and $N_{t}$ as the total number of samples that enters the test

## Identification trees

What is the value of Q in this case? In this case, the smallest the better!


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## Identification trees

What is the value of Q in this case?


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What is the value of Q in this case?


## Identification trees

What is the score of each second test?

Shadow

## Identification trees



## Identification trees



We can convert this tree into a set of rules to classify

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If Shadow ? and Garlic Y -> not a vampire

## Identification trees



We can convert this tree into a set of rules to classify

If Shadow ? and Garlic Y -> not a vampire<br>If Shadow ? and Garlic N -> vampire

## Identification trees



We can convert this tree into a set of rules to classify

```
If Shadow ? and Garlic Y -> not a vampire
If Shadow ? and Garlic N -> vampire
```

Note: we might not need both rules in practice In our data if Garlic is $N$ we have a vampire independently of the Shadow

## Quantifying disorder

There are also other metrics such as the Gini impurity

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Let us consider a group of N items

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We can define the probability $p_{i}$ for each category as $p_{i}=\frac{N_{i}}{N}$

## Quantifying disorder

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Let us consider a group of N items
Let us assume that they belong to one of K categories
We can define the probability $p_{i}$ for each category as $p_{i}=\frac{N_{i}}{N}$
The Gini impurity of this population is then defined as

## Quantifying disorder

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Let us consider a group of N items
Let us assume that they belong to one of K categories
We can define the probability $p_{i}$ for each category as $p_{i}=\frac{N_{i}}{N}$
The Gini impurity of this population is then defined as

$$
G I=1-\sum_{i=1}^{k} p_{i}^{2}
$$

## Quantifying disorder

In this example $N=7$

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$$
p_{\text {red }}=\frac{4}{7}
$$

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$$
p_{\text {red }}=\frac{4}{7} \quad p_{\text {violet }}=\frac{2}{7}
$$

## Quantifying disorder

In this example $N=7$

$$
p_{\text {red }}=\frac{4}{7} \quad p_{\text {violet }}=\frac{2}{7} \quad p_{\text {orange }}=\frac{1}{7}
$$

## Quantifying disorder

In this example $N=7$

$$
p_{\text {red }}=\frac{4}{7} \quad p_{\text {violet }}=\frac{2}{7} \quad p_{\text {orange }}=\frac{1}{7}
$$

Thus

## Quantifying disorder

In this example $N=7$

$$
p_{\text {red }}=\frac{4}{7} \quad p_{\text {violet }}=\frac{2}{7} \quad p_{\text {orange }}=\frac{1}{7}
$$

Thus

$$
G I=1-\left(\frac{4}{7}\right)^{2}-\left(\frac{2}{7}\right)^{2}-\left(\frac{1}{7}\right)^{2}=1-\frac{21}{49}=0.57
$$

## Quantifying disorder

In this example, they are all different $\quad K=N=7$

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$$
p_{i}=\frac{1}{N}
$$

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$$
p_{i}=\frac{1}{N}
$$

Thus

## Quantifying disorder

In this example, they are all different $\quad K=N=7$

$$
p_{i}=\frac{1}{N}
$$

Thus

$$
G I=1-\sum_{i=1}^{K} \frac{1}{N^{2}}=1-\frac{K}{N^{2}}=1-\frac{N}{N^{2}}=1-\frac{1}{N}=\frac{N-1}{N} \sim 1
$$

## Quantifying disorder

In this example, they are all the same

$$
N=7 \quad K=1
$$

## Quantifying disorder

In this example, they are all the same

$$
N=7 \quad K=1
$$

$$
p_{1}=1
$$

## Quantifying disorder

In this example, they are all the same

$$
N=7 \quad K=1
$$

$$
p_{1}=1
$$

Thus

## Quantifying disorder

In this example, they are all the same

$$
N=7 \quad K=1
$$

$$
p_{1}=1
$$

Thus

$$
G I=1-p_{1}^{2}=0
$$

## Quantifying disorder

In this example, they are all the same

$$
\begin{array}{ll}
N=7 \quad K=1 & \\
& p_{1}=1
\end{array}
$$

Thus

$$
G I=1-p_{1}^{2}=0
$$

Hence, the Gini impurity is zero for "pure" samples and 1 for maximally "impure"

## Quantifying disorder

What is the Gini impurity of the outcome of each test?


## Quantifying disorder

What is the Gini impurity of the outcome of each test?


We have, in this case, three groups (leafs), we start by computing their Gl

## Quantifying disorder

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What is the Gini impurity of the outcome of each test?


$$
G I_{?}=1-\left(\frac{2}{4}\right)^{2}-\left(\frac{2}{4}\right)^{2}=\frac{1}{2}
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?


$$
G I_{?}=1-\left(\frac{2}{4}\right)^{2}-\left(\frac{2}{4}\right)^{2}=\frac{1}{2} \quad G I_{Y}=0
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?


$$
G I_{?}=1-\left(\frac{2}{4}\right)^{2}-\left(\frac{2}{4}\right)^{2}=\frac{1}{2} \quad G I_{Y}=0 \quad G I_{N}=0
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?


$$
G I_{?}=1-\left(\frac{2}{4}\right)^{2}-\left(\frac{2}{4}\right)^{2}=\frac{1}{2} \quad G I_{Y}=0 \quad G I_{N}=0
$$

We can combined them using a weighted average, considering the different number of people in each leaf

Quantifying disorder


$$
G I_{\text {shadow }}=w_{?} G I_{?}+w_{Y} G I_{Y}+w_{N} G I_{N}
$$

Quantifying disorder


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Quantifying disorder


$$
\begin{aligned}
G I_{\text {shadow }}=w_{?} G I_{?}+w_{Y} G I_{Y}+w_{N} G I_{N} & \\
& w_{?}=\frac{4}{8}=\frac{1}{2}
\end{aligned} w_{Y}=\frac{3}{8} \quad w_{N}=\frac{1}{8}
$$

Quantifying disorder

$$
G I_{\text {shadow }}=w_{?} G I_{?}+w_{Y} G I_{Y}+w_{N} G I_{N} \quad \text { Shadow } \quad w_{N}=\frac{1}{8}
$$

## Quantifying disorder

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$$
G I_{Y}=0
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?
$G I_{Y}=0$


## Quantifying disorder

What is the Gini impurity of the outcome of each test?

$$
\begin{gathered}
\text { Garlic } \\
G I_{Y}=0 \quad G I_{N}=1-\left(\frac{3}{5}\right)^{2}-\left(\frac{2}{5}\right)^{2}=0.48 \\
G I_{\text {garlic }}=w_{N} G I_{N}+w_{Y} G I_{Y}=\frac{5}{8} 0.48=0.3
\end{gathered}
$$

## Quantifying disorder

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## Quantifying disorder

What is the Gini impurity of the outcome of each test?

|  | Complexion |
| :---: | :---: |
| Pale |  |
| 2 N | 1 N |
|  | 2 Y |

$$
G I_{\text {Pale }}=0 \quad G I_{\text {ave }}=1-\left(\frac{1}{3}\right)^{2}-\left(\frac{2}{3}\right)^{2}=0.44
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?


$$
G I_{\text {Pale }}=0 \quad G I_{\text {ave }}=1-\left(\frac{1}{3}\right)^{2}-\left(\frac{2}{3}\right)^{2}=0.44 \quad G I_{\text {ruddy }}=0.44
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?

$$
\begin{gathered}
\text { Complexion } \\
G I_{\text {Pale }}=0 \quad G I_{\text {ave }}=1-\left(\frac{1}{3}\right)^{2}-\left(\frac{2}{3}\right)^{2}=0.44 \quad G I_{\text {ruddy }}=0.44 \\
G I_{\text {complexion }}=2 \frac{3}{8} 0.44=0.33
\end{gathered}
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?


## Quantifying disorder

What is the Gini impurity of the outcome of each test?


$$
G I_{\text {none }}=0.44
$$

## Quantifying disorder

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## Quantifying disorder

What is the Gini impurity of the outcome of each test?

| Accent |  |  |
| :---: | :---: | :---: |
| None |  | dd |
| 1 Y | 1 Y | 1 Y |
| 2 N | 2 N | 1 N |

$$
G I_{\text {none }}=0.44
$$

$$
G I_{\text {heavy }}=0.44
$$

$$
G I_{o d d}=0.5
$$

## Quantifying disorder

What is the Gini impurity of the outcome of each test?

$$
\begin{gathered}
\text { Accent } \\
G I_{\text {none }}=0.44 \quad \text { Odd } \\
2 \mathrm{~N} \quad 2 \mathrm{~N} \\
G I_{\text {heavy }}=0.44 \\
G I_{\text {complexion }}= \\
\hline \frac{3}{8} 0.44+\frac{2}{8} 0.5=0.45
\end{gathered} \quad G I_{\text {odd }}=0.5
$$

## Identification trees

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Imagine that we have another variable that takes numeric values

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We can set a threshold and transform the variable in categorical

## Identification trees

What if we have numeric values? Can we use the method?

Imagine that we have another variable that takes numeric values


We can set a threshold and transform the variable in categorical How do I select such threshold?

## Identification trees

Imagine that we get another variable

| Shadow | Garlic | Complexion Accent | Height | Vampire |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | 162 | No |
| Yes | Yes | Ruddy | None | 173 | No |
| $?$ | No | Ruddy | None | 198 | Yes |
| No | No | Average | Heavy | 185 | Yes |
| $?$ | No | Average | Odd | 197 | Yes |
| Yes | No | Pale | Heavy | 187 | No |
| Yes | No | Average | Heavy | 175 | No |
| $?$ | Yes | Ruddy | Odd | 168 | No |

## Identification trees

We first order the data according to the numeric values

| Height | Vampire |
| :--- | :--- |
|  |  |
| 162 | No |
| 168 | No |
| 173 | No |
| 175 | No |
| 185 | Yes |
| 187 | Yes |
| 197 | Yes |
| 198 | Yes |

## Identification trees

Then we compute the average for each pair

| Height | Vampire |
| :--- | :--- |
|  |  |
| 162 | No |
| 168 | No |
| 173 | No |
| 175 | No |
| 185 | Yes |
| 187 | Yes |
| 197 | Yes |
| 198 | Yes |

## Identification trees

Then we compute the average for each pair

| Height |  | Vampire |
| :---: | :--- | :--- |
| 165162 | No |  |
| 170.5 | 168 | No |
| 174 | No |  |
| 170 | 175 | No |
| 186 | 185 | Yes |
| 192 | Yes |  |
| 197.5 | 197 | Yes |
| 198 | Yes |  |

## Identification trees

The we use each average as threshold and compute the disorder of the test done with that value

|  | Height | Vampire |
| :--- | :--- | :--- |
| 165 | 162 | No |
| 170.5 | 168 | No |
| 174 | 173 | No |
| 180 | 175 | No |
| 186 | 185 | Yes |
| 192 | 187 | Yes |
| 197.5 | 197 | Yes |
| 198 | Yes |  |



## Identification trees

The we use each average as threshold and compute the disorder of the test done with that value

| Height |  |  |
| :--- | :--- | :--- |
|  | Vampire |  |
| 165 | 162 | No |
| 170.5 | 168 | No |
| 174 | 173 | No |
| 180 | 185 | No |
| 186 | 185 | Yes |
| 192 | 187 | Yes |
| 197.5 | Yes |  |
| 198 | Yes |  |



## Identification trees

The we use each average as threshold and compute the disorder of the test done with that value

| Height |  |  |
| :--- | :--- | :--- |
|  | Vampire |  |
| 165 | 162 | No |
| 170.5 | 168 | No |
| 174 | 173 | No |
| 180 | 185 | No |
| 186 | 185 | Yes |
| 192 | 187 | Yes |
| 197.5 | Yes |  |
| 198 | Yes |  |



## Identification trees

The we use each average as threshold and compute the disorder of the test done with that value

|  | Height | Vampire |
| :--- | :--- | :--- |
| 165 | 162 | No |
| 170.5 | 168 | No |
| 174 | No |  |
| 173 | 175 | No |
| 186 | 185 | Yes |
| 192 | 187 | Yes |
| 197.5 | Yes |  |
| 198 | Yes |  |

$$
\begin{gathered}
\text { Height<165 } \\
G I_{Y}=0 \quad 3 \mathrm{Y} \\
G I_{\text {Height }<165}=\frac{7}{8} 0.49=0.42
\end{gathered}
$$

## Identification trees

We then try this with all possible values and get the smallest!

| Height |  |  |
| :---: | :--- | :--- |
|  | Vampire |  |
| 165 | 162 | No |
| 170.5 | 168 | No |
| 174 | No |  |
| 170 | 175 | No |
| 186 | 185 | Yes |
| 192 | Yes |  |
| 197.5 | Yes |  |
| 198 | Yes |  |

## Identification trees

Often numeric data is represented in this way


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Decision boundaries must be parallel to one of the axes! They are defined by a threshold


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## Identification trees

Nearest neighbors could give us this


Random forests

Trees are, as we saw, very simple and intuitive

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## Random forests

Trees are, as we saw, very simple and intuitive In their simplest form however they are inaccurate

They might be good in the training set, but they are not as good in validation

A possible solution (and there are many) is using so-called random forests!
Random forests are one of the many ensemble methods

## Random forests

The main idea of random forests is very similar to boostrapping for regressions

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They allow "sampling" data and many different identification trees by considering a random number of features

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They allow "sampling" data and many different identification trees by considering a random number of features

The classification is done considering a majority vote across many different trees

## Random forests

First step to build a random forest is to get a boostrapped dataset

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This is the same things we did for the regression case!

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First step to build a random forest is to get a boostrapped dataset
This is the same things we did for the regression case!

Pick $s$ samples at random with replacement from the original dataset

Random forests

| Shadow | Garlic | Complexio <br> n | Accent | Vampire |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No |  |
| Yes | Yes | Ruddy | None | No |  |
| $?$ | No | Ruddy | None | Yes |  |
| No | No | Average | Heavy | Yes |  |
| $?$ | No | Average | Odd | Yes |  |
| Yes | No | Pale | Heavy | No |  |
| Yes | No | Average | Heavy | No |  |
| $?$ |  | Yes | Ruddy | Odd | No |

Original dataset

Random forests

| Shadow | Garlic | Complexio <br> n | Accent | Vampire |
| :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No |
| Yes | Yes | Ruddy | None | No |
| $?$ | No | Ruddy | None | Yes |
| No | No | Average | Heavy | Yes |
| $?$ | No | Average | Odd | Yes |
| Yes | No | Pale | Heavy | No |
| Yes | No | Average | Heavy | No |
| $?$ | Yes | Ruddy | Odd | No |

Original dataset

## Random forests

| Shadow | Garlic | Complexio <br> n | Accent | Vampire |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No |
| Yes | Yes | Ruddy | None | No |
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| Yes | No | Average | Heavy | No |
| $?$ | Yes | Ruddy | Odd | No |



Original dataset
Boostrapped dataset

## Random forests

## Same sample are repeated!

| Shadow | Garlic | Complexio <br> n | Accent | Vampire |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No |  |
| Yes | Yes | Ruddy | None | No |  |
| $?$ | No | Ruddy | None | Yes |  |
| No | No | Average | Heavy | Yes |  |
| $?$ | No | Average | Odd | Yes |  |
| Yes | No | Pale | Heavy | No |  |
| Yes | No | Average | Heavy | No |  |
| $?$ |  | Yes | Ruddy | Odd | No |


| Shadow | Garlic | Complexion Accent | Vampire |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | No | No | Average | Heavy | Yes |
| $?$ | ? | No | Ruddy | None | Yes |
| No | No | Average | Heavy | Yes |  |
| ? |  | No | Average | Odd | Yes |
| Yes | No | Po | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |  |

Original dataset
Boostrapped dataset

## Random forests

Second step is to create decision trees from the bootstrapped dataset

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Second step is to create decision trees from the bootstrapped dataset

Key aspect: only a random number of variables are used!

Random forests
We could pick these two

| Shadow | Garlic | Complexion | Accent | Vampire |
| :---: | :---: | :---: | :---: | :---: |
| No | No | Average | Heavy | Yes |
| ? | No | Ruddy | None | Yes |
| ? | No | Ruddy | None | Yes |
| No | No | Average | Heavy | Yes |
| ? | No | Average | Odd | Yes |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |

## Random forests

Imagine that "shadow" is the best, between the two, to split the sample
So, it will be the root of our tree


| Shadow | Garlic | Complexion | Accent | Vampire |
| :--- | :--- | :--- | :--- | :--- |
| No | No | Average | Heavy | Yes |
| $? ?$ | No | Ruddy | None | Yes |
| $?$ | No | Ruddy | None | Yes |
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| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |

## Random forests

Imagine that "shadow" is the best, between the two, to split the sample
So, it will be the root of our tree


Then we keep building the tree by selecting again at random two other variables

| Shadow | Garlic | Complexion | Accent | Vampire |
| :--- | :--- | :--- | :--- | :--- |
| No | No | Average | Heavy | Yes |
| $? ?$ | No | Ruddy | None | Yes |
| $? ?$ | No | Ruddy | None | Yes |
| No | No | Average | Heavy | Yes |
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| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |

## Random forests

So we keep building the tree


| Shadow | Garlic | Complexion | Accent | Vampire |
| :--- | :--- | :--- | :--- | :--- |
| No | No | Average | Heavy | Yes |
| $?$ | No | Ruddy | None | Yes |
| $?$ | No | Ruddy | None | Yes |
| No | No | Average | Heavy | Yes |
| $?$ | No | Average | Odd | Yes |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |

## Random forests

So we keep building the tree


| Shadow | Garlic | Complexion | Accent | Vampire |
| :--- | :--- | :--- | :--- | :--- | :--- |
| No | No | Average | Heavy | Yes |
| $?$ | No | Ruddy | None | Yes |
| $?$ | No | Ruddy | None | Yes |
| No | No | Average | Heavy | Yes |
| $?$ | No | Average | Odd | Yes |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |
| Yes | No | Pale | Heavy | No |

We keep going as usual until we have found all the leafs

## Random forests

Then we go back to step 1 and repeat and get another tree many times


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Then we go back to step 1 and repeat and get another tree many times


This builds our forest!

## Random forests

The variety that of decision trees that we build it turns out to improve their precision

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But, how do we use it for real?

## Random forests

It is very simple, we get a new data point that we need to classify

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| :--- | :--- | :--- | :--- |
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## Random forests

It is very simple, we get a new data point that we need to classify

| Shadow | Garlic | Complexion Accent | Vampire |
| :--- | :--- | :--- | :--- |
| No | No | Average Heavy |  |

Then we run this data point in each decision tree in the forest

Random forests


## Random forests



In this simple case, the new data point is classified as a vampire 2 times over 3

Random forests


## Random forests



The option with the majority of "votes" is the solution!

## Random forests

Key question: how do we know or estimate the precision of the forest?

## Random forests

In the boostrapped dataset, how many samples are not selected, on average?

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Probability of NOT being selected after s draws is $\left(1-\frac{1}{s}\right)^{s} \xrightarrow{s \rightarrow \infty} \frac{1}{e}$
So, we can use this $36 \%$ of the data for evaluation!
This subsample is called out-of-bag sample

## Random forests

However, how do we pick the number of random variables to build the forest?

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We use this number of hyper-parameter and confront the out-of-bag error

## Random forests

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We use this number of hyper-parameter and confront the out-of-bag error

The starting point is often the square-root of the number of variables, then you consider values below and above this

## AdaBoost (adaptive boosting)

So far, we have used either one or multiple "full" decision trees

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It turns out that we can use many weak leaners (i.e., stumps) instead

We use a forest of stumps

## AdaBoost

This was our first full tree


## AdaBoost

In AdaBoost we will be using stumps


## AdaBoost VS random forest

In random forests, each tree had an equal weight on the final decision

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## AdaBoost VS random forest

In random forests, each tree had an equal weight on the final decision
In a forest of stumps made with AdaBoost, some will be considered as more important than others

In random forests, each tree was independent of the others
In a forest of stumps made with AdaBoost, order is key
In particular, the error that the first stump makes influence how the second stump is made, the error of the second stump influence the third etc..

AdaBoost
Let us now see how this is done

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Let us now see how this is done
We start adding a weight defining how important is to correctly classify each sample

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| Shadow | Garlic | Complexion | Accent | Vampire | Weight |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $? ?$ | Yes | Pale | None | No | $1 / 8$ |
| Yes | Yes | Ruddy | None | No | $1 / 8$ |
| $? ?$ | No | Ruddy | None | Yes | $1 / 8$ |
| No | No | Average | Heavy | Yes | $1 / 8$ |
| $?$ | No | Average | Odd | Yes | $1 / 8$ |
| Yes | No | Pale | Heavy | No | $1 / 8$ |
| Yes | No | Average | Heavy | No | $1 / 8$ |
| $?$ | Yes | Ruddy | Odd | No | $1 / 8$ |

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| $? ?$ | Yes | Pale | None | No | $1 / 8$ |
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| $?$ | No | Ruddy | None | Yes | $1 / 8$ |
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| $?$ | No | Average | Odd | Yes | $1 / 8$ |
| Yes | No | Pale | Heavy | No | $1 / 8$ |
| Yes | No | Average | Heavy | No | $1 / 8$ |
| $?$ | Yes | Ruddy | Odd | No | $1 / 8$ |

At the start each weight is the same: $\frac{1}{S}$

## AdaBoost

We then evaluate which stump does the best job classifying the data using a majority rule

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| Shadow | Garlic | Complexi <br> on | Accent | Vampire | Weight |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No | $1 / 8$ |
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| $?$ |  |  |  |  |  |

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We then evaluate which stump does the best job classifying the data using a majority rule


Classification

| Shadow | Garlic | Complexi <br> on | Accent | Vampire | Weight |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No | $1 / 8$ |
| Yes | Yes | Ruddy | None | No | $1 / 8$ |
| $? ?$ | No | Ruddy | None | Yes | $1 / 8$ |
| No | No | Average | Heavy | Yes | $1 / 8$ |
| $?$ |  |  |  |  |  |
| $?$ | No | Average | Odd | Yes | $1 / 8$ |
| Yes | No | Pale | Heavy | No | $1 / 8$ |
| Yes | No | Average | Heavy | No | $1 / 8$ |


| Yes | Ruddy | Odd | No | $1 / 8$ |
| :--- | :--- | :--- | :--- | :--- |

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We then evaluate which stump does the best job classifying the data using a majority rule


Classification If no -> yes

| Shadow | Garlic | Complexi <br> on | Accent | Vampire | Weight |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No | $1 / 8$ |
| Yes | Yes | Ruddy | None | No | $1 / 8$ |
| $?$ | No | Ruddy | None | Yes | $1 / 8$ |
| No | No | Average | Heavy | Yes | $1 / 8$ |
| $?$ | No | Average | Odd | Yes | $1 / 8$ |
| Yes | No | Pale | Heavy | No | $1 / 8$ |
| Yes | No | Average | Heavy | No | $1 / 8$ |
| $?$ |  |  |  |  |  |
|  | Yes | Ruddy | Odd | No | $1 / 8$ |

## AdaBoost

We then evaluate which stump does the best job classifying the data using a majority rule


Classification
If no -> yes
If yes -> no

| Shadow | Garlic | Complexi <br> on |  | Vccent | Vampire |
| :--- | :--- | :--- | :--- | :--- | :--- | Weight

## AdaBoost

We then evaluate which stump does the best job classifying the data using a majority rule


Classification
If no -> yes
If yes -> no
If ? -> yes (or no it is the same!)

| Shadow | Garlic | Complexi <br> on | Accent | Vampire | Weight |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No | $1 / 8$ |
| Yes | Yes | Ruddy | None | No | $1 / 8$ |
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| Yes | No | Pale | Heavy | No | $1 / 8$ |
| Yes | No | Average | Heavy | No | $1 / 8$ |
| $?$ |  |  |  |  |  |

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| Shadow | Garlic | Complexi <br> on | Accent | Vampire | Weight |
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| Yes | No | Pale | Heavy | No | $1 / 8$ |
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We then evaluate which stump does the best job classifying the data using a majority rule


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| $?$ |  |  |  |  |  |

## AdaBoost

We then which stump does the best job classifying the data

| Garlic |  |
| :---: | :---: |
|  | N |
| N | 3 Y |
|  | 2 N |

Classification

| If yes $->$ no | 2 mistakes |
| :--- | :--- |
| If no $->$ yes | 6 correct |


| Shadow | Garlic | Complexi <br> on |  | Vccent | Vampire | Weight |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No | $1 / 8$ |  |
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| Yes | No | Pale | Heavy | No | $1 / 8$ |  |
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| $?$ |  |  |  |  |  |  |
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We then which stump does the best job classifying the data


Classification
If Pale -> no
If Ave -> yes
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Since the stump made two mistakes and each data sample had the same weight t total error is

$$
E_{t}=\frac{1}{8}+\frac{1}{8}=\frac{1}{4}
$$

## AdaBoost

Using the total error of the stump we can calculate its weight as

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$$
w_{\text {stump }}=\frac{1}{2} \ln \left(\frac{1-E_{t}}{E_{t}}\right) \sim 0.54
$$

## AdaBoost

Using this information we can modify the weights of the samples

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$$
w_{s_{i}}=s_{i} e^{w_{\text {sump }}}=\frac{1}{8} e^{0.54} \sim 0.21
$$

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$$

We then decrease the sample weights for the correctly classified samples as

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$$
w_{s_{i}}=s_{i} e^{w_{\text {sump }}}=\frac{1}{8} e^{0.54} \sim 0.21
$$

We then decrease the sample weights for the correctly classified samples as

$$
w_{s_{i}}=s_{i} e^{-w_{\text {stump }}}=\frac{1}{8} e^{-0.54} \sim 0.07
$$

## AdaBoost

Hence, we will have

| Shadow | Garlic | Complexi <br> on |  | Accent | Vampire |
| :--- | :--- | :--- | :--- | :--- | :--- | Weight

We need to normalize the weight!

## AdaBoost

Hence, we will have

| Shadow | Garlic | Complexi <br> on |  | Accent | Vampire | Weight |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $?$ | Yes | Pale | None | No | 0.25 |  |
| Yes | Yes | Ruddy | None | No | 0.083 |  |
| $?$ | No | Ruddy | None | Yes | 0.083 |  |
| No | No | Average | Heavy | Yes | 0.083 |  |
| $?$ | No | Average | Odd | Yes | 0.083 |  |
| Yes | No | Pale | Heavy | No | 0.083 |  |
| Yes | No | Average | Heavy | No | 0.083 |  |
| $?$ |  |  |  |  |  |  |
|  | Yes | Ruddy | Odd | No | 0.25 |  |

## AdaBoost

Now we can create a boostrapped version of the sample, using the weights to sampling

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Then, we forget about the initial dataset, we set all the sample weights to zero and repeat

## AdaBoost

Hence, we will have a range of stumps, each with their weight

## AdaBoost

For example

$w_{\text {stump }}=0.4$
$w_{\text {stump }}=0.34$


## AdaBoost

Imagine we get a new data point, stumps on the left classify it as vampire, those on the left as not a vampire. We pick the classification by summing the weights of each stump!


$$
w_{\text {stump }}=0.54
$$



$$
w_{\text {stump }}=0.6
$$



$$
w_{\text {stump }}=0.3
$$



## AdaBoost

So, in this case, the data point will be classified as a vampire


$$
w_{\text {stump }}=0.54
$$


$w_{\text {stump }}=0.6$


$$
\begin{aligned}
& w_{\text {stump }}=0.4 \\
& \\
& w_{\text {stump }}=0.34
\end{aligned}
$$

$$
w_{\text {stump }}=0.3
$$



