Lecture 2: Decision Trees DD2421

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- Lecture 1: Nearest Neighbour Classifier (Memory-based)
- Lecture 2: Decision Trees (Logical inference, Rule-based)
- Lecture 3: Challenges in Machine Learning

- 1 Decision Trees
 - The representation
 - Training
- 2 Unpredictability he to atom head Se tree
 - Entropy
 - Information gain
 - Gini impurity
- 3 Overfitting
 - Overfitting
 - Occam's principle
 - Training and validation set approach
 - Extensions



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Basic Idea: Test the attributes (features) sequentially

= Ask questions about the target/status sequentially

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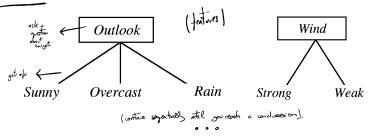
= Ask questions about the target/status sequentially

Example: building a concept of whether someone would like to play tennis.

Basic Idea: Test the attributes (features) sequentially

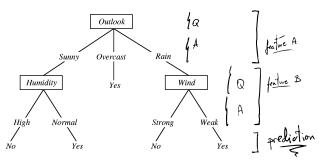
= Ask questions about the target/status sequentially

Example: building a concept of whether someone would like to play tennis.



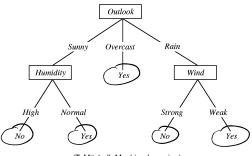
Useful also (but not limited to) when nominal data are involved, e.g. in medical diagnosis, credit risk analysis etc.

The whole analysis strategy can be seen as a tree.



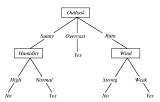
(T. Mitchell, Machine Learning)

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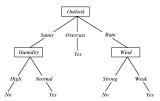


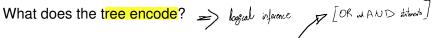
(T. Mitchell, Machine Learning)

Each leaf node bears a category label, and the test pattern is assigned the category of the leaf node reached.

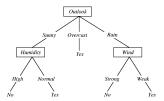


What does the tree encode?





 $(Sunny \land Normal Humidity) \lor (Cloudy) \lor (Rainy \land Weak Wind)$



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 $(Sunny \land Normal Humidity) \lor (Cloudy) \lor (Rainy \land Weak Wind)$

Logical expressions of the conjunction of decisions along the path.

Arbitrary boolean functions can be represented!

How to grow/construct the tree automatically?

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 Choose the best question (according to the information gain), and split the input data into subsets

be justing not give information about the different Split should be done and data is expectedly once modely dosephable.



How to grow/construct the tree automatically?

- Choose the best question (according to the information gain), and split the input data into subsets
- Terminate: call branches with a unique class labels leaves (no need for further quesitons)



How to grow/construct the tree automatically?

- Choose the best question (according to the information gain), and split the input data into subsets
- 2 Terminate: call branches with a unique class labels leaves (no need for further quesitons)
- Grow: recursively extend other branches (with subsets bearing mixtures of labels)

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Quize time - Game of "sixty-three"

x drawn from {0,1,2,3,4, ..., 63}

- I pick a number x from the set.
- You ask me yes/now questions.

How many (and what) questions will you ask me to get the number x as rapidly as possible?

How to measure information gain?

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The Shannon information content of an outcome is:

$$\begin{bmatrix}
\log_2 \frac{1}{p_i} \\
\downarrow
\end{bmatrix} \quad \text{(information measurement)}$$

 $(p_i : probability for event i)$

How to measure information gain?

The Shannon information content of an outcome is:

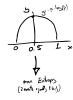
$$\log_2 \frac{1}{p_i}$$

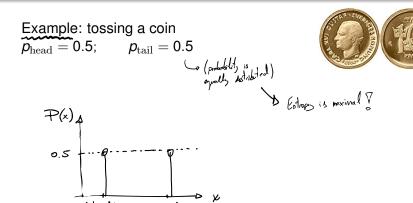
 $(p_i : probability for event i)$

The Entropy — measure of uncertainty (unpredictability)

Entropy =
$$\sum_{i} -p_i \log_2 p_i$$

is a sensible measure of expected information content.





$$p_{\rm head} = 0.5; \qquad p_{\rm tail} = 0.5$$



$$Entropy = \sum_{i} -p_{i} \log_{2} p_{i} \quad \Longrightarrow_{i} \text{ analler when brased}$$
1 e. see eacts are not likely.

$$p_{\rm head} = 0.5; \qquad p_{\rm tail} = 0.5$$



$$\begin{aligned} \text{Entropy} &= \sum_{i} -p_{i} \log_{2} p_{i} = \\ &= -0.5 \log_{2} 0.5 - 0.5 \log_{2} 0.5 \quad \text{for any like with} \\ &= \widehat{P_{i}} \quad \widehat{P_{i}} \quad \widehat{P_{i}} \quad \widehat{P_{i}} \quad \widehat{P_{i}} \quad \widehat{P_{i}} \end{aligned}$$

$$p_{\rm head} = 0.5; \qquad p_{\rm tail} = 0.5$$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

= $-0.5 \underbrace{\log_{2} 0.5}_{-1} -0.5 \underbrace{\log_{2} 0.5}_{-1}$

$$p_{\rm head} = 0.5; \qquad p_{\rm tail} = 0.5$$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

$$= -0.5 \log_{2} 0.5 - 0.5 \log_{2} 0.5 =$$

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Example: tossing a coin

$$p_{\text{head}} = 0.5;$$
 $p_{\text{tail}} = 0.5$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

= $-0.5 \underbrace{\log_{2} 0.5}_{-1} -0.5 \underbrace{\log_{2} 0.5}_{-1} =$

= 1

The result of a coin-toss has 1 bit of information

Example: rolling a die
$$p_1 = \frac{1}{6}$$
; $p_2 = \frac{1}{6}$; ... $p_6 = \frac{1}{6}$

$$\text{Entropy} = \sum_{i} -p_{i} \log_{2} p_{i}$$



Example: rolling a die
$$p_1 = \frac{1}{6}; \quad p_2 = \frac{1}{6}; \dots \quad p_6 = \frac{1}{6}$$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

= $6 \times (-\frac{1}{6} \log_{2} \frac{1}{6})$

Example: rolling a die
$$p_1 = \frac{1}{6}$$
; $p_2 = \frac{1}{6}$; ... $p_6 = \frac{1}{6}$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i}$$
 =
$$= 6 \times \left(-\frac{1}{6} \log_{2} \frac{1}{6}\right) =$$

$$= -\log_{2} \frac{1}{6} = \log_{2} 6 \approx 2.58$$

Example: rolling a die
$$p_1 = \frac{1}{6}$$
; $p_2 = \frac{1}{6}$; ... $p_6 = \frac{1}{6}$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

= $6 \times (-\frac{1}{6} \log_{2} \frac{1}{6}) =$
= $-\log_{2} \frac{1}{6} = \log_{2} 6 \approx 2.58$

The result of a die-roll has 2.58 bit of information



Example: rolling a fake die
$$p_1 = 0.1; \dots p_5 = 0.1; p_6 = 0.5$$

$$\text{Entropy} = \sum_i -p_i \log_2 p_i$$



Example: rolling a fake die

$$p_1 = 0.1; \dots p_5 = 0.1; p_6 = 0.5$$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

= $-5 \cdot 0.1 \log_{2} 0.1 - 0.5 \log_{2} 0.5$

Example: rolling a fake die

$$p_1 = 0.1; \dots p_5 = 0.1; p_6 = 0.5$$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

= $-5 \cdot 0.1 \log_{2} 0.1 - 0.5 \log_{2} 0.5 =$
 ≈ 2.16

Example: rolling a fake die

$$p_1 = 0.1; \dots p_5 = 0.1; p_6 = 0.5$$



Entropy =
$$\sum_{i} -p_{i} \log_{2} p_{i} =$$

= $-5 \cdot 0.1 \log_{2} 0.1 - 0.5 \log_{2} 0.5 =$
 ≈ 2.16

was numbers are more that, so it becomes more productible, i.e. kess into is needed to gress.

A real die is more unpredictable (2.58 bit) than a fake (2.16 bit)

Unpredictability of a dataset

• 100 examples, 42 positive

• 100 examples, 3 positive

Entropy

Unpredictability of a dataset

• 100 examples, 42 positive

$$-\frac{58}{100}\log_2\frac{58}{100} - \frac{42}{100}\log_2\frac{42}{100} = \underbrace{0.981}_{\leqslant}$$

• 100 examples, 3 positive



Entropy

Unpredictability of a dataset

• 100 examples, 42 positive

$$-\frac{58}{100}\log_2\frac{58}{100}-\frac{42}{100}\log_2\frac{42}{100}=0.981$$

• 100 examples, 3 positive

$$-\frac{97}{100}\log_2\frac{97}{100} - \frac{3}{100}\log_2\frac{3}{100} = 0.194$$

Entropy

Unpredictability of a dataset (think of a subset at a node)

• 100 examples, 42 positive

$$-\frac{58}{100}\log_2\frac{58}{100}-\frac{42}{100}\log_2\frac{42}{100}=0.981$$

100 examples, 3 positive

$$-\frac{97}{100}\log_2\frac{97}{100}-\frac{3}{100}\log_2\frac{3}{100}=0.194$$

Back to the decision trees

Smart idea:

Ask about the attribute which maximizes the expected reduction of the entropy.

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manumized entrops of
Co (alk a partial above assure
led to a most of spital data)
```

Back to the decision trees

Smart idea:

Ask about the attribute which maximizes the expected reduction of the entropy.

Information gain

Ask about attribute A for a data set S that has Entropy Ent(S),

$$\frac{\text{Gain}}{\text{Ent}(S)} - \underbrace{\text{Ent}(S)}_{\text{before}} - \underbrace{\text{Ent}(S)}_{\text{before}}$$

Back to the decision trees

Smart idea:

Ask about the attribute which maximizes the expected reduction of the entropy.

Information gain

Ask about attribute A for a data set S that has Entropy Ent(S), and get subsets S_V according to the value of A

$$Gain = \underbrace{\operatorname{Ent}(S)}_{\text{before}} - \underbrace{\sum_{v \in \operatorname{Values}(A)} \frac{|S_v|}{|S|}}_{\text{before}} \underbrace{\operatorname{Ent}(S_v)}_{\text{after}} \underbrace{\operatorname{Ent}(S_v)}_{\text{after}} \\
\underbrace{\operatorname{Ent}(S)}_{\text{after}} - \underbrace{\sum_{v \in \operatorname{Values}(A)} \frac{|S_v|}{|S|}}_{\text{after}} \underbrace{\operatorname{Ent}(S_v)}_{\text{after}} \\
\underbrace{\operatorname{Ent}(S)}_{\text{(a)twist}} - \underbrace{\operatorname{Ent}(S_v)}_{\text{(a)twist}} \underbrace{\operatorname{Ent}(S_v)}_{\text{(a)twist}} \\
\underbrace{\operatorname{Ent}(S)}_{\text{(a)twist}} - \underbrace{\operatorname{Ent}(S_v)}_{\text{(a)twist}} \underbrace{\operatorname{Ent}(S_v)}_{\text{(a)twist}} \\
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\underbrace{\operatorname{Ent}(S_v)}_{\text{(a)twist}} - \underbrace{\operatorname{Ent}(S_v)}_{\text{(a)twist}} \\
\underbrace{\operatorname{Ent}(S_v)}_{\text{(a)twist}} - \underbrace{\operatorname{Ent}(S_v)}$$

Q: is glas, B, E, C, Of: Jentine + ?

A: Black/white

torget: +, non + ...

Lo which feature is the best greation?

Α	В	C	D	7
0	•	•	0	+
•	•	0	0	+
0	0	•	0	
0	•	•	•	+
0	•	0	0	+
•	0	•	0	
0	•	•	0	+
o •	0	0	0	
•	0	0	0	
0	•	•	0	+
0	0	0	•	+
•	•	•	0	
	•	•	0	+
0	•	0	•	
0	0	0	0	
0	0	•	•	
0	•	•	•	
0	•	0	0	+
0	0	•	0	
•	•	0	0	
0	•	0	0	+
0	0	•	•	+
•	•	0	0	+
0	0	0	0	
0	0	•	0	

$$\mathrm{Ent} = -\frac{12}{25} \log_2 \frac{12}{25} - \frac{13}{25} \log_2 \frac{13}{25} \approx \mathbf{0.9988}$$

Lo which of the four justices {A,B,C,D} is the last split?

				ı
Α	В	C	D	
0	•		0	+
•	•	0	0	+
0	0	0	0	
0	0	•	•	+
0	•	0	0	+
•	0	•	0	
0	•	•	0	+
0	0	0	0	
•	0	0	0	
0	•	•	0	+
0	0	0	•	+
0	0	•	0	
•	•	•	0	+
0	•	0	•	
0	0	0	0	
0	0	•	0	
0	•	•	•	
0	•	0	0	+
0	0	•	0	
•	0	0	0	
0	•	0	0	+
0	0	•	•	+
•	•	0	0	+
0	0	0	0	
0	0	•	0	



$$Ent = -\frac{12}{25}\log_2\frac{12}{25} - \frac{13}{25}\log_2\frac{13}{25} \approx \mathbf{0.9988}$$

$$A = \bullet$$
: $\frac{3}{6}$ positive $\rightarrow 1.0$ (where $t \neq 0.50$ cm).

$$A=\circ: \frac{9}{19} \text{ positive} o 0.9980 \text{ (whop) for white } \mathcal{Y}_s \text{)}$$

Expected: $\frac{6}{25} \cdot 1.0 + \frac{19}{25} \cdot 0.9980 \approx 0.9985$

acrage evitrops for bours classification problem.

Α	B	С	D	I
0	•	•	0	+
•	•	0	0	+
0	0	•	•	
0	0	•	•	+
0	•	0	0	+
•	0	•	0	
0	•	•	0	+
•	0	0	0	
	0	0	0	
0	•	•	0	+
0	0	0	•	+
•	0	•	0	
•	•	•	•	+
0	•	0	•	
0	0	0	0	
0	0	•	0	
0	•	•	•	
0	•	•	0	+
•	0		0	
•	0	0	0	
0	•	0	0	+
0	•	•	•	+
•	•	0	0	+
0	0	0	0	
0	0	•	0	

$$Ent = -\frac{12}{25}\log_2\frac{12}{25} - \frac{13}{25}\log_2\frac{13}{25} \approx \textbf{0.9988}$$

$$A = \bullet$$
: $\frac{3}{6}$ positive $\rightarrow 1.0$

$$A = \circ$$
: $\frac{9}{19}$ positive $\rightarrow 0.9980$

Expected:
$$\frac{6}{25} \cdot 1.0 + \frac{19}{25} \cdot 0.9980 \approx 0.9985$$

$$B = \bullet$$
: $\frac{9}{11}$ positive $\rightarrow 0.684$

$$B = \circ$$
: $\frac{3}{14}$ positive $\rightarrow 0.750$

Expected: **0.721**

Α	B	l C	D	ı
0	•	C	0	+
•	•	0	0	+
0	0	0	0	
0	0	•	•	+
	•	0	0	+
•	0	•	0	
0	•	•	0	+
0	0	0	0	
•	0	0	0	
0	•	•	0	+
0	0	0	•	+
0	0	•	0	
•	•	•	0	+
0	•	0	•	
0	0	0	0	
0	0	•	0	
0	•	•	•	
0	•	0	0	+
0	0	•	0	
•	0	0	0	
0	•	0	0	+
0	0	•	•	+
•	•	0	0	+
0	0	0	0	
0	0	•	0	

$$Ent = -\frac{12}{25}\log_2\frac{12}{25} - \frac{13}{25}\log_2\frac{13}{25} \approx \textbf{0.9988}$$

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Expected:
$$\frac{6}{25} \cdot 1.0 + \frac{19}{25} \cdot 0.9980 \approx 0.9985$$

$$B = \bullet$$
: $\frac{9}{11}$ positive $\rightarrow 0.684$

$$B = \circ$$
: $\frac{3}{14}$ positive $\rightarrow 0.750$

Expected: 0.721

$$C = \bullet$$
: $\frac{6}{12}$ positive $\rightarrow 1.0$

$$C = \circ$$
: $\frac{6}{13}$ positive $\rightarrow 0.9957$

Expected: **0.9977**

Α	B	С	D	ı
	•	C •	0	+
•	•	0	0	+
0	0	0	0	
0	0	•	•	+
•	•	0	0	+
•	0	•	0	
0	•	•	0	+
0	0	0	0	
•	0		0	
0	•	•	0	+
0	0	0	•	+
•	0	•	0	
•	•	•	0	+
0	•	0	•	
0	0	0	0	
0	0	•	0	
0	•	•	•	
0	•	0	0	+
0	0	•	0	
•	0	0	0	
0	•	0	0	+
0	0	•	•	+
•	•	0	0	+
0	0	•	0	
0	0	•	0	

$$Ent = -\frac{12}{25}\log_2\frac{12}{25} - \frac{13}{25}\log_2\frac{13}{25} \approx \mathbf{0.9988}$$

$$A = \bullet$$
: $\frac{3}{6}$ positive $\rightarrow 1.0$

$$A = \circ$$
: $\frac{9}{19}$ positive $\rightarrow 0.9980$

Expected:
$$\frac{6}{25} \cdot 1.0 + \frac{19}{25} \cdot 0.9980 \approx 0.9985$$

$$B = \bullet$$
: $\frac{9}{11}$ positive $\rightarrow 0.684$

$$B = \circ$$
: $\frac{3}{14}$ positive $\rightarrow 0.750$

Expected: 0.721

$$C = \bullet$$
: $\frac{6}{12}$ positive $\rightarrow 1.0$

$$C = \circ$$
: $\frac{6}{13}$ positive $\rightarrow 0.9957$

Expected: **0.9977**

$$D = \bullet$$
: $\frac{3}{5}$ positive $\rightarrow 0.9710$

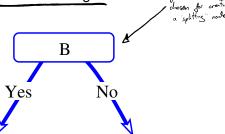
$$D = \circ$$
: $\frac{9}{20}$ positive $\rightarrow 0.9928$

Expected: **0.9884**

	D		В	Α
		C		
+	0		•	•
+	0	0	•	•
	0	0	0	0
+	•	•	0	0
+	0	•	•	•
	0	•	0	
+	0	•	•	0
	0	0 0	0	•
	0	0	0	
+	0	•	•	0
+	•	•	0	0
	0	•	0	•
+	0	•	•	•
	•	0	•	0
	0	0	0	0
	0	•	0	0
	•	•	•	0
+	0	•	•	0
	0	•	0	0
	0	0	•	•
+	•	0	•	0
+	•	•	0	0
+	0	0	•	•
	0	•	0	0
	0	• • <u>≡</u>	o = >	0

$$Gain(A) = 0.9988 - 0.9985 = 0.0003$$
 $Gain(B) = 0.9988 - 0.7210 = 0.2778$
 $Gain(C) = 0.9988 - 0.9977 = 0.0011$
 $Gain(D) = 0.9988 - 0.9884 = 0.0104$

$$Gain(A) = 0.9988 - 0.9985 =$$
0.0003 $Gain(B) = 0.9988 - 0.7210 =$ **0.2778** $Gain(C) = 0.9988 - 0.9977 =$ **0.0011** $Gain(D) = 0.9988 - 0.9884 =$ **0.0104** Attribute B gives most information gain





Examples where

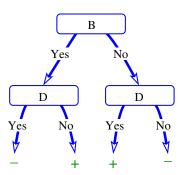
$$B = \bullet$$

l	D	C	В	Α
+	0	•	•	0
+	0	0	•	•
+	0	0	•	0
+	0	•	•	0
+	0	•	•	0
+	0	•	•	•
	•	0	•	0
	•	•	•	0
+	0	0	•	0
+	0	0	•	0
+	0	0	•	•

Examples where

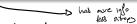
$$B = \circ$$

Α	В	C	D	
0	0	0	0	
0	0	•	•	+
•	0	•	0	
0	0	0	0	
•	0	0	0	
0	0	0	•	+
0	0	•	0	
0	0	0	0	
0	0	•	0	
•	0	0	0	
0	0	•	0	
0	0	•	•	+
0	0	0	0	
0	0	•	0	



Greedy approach to choose a question:

Choose the attribute which tells us most about the answer



In sum, we need to find good questions to ask.

(more than one attribute could be involved in one question)

Gini impurity: Another definition of predictability (impurity).

$$\sum_{i} p_{i}(1-p_{i}) = 1 - \sum_{i} p_{i}^{2}$$

$$(p_{i} : \text{probability for event } i)$$

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Similar to the entropy but more strongly peaked at equal probabilities.

- Decision Trees
 - The representation
 - Training
- 2 Unpredictability
 - Entropy
 - Information gain
 - Gini impurity
- 3 Overfitting
 - Overfitting
 - Occam's principle
 - Training and validation set approach
 - Extensions



Overfitting

When the learned models are overly specialized for the training samples.

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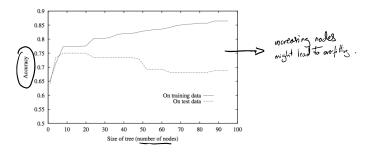
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Overfitting

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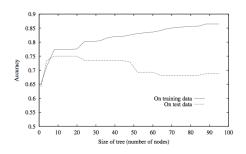
Good results on training data, but generalizes poorly.

- When does this occur?
 - Non-representative sample
 - Noisy examples
 - Too complex model



(T. Mitchell, Machine Learning)

What can be done about it?



(T. Mitchell, Machine Learning)

What can be done about it?
Choose a simpler model and accept some errors for the training examples

> fluit adopts better to new samples (test data).

Which hypothesis should be preferred when several are compatible with the data?

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Occam's principle (Occam's razor)

William from Ockham, Theologian and Philosopher (1288–1348)

"Entities should not be multiplied beyond necessity"

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Occam's principle (Occam's razor)

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"Entities should not be multiplied beyond necessity"

The simplest explanation compatible with data tends to be the right one



Separate the available data into two sets of examples

- Training set T: to form the learned model
- Validation set V: to evaluate the accuracy of this model

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- The validation set to provide a <u>safety check</u> against overfitting the spurious characteristics of the training set

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(*V* need be large enough to provide statistically meaningful instances)



Reduced-Error Pruning

Split data into training and validation set

Do until further pruning is harmful:



- Evaluate impact on validation set of pruning each possible node (plus those below it)
- Greedily remove the one that most improves validation set accuracy

Produces smallest version of most accurate subtree

Possible ways of improving/extending the decision trees

- Avoid overfitting
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A collection of trees (Ensemble learning: in Lecture 10)

- Bootstrap aggregating (bagging)
- Decision Forests