CS 760: Machine Learning
Supervised Learning I

Josiah Hanna

University of Wisconsin — Madison

9/14/2023

Announcements

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- Enrollment:
  - Email me today if you’re still on waitlist AND have a reason for additional priority.
  - It will be offered next semester if you don’t get in.

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  - Please look at homework 1 before add/drop deadline.

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- Background Knowledge:
  - Please look at homework 1 before add/drop deadline.
  - Please take background survey on Piazza.
- Homework 1 is due at 9:30 AM on Tuesday, September 19.
- Sign-up for Piazza (link on webpage)
  - Passcode: mlfall23

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  - You will be able to explain the concept of an inductive bias.
  - You will be able to explain how a decision tree classifies instances.

Outline

- **Review from last time**
  - Features, labels, hypothesis class, training, generalization
- **Instance-based learning**
  - k-NN classification/regression, locally weighted regression, strengths & weaknesses, inductive bias
- **Decision trees**
  - Setup, splits, learning, information gain, strengths and weaknesses

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Supervised Learning: Formal Setup

Problem setting

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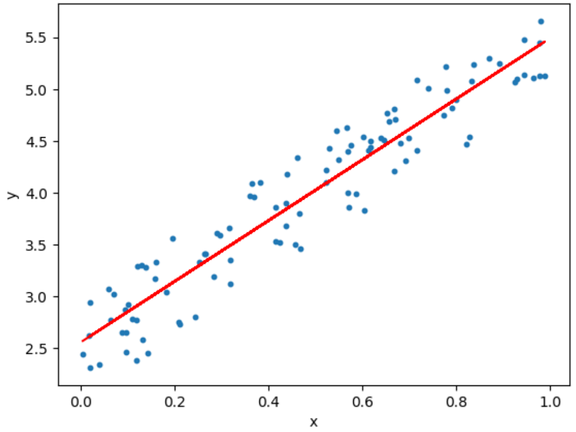

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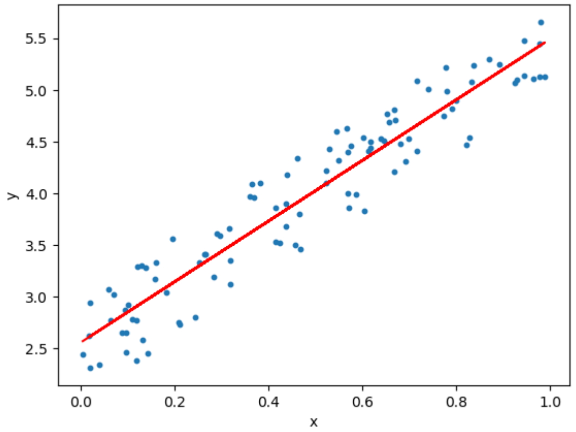

- There are other types…

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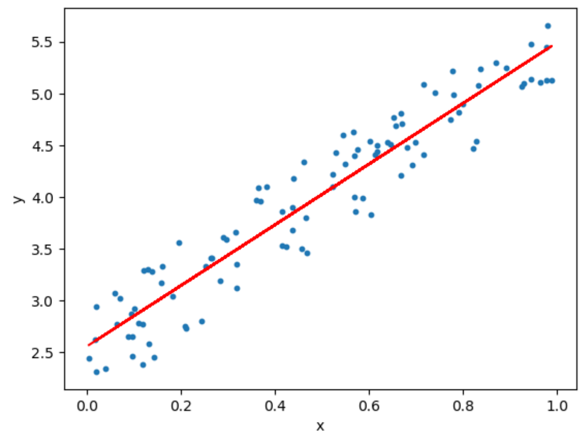

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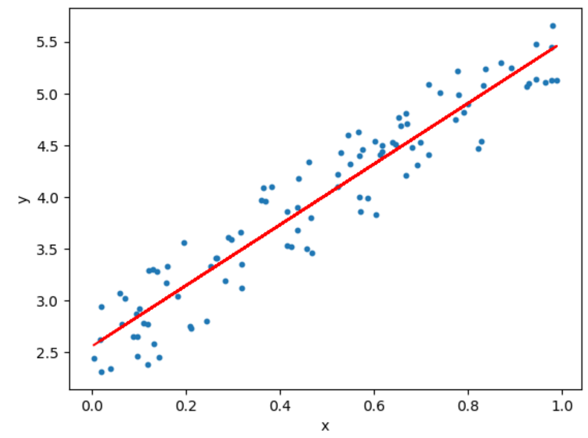

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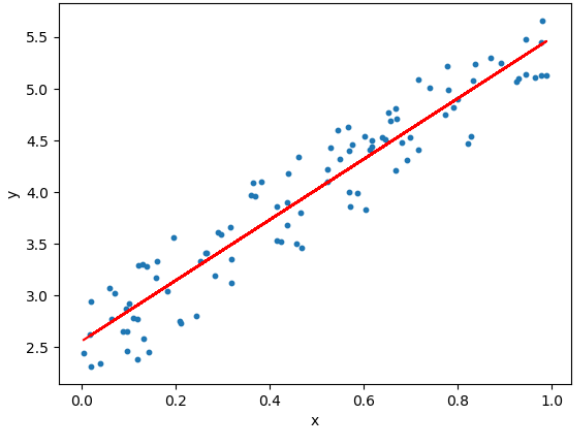

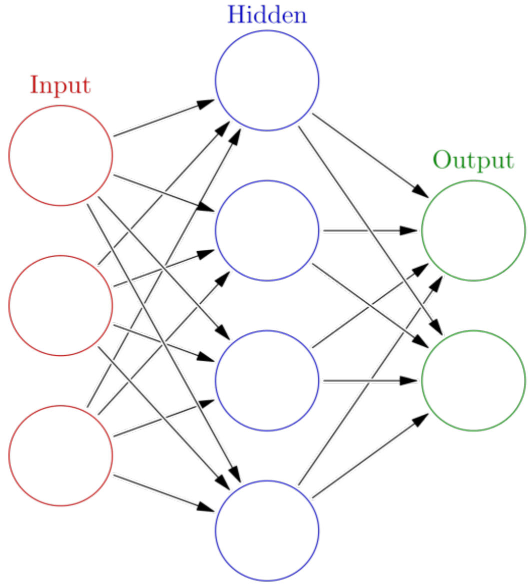

Wikipedia

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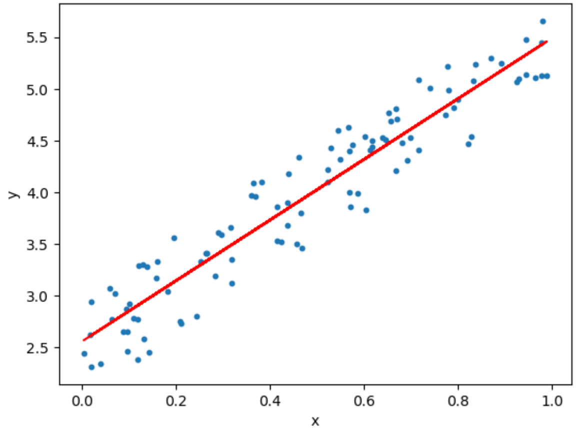
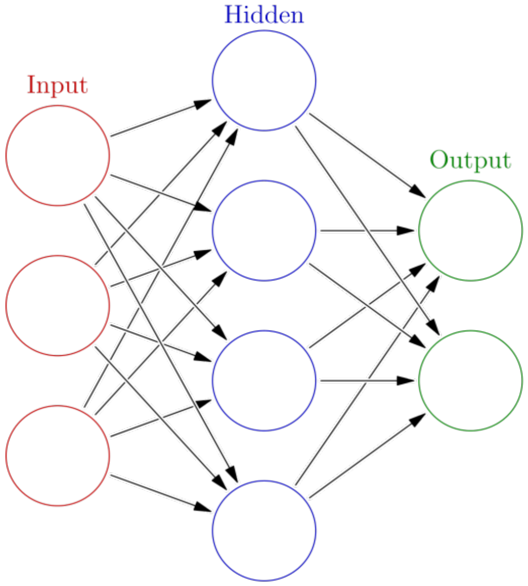


$$f^{(0)}(x) = x$$

$$f^{(k)}(x) = \sigma(W_k^T f^{(k-1)}(x)))$$



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Supervised Learning: Training & Generalization

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  - Do well on future (test) data points, not just on training data.

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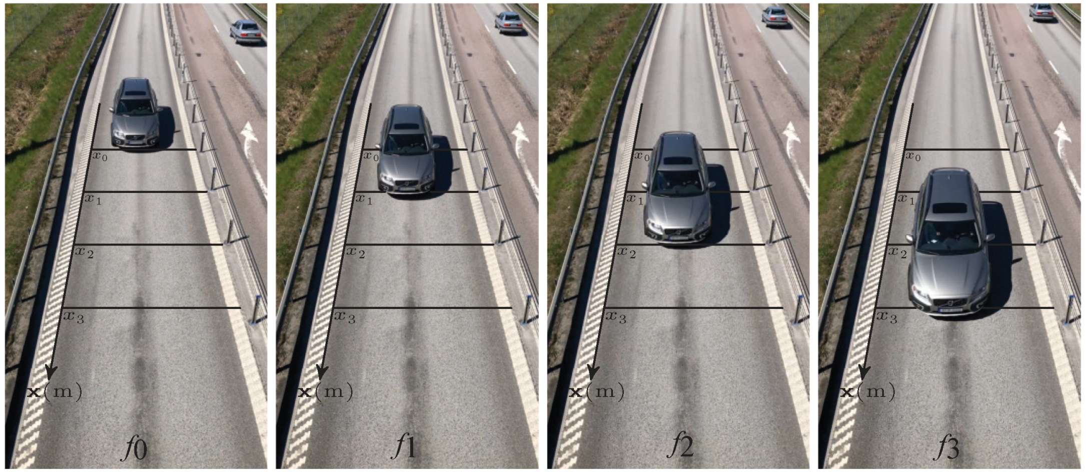

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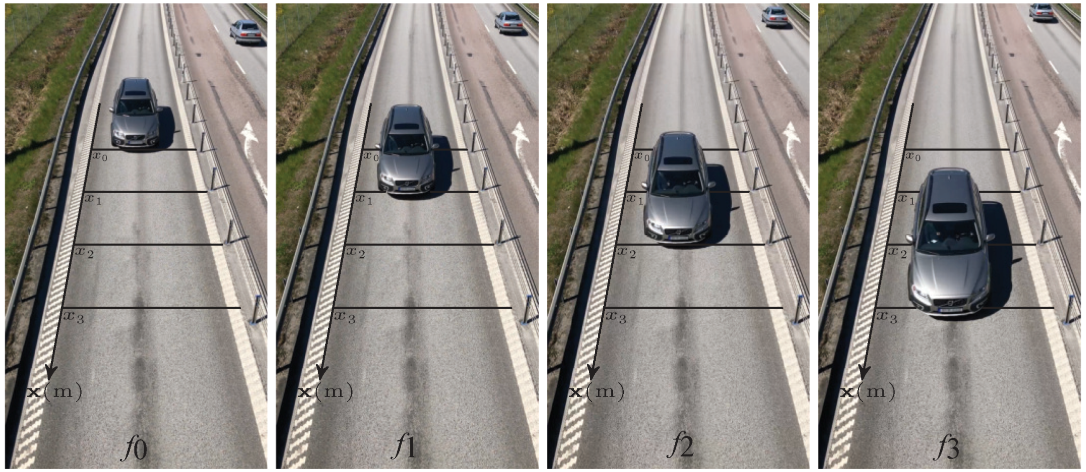

Nearest Neighbors: Idea

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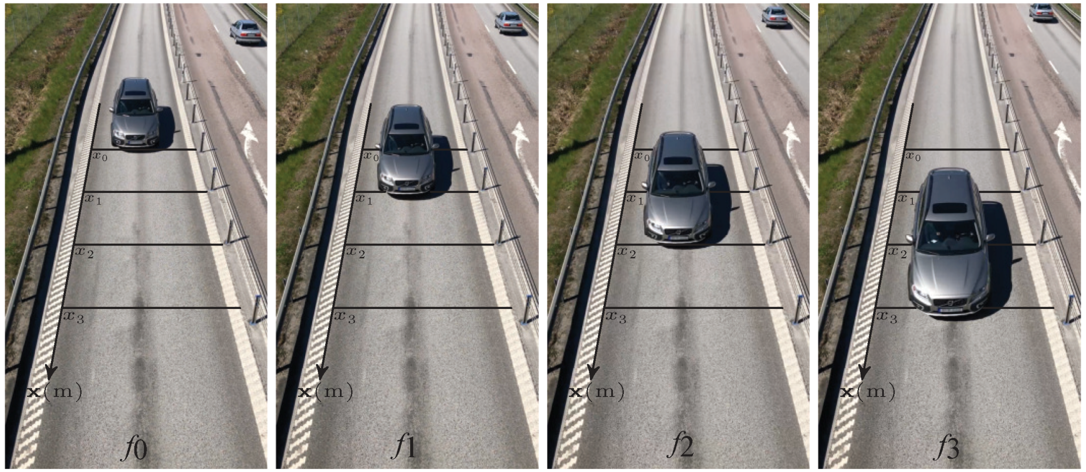
- **Example**: classify car/no car
  - Everything is similar, except the location of car
- What does "nearby" mean?



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Prediction: for x , find nearest training point $x^{(j)}$

Return $y^{(j)}$ poisonous

x

1NN: Decision Regions

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Defined by “**Voronoi Diagram**”

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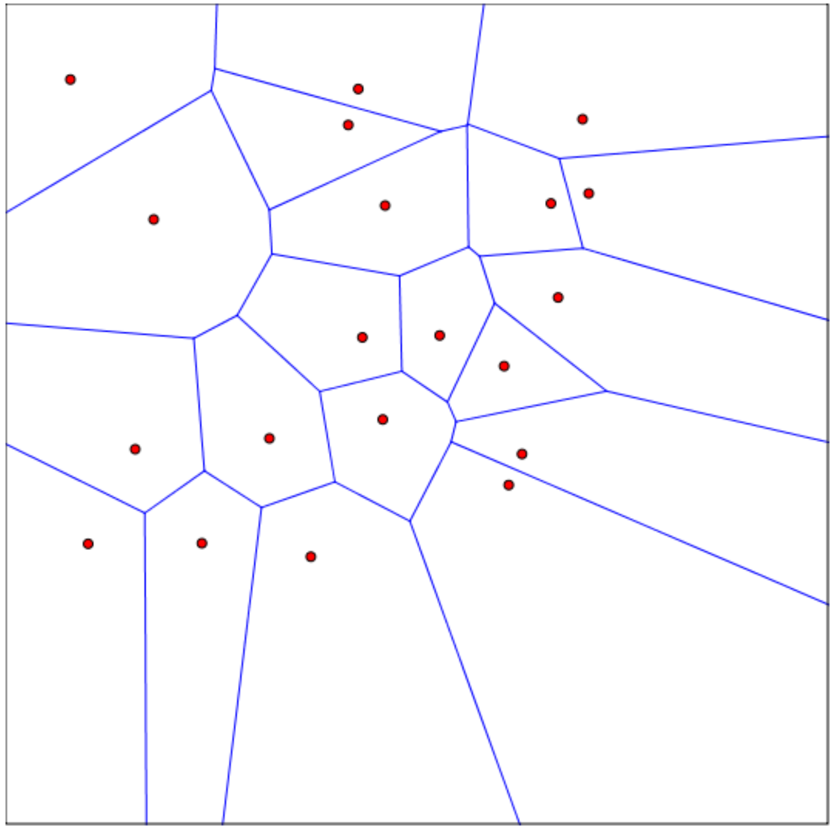

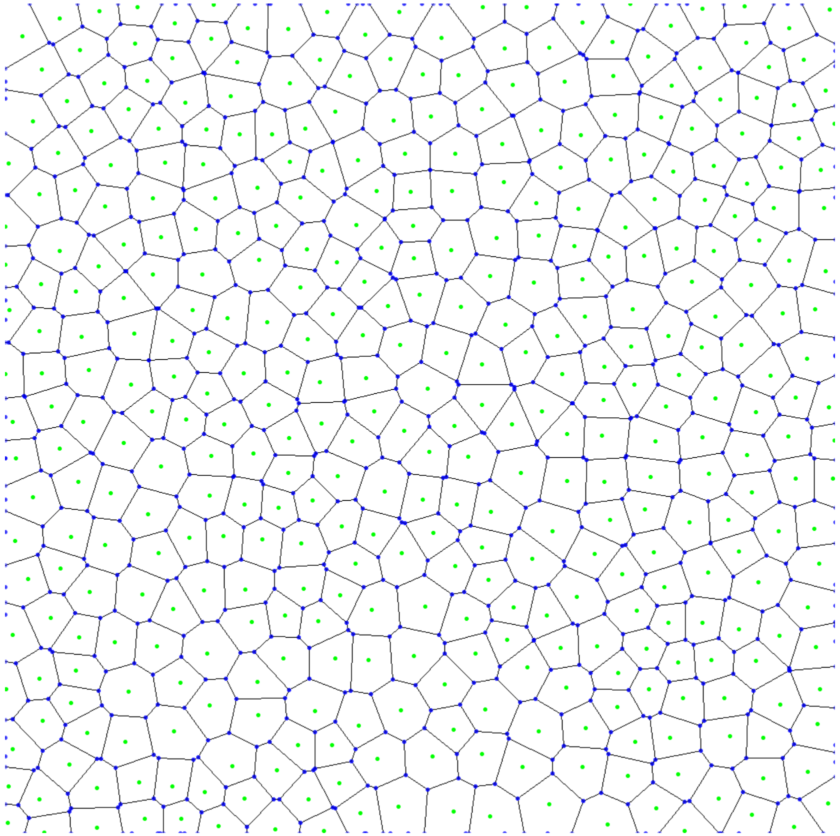

k-Nearest Neighbors: Classification

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- I.e., among the ***k*** most similar points, output most popular class.

k-Nearest Neighbors: Distances

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Discrete features: Hamming distance

Ex: d([‘a’, ‘b’, ‘c’], [‘d’, ‘b’, ‘e’]) = 2

$$d_H(x^{(i)}, x^{(j)}) = \sum_{a=1}^{d} 1\{x_a^{(i)} \neq x_a^{(j)}\}$$

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Continuous features:

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Ex: d([0, 0], [4, 4]) = $\sqrt{32}$

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Continuous features:

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$$d(x^{(i)}, x^{(j)}) = \left(\sum_{a=1}^{d} (x_a^{(i)} - x_a^{(j)})^2 \right)^{\frac{1}{2}}$$

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$$d_H(x^{(i)}, x^{(j)}) = \sum_{a=1}^{d} 1\{x_a^{(i)} \neq x_a^{(j)}\}$$

Continuous features:

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$$d(x^{(i)}, x^{(j)}) = \left(\sum_{a=1}^{d} (x_a^{(i)} - x_a^{(j)})^2\right)^{\frac{1}{2}}$$

Ex: d([0, 0], [4, 4]) = $\sqrt{32}$

- L1 (Manhattan) dist.:

k-Nearest Neighbors: Distances

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Prevents high magnitude / variance features from dominating distance calculation.

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- Might need **normalization**, (e.g. normalize individual distances to maximum value of 1)

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Training/learning: given

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- I.e., among the ***k*** points, output mean label.

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$$\hat{y} \leftarrow \frac{\sum_{i=1}^{k} y^{(i)} / d(x, x^{(i)})^2}{\sum_{i=1}^{k} 1 / d(x, x^{(i)})^2}$$

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One relevant feature x_1

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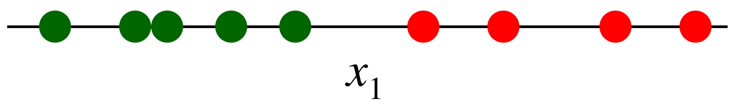

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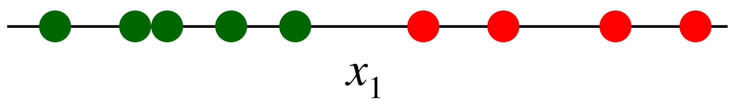

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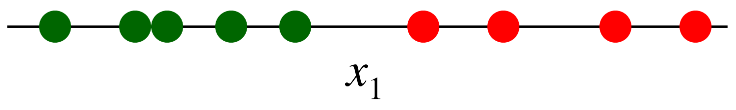

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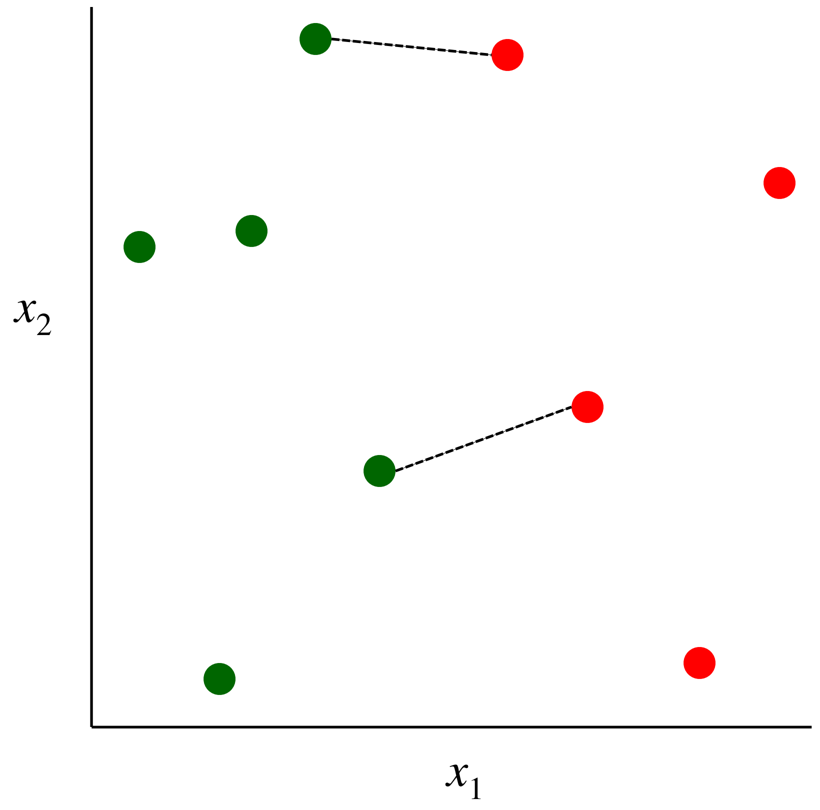

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- No “model” to interpret

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learner	hypothesis space bias	preference bias
k-NN	Decomposition of space determined by nearest neighbors	Instances in neighborhood belong to same class

Break & Quiz

Q2-1: Table shows all the training points in 2D space and their labels. Assume a 3-NN classifier and Euclidean distance. What should be the labels of the points A: (1, 1) and B(2, 1)?

1. A: +, B: -
2. A: -, B: +
3. A: -, B: -
4. A: +, B: +

x	y	label
0	0	+
1	0	+
2	0	+
2	2	+
0	1	-
0	2	-
1	2	-
3	1	-

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3	1	-

3 nearest neighbors to point A are (0, 1) [-], (1, 0) [+], (1, 2) [-]. Hence, the label should be **[-]**

3 nearest neighbors to point B are (2, 0) [+], (2, 2) [+], (3, 1) [-]. Hence, the label should be **[+]**

Q2-2: In a distance-weighted nearest neighbor, which of the following weight is **NOT** appropriate? Let p be the test data point and x_i {i = 1: N} be training data points.

1. $w_i = d(p, x_i)^{1/2}$
2. $w_i = d(p, x_i)^{-2}$
3. $w_i = \exp(-d(p, x_i))$
4. $w_i = 1$

Q2-2: In a distance-weighted nearest neighbor, which of the following weights is **NOT** appropriate? Let p be the test data point and x_i {i = 1: N} be training data points.

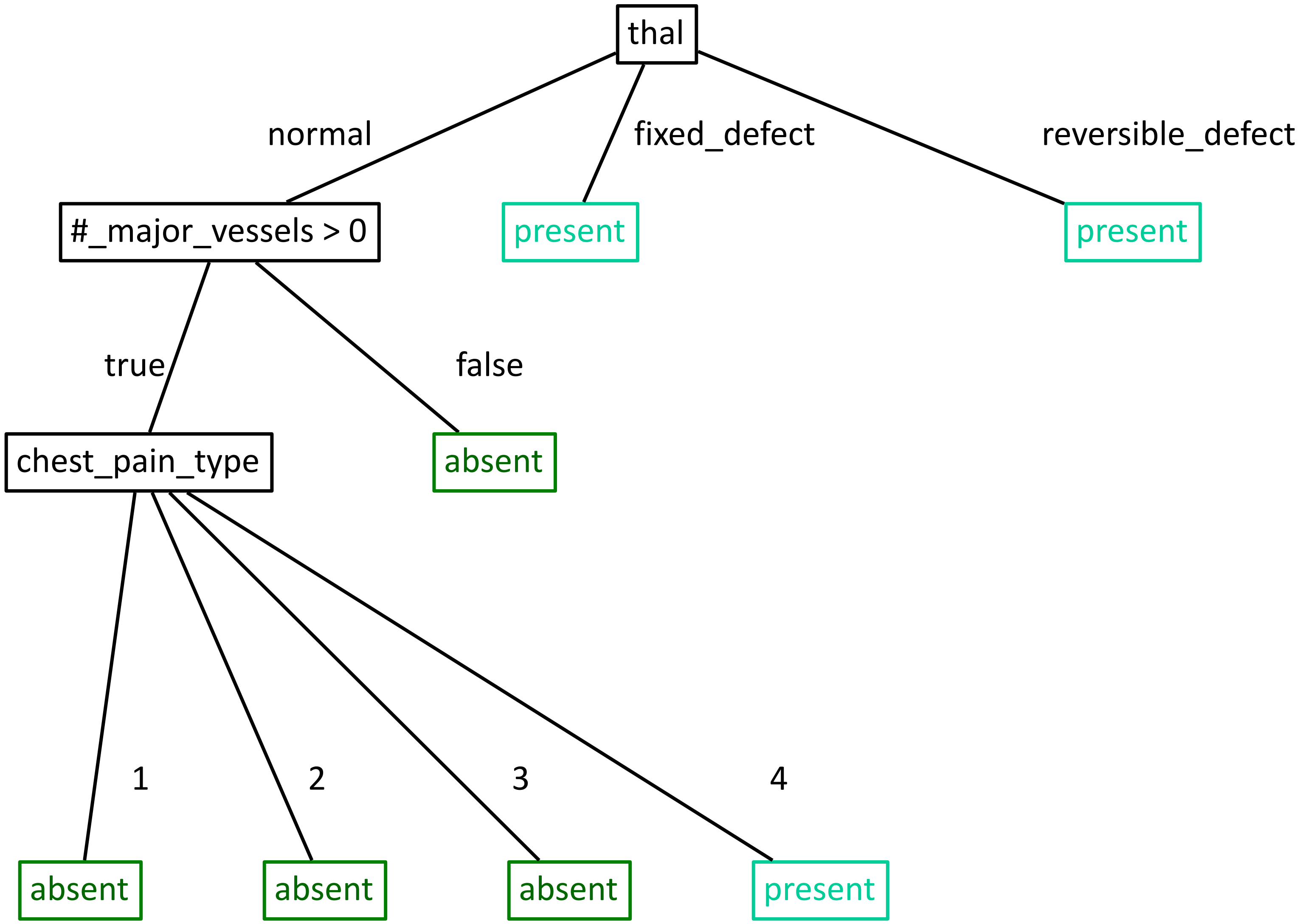
1. $w_i = d(p, x_i)^{½}$
2. $w_i = d(p, x_i)^{-2}$
3. $w_i = \exp(-d(p, x_i))$
4. $w_i = 1$

The intuition behind weighted kNN, is to give more weight to the points which are nearby and less weight to the points which are farther away. Any function whose value decreases as the distance increases can be used as a function for the weighted knn classifier. w = 1 is also **OK** as it reduces to our traditional nearest-neighbor algorithm.

Outline

- **Review from last time**
  - Features, labels, hypothesis class, training, generalization
- **Instance-based learning**
  - k-NN classification/regression, locally weighted regression, strengths & weaknesses, inductive bias
- **Decision trees**
  - Setup, splits, learning, information gain, strengths and weaknesses

Decision Trees: Heart Disease Example



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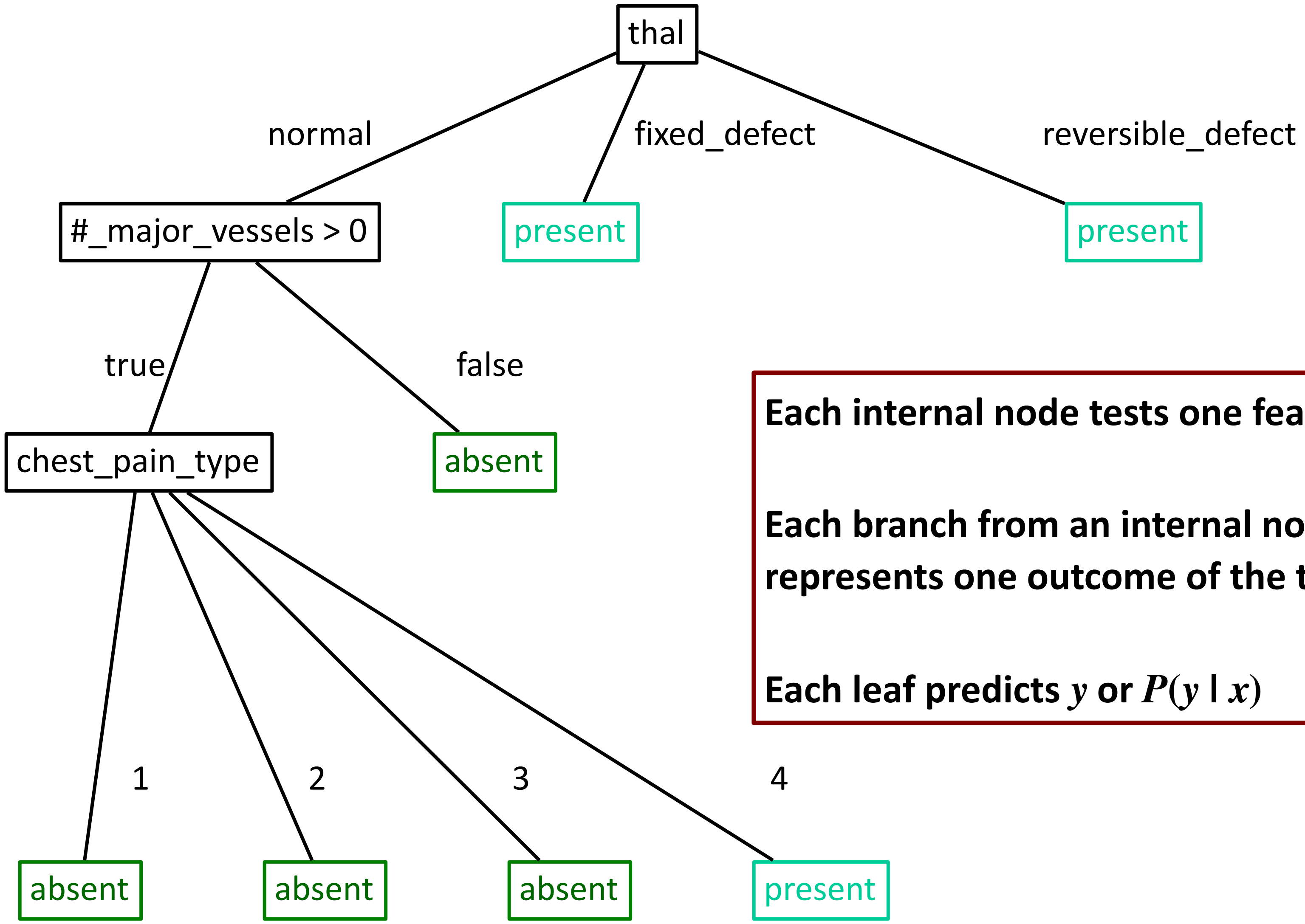

Each internal node tests one feature x_i

Each branch from an internal node represents one outcome of the test

Each leaf predicts y or $P(y \mid x)$

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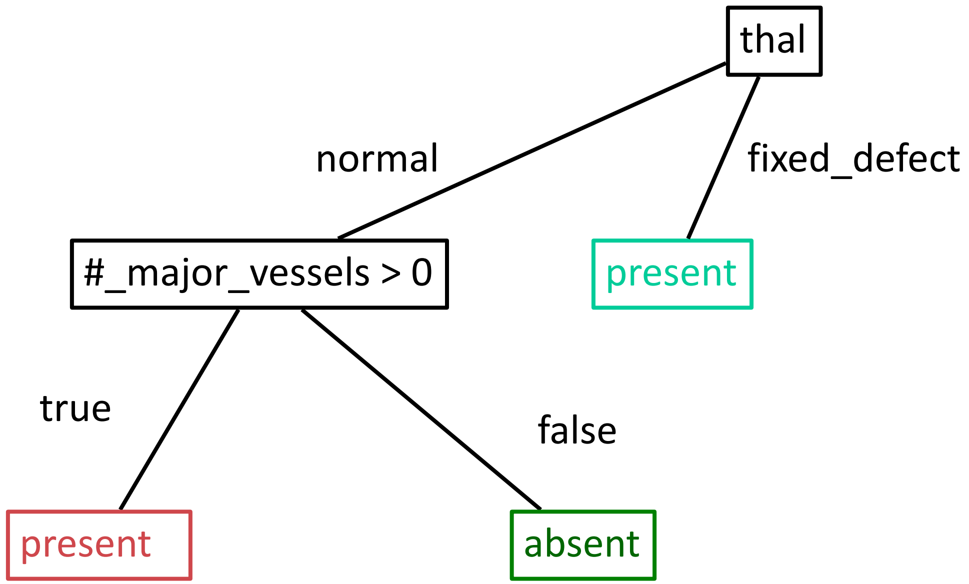

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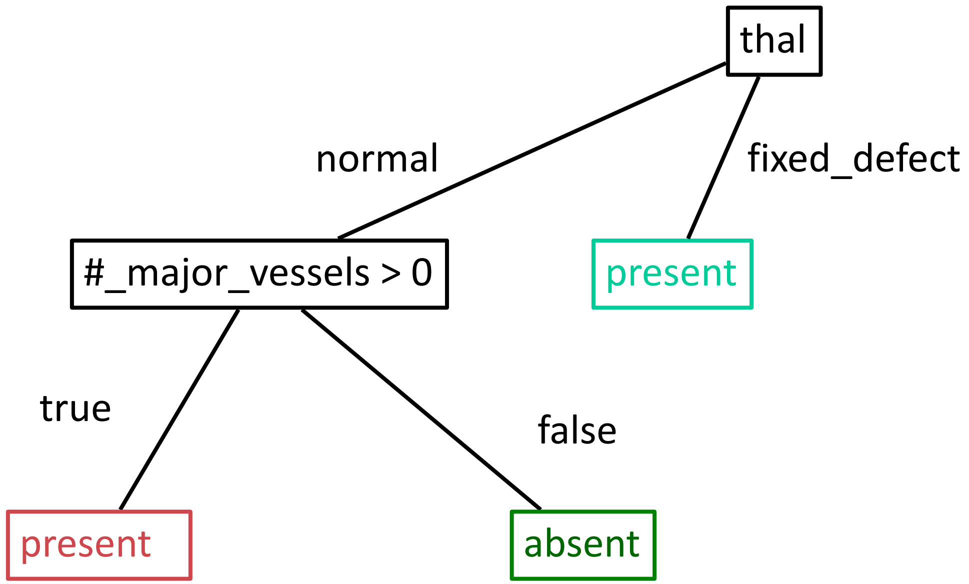

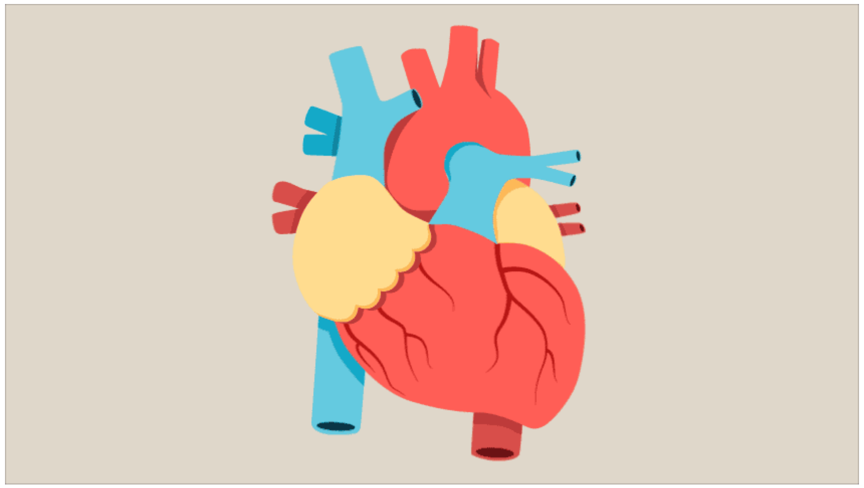

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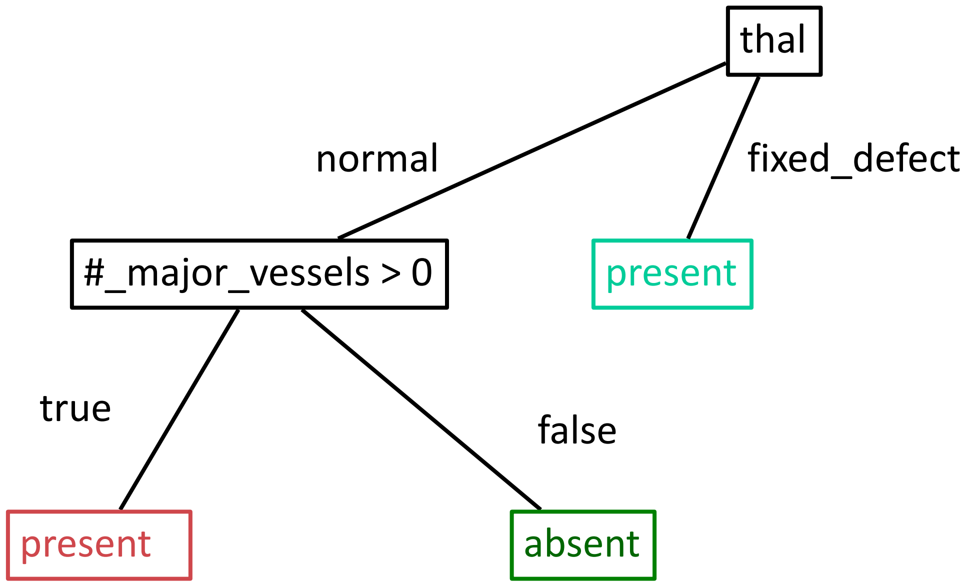

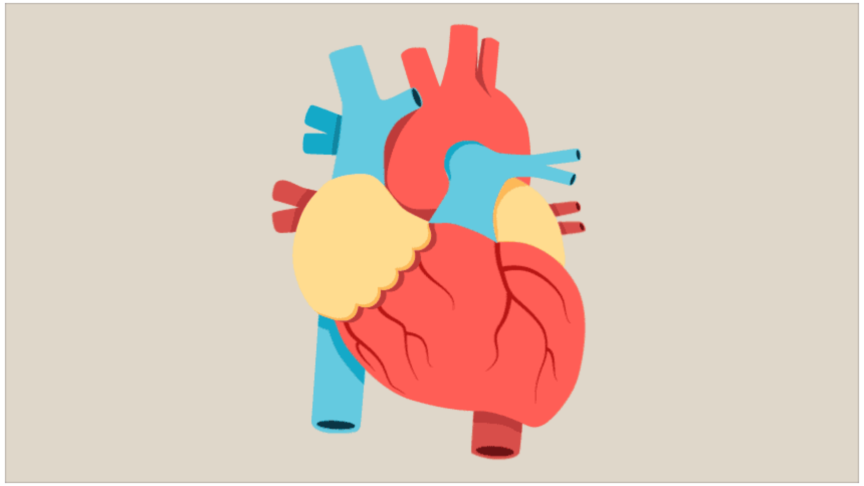

thal = normal

[#_major_vessels > 0] = true: present

[#_major_vessels > 0] = false: absent

thal = fixed_defect: present

Decision Trees: Mushrooms Example

```
odor = a: e (400.0)
odor = c: p (192.0)
odor = f: p (2160.0)
odor = l: e (400.0)
odor = m: p (36.0)
odor = n
|   spore-print-color = b: e (48.0)
|   spore-print-color = h: e (48.0)
|   spore-print-color = k: e (1296.0)
|   spore-print-color = n: e (1344.0)
|   spore-print-color = o: e (48.0)
|   spore-print-color = r: p (72.0)
|   spore-print-color = u: e (0.0)
|   spore-print-color = w
|   |   gill-size = b: e (528.0)
|   |   gill-size = n
|   |   |   gill-spacing = c: p (32.0)
|   |   |   gill-spacing = d: e (0.0)
|   |   |   gill-spacing = w
|   |   |   |   population = a: e (0.0)
|   |   |   |   population = c: p (16.0)
|   |   |   |   population = n: e (0.0)
|   |   |   |   population = s: e (0.0)
|   |   |   |   population = v: e (48.0)
|   |   |   |   population = y: e (0.0)
|   spore-print-color = y: e (48.0)
odor = p: p (256.0)
odor = s: p (576.0)
odor = y: p (576.0)
```

if odor=almond, predict edible

if odor=none ∧
spore-print-color=white ∧
gill-size=narrow ∧
gill-spacing=crowded,
predict poisonous

Decision Trees: Learning

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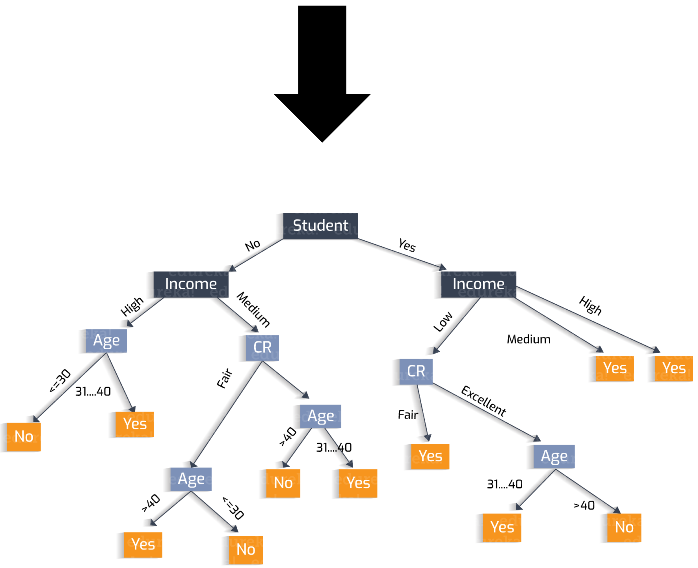

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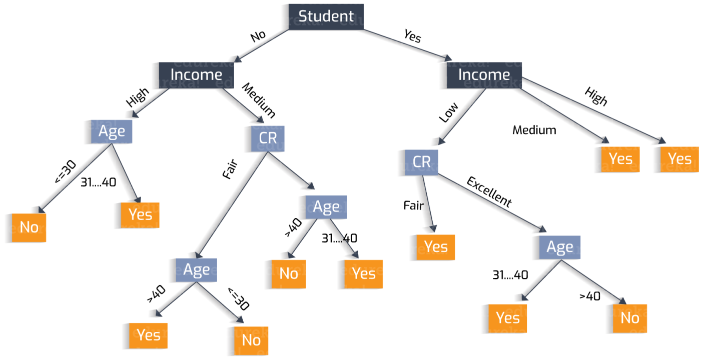

MakeSubtree(set of training instances D)

C = DetermineCandidateSplits(D)

if stopping criteria is met

  make a leaf node N

  determine class label for N

else

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  S = FindBestSplit(D, C)

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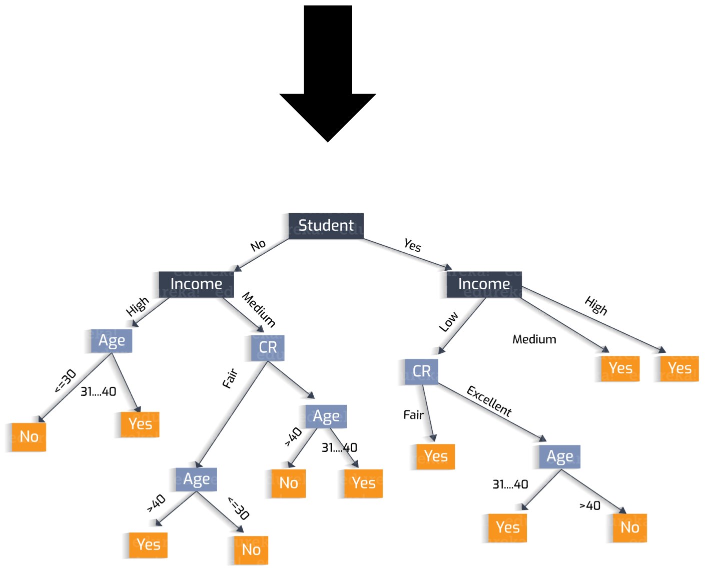

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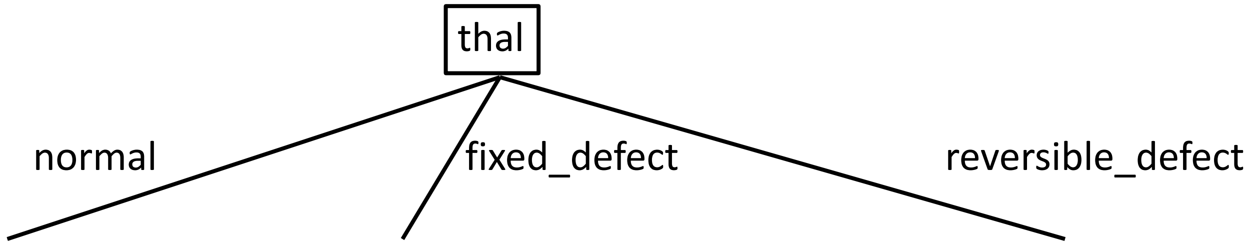

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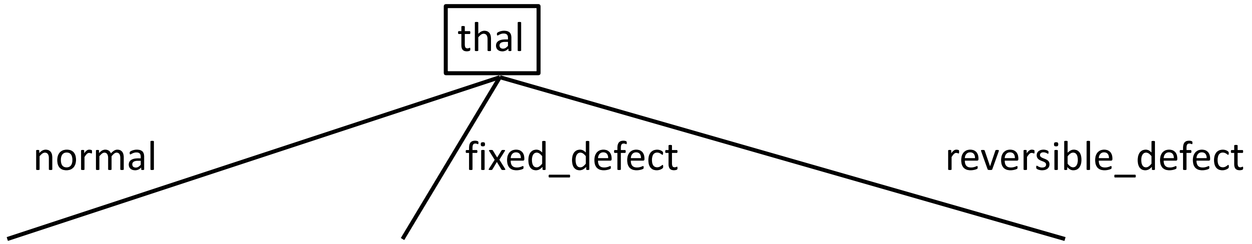

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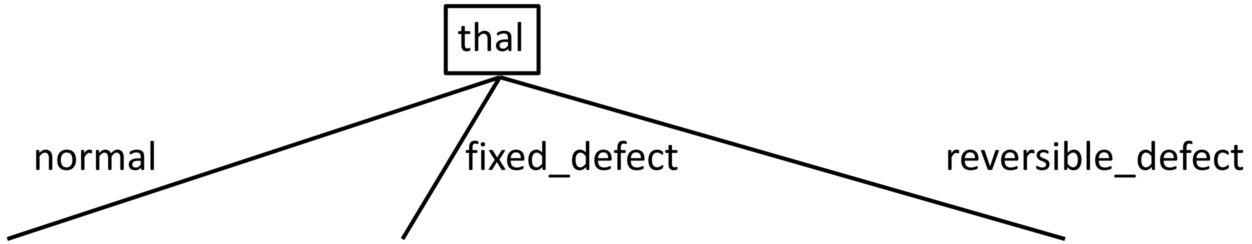

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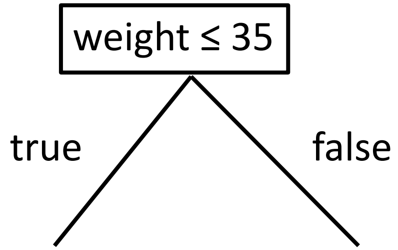

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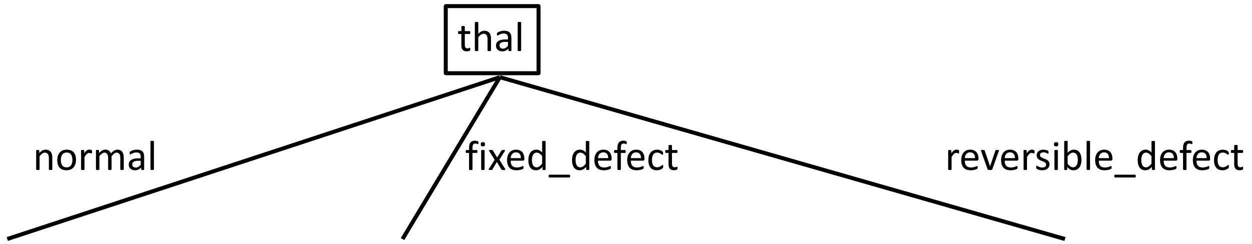

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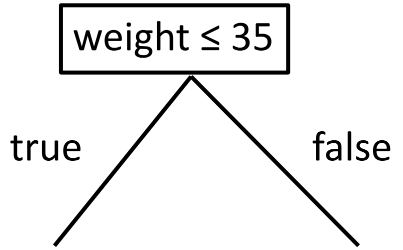

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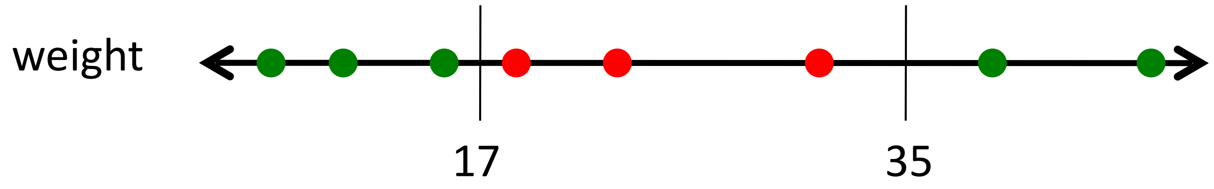

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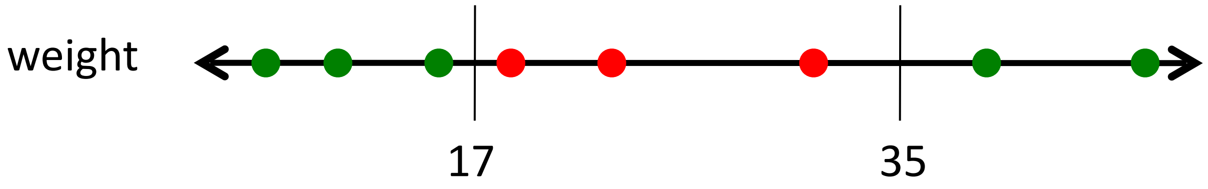
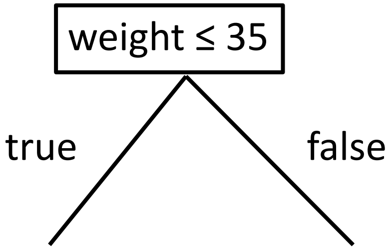
Given a set of training instances D and a specific feature X_i

- Sort the values of X_i in D
- Evaluate split thresholds in intervals between instances of different classes





Numeric Feature Splits Algorithm

// Run this subroutine for each numeric feature at each node of DT induction

DetermineCandidateNumericSplits(set of training instances D, feature X_i)

$C = \{\}$ // initialize set of candidate splits for feature X_i

let v_j denote the value of X_i for the j^{th} data point

sort the dataset using v_j as the key for each data point

for each pair of adjacent v_j, v_{j+1} in the sorted order

if the corresponding class labels are different

add candidate split $X_i \leq (v_j + v_{j+1})/2$ to C

return C

DT: Splits on Nominal Features

Instead of using k-way splits for k-valued features, could require binary splits on all nominal features.

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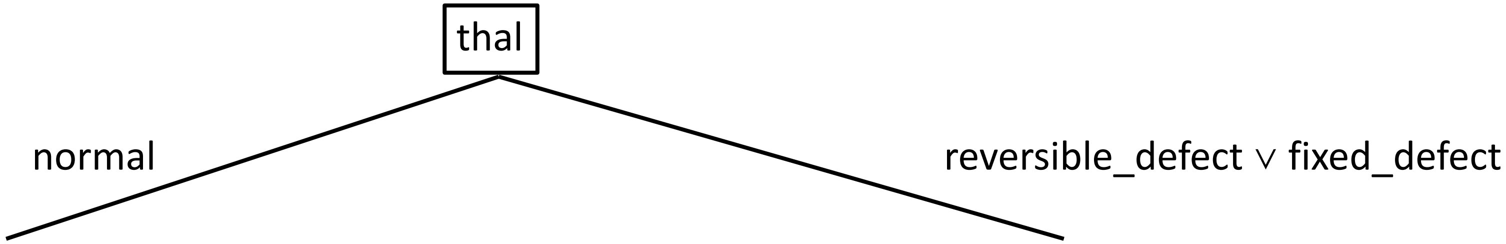

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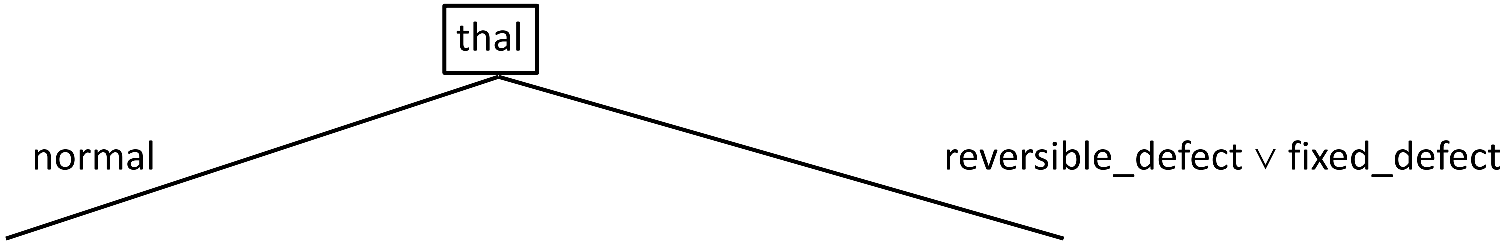

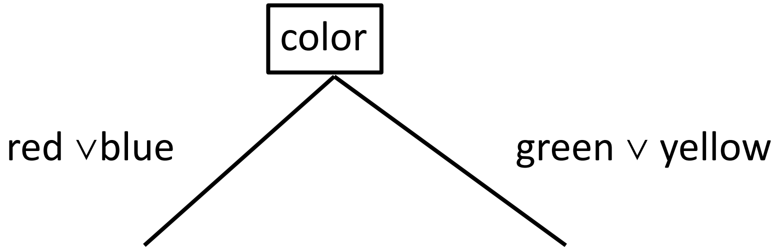

Decision Trees: Learning

- **Learning Algorithm**:

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$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})\}$$

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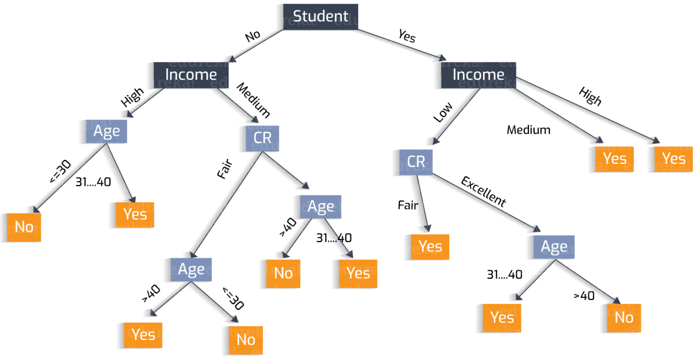

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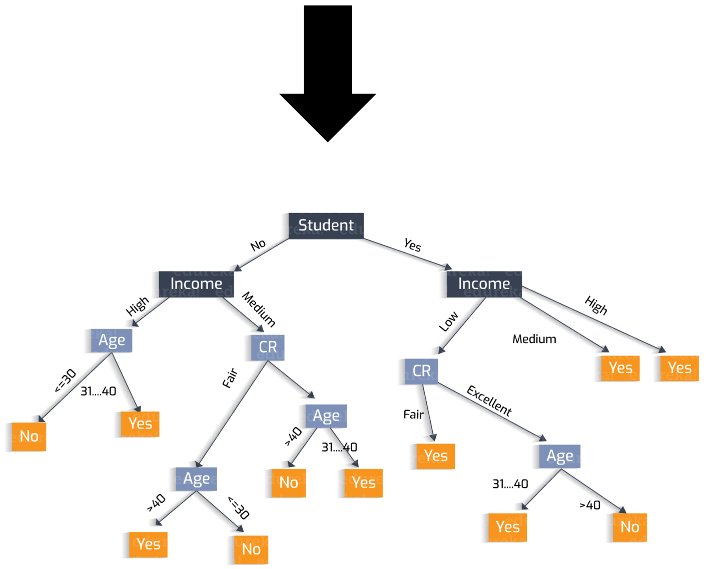

MakeSubtree(set of training instances D)

C = **DetermineCandidateSplits**(D)

if **stopping criteria** is met

make a leaf node N

determine class label for N

else

make an internal node N

S = **FindBestSplit**(D, C)

for each group k of S

D_k = subset of training data in group k

k^{th} child of N = MakeSubtree(D_k)

return subtree rooted at N

Decision tree Learning: Finding the Best Splits

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- "when you have two competing theories that make the same predictions, the simpler one is the better"

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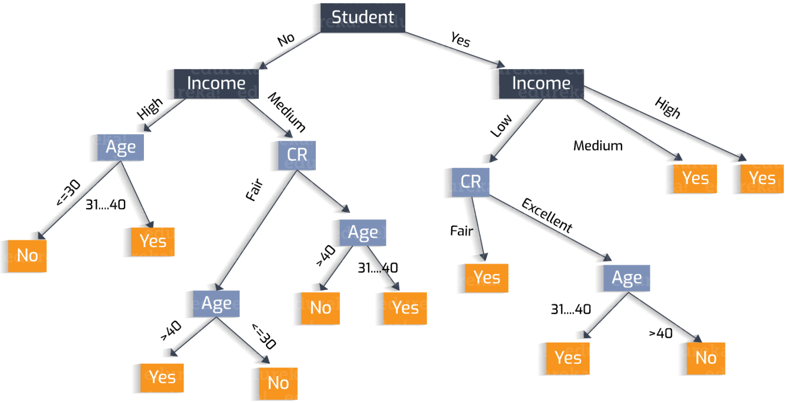
DT Learning: Finding Optimal Splits?

Can we find and return the smallest possible decision tree that accurately classifies the training set?



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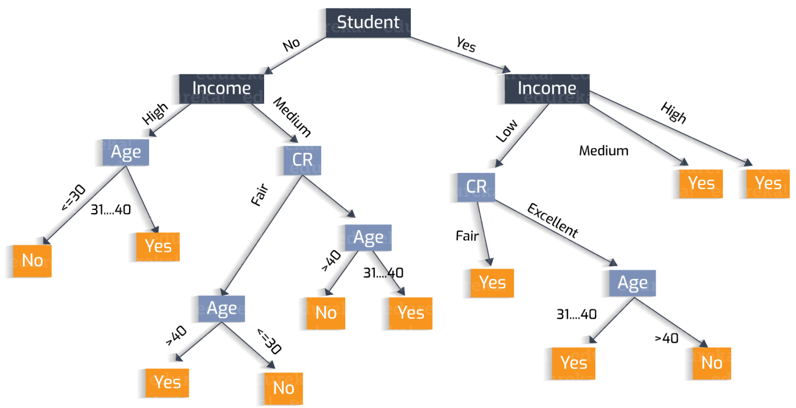

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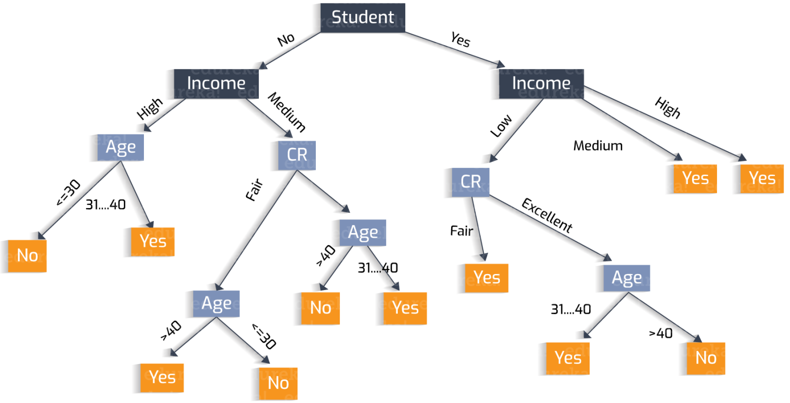

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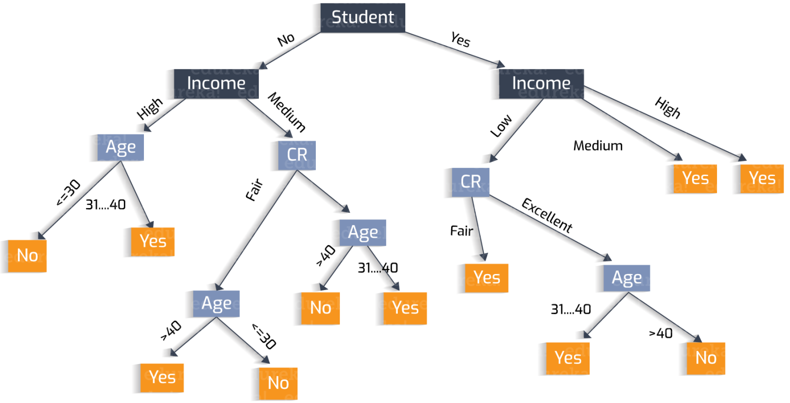
- Instead, we'll use an information-theoretic heuristic to greedily choose splits



Information Theory: Super-Quick Intro

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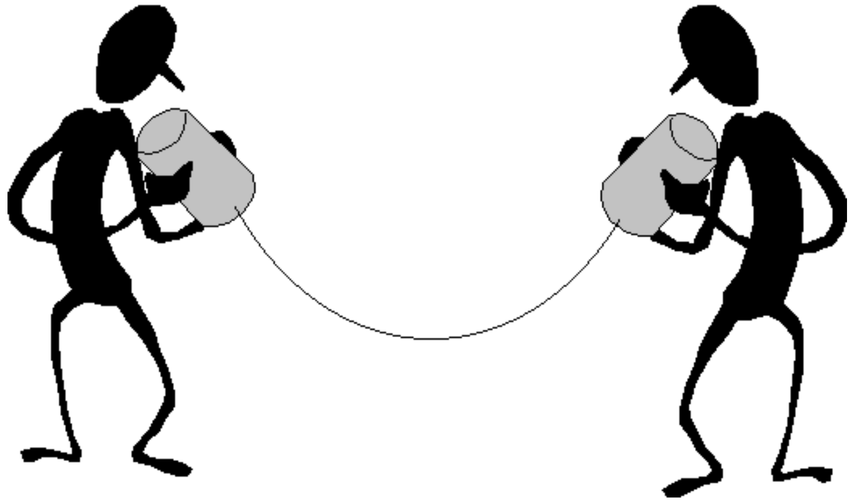

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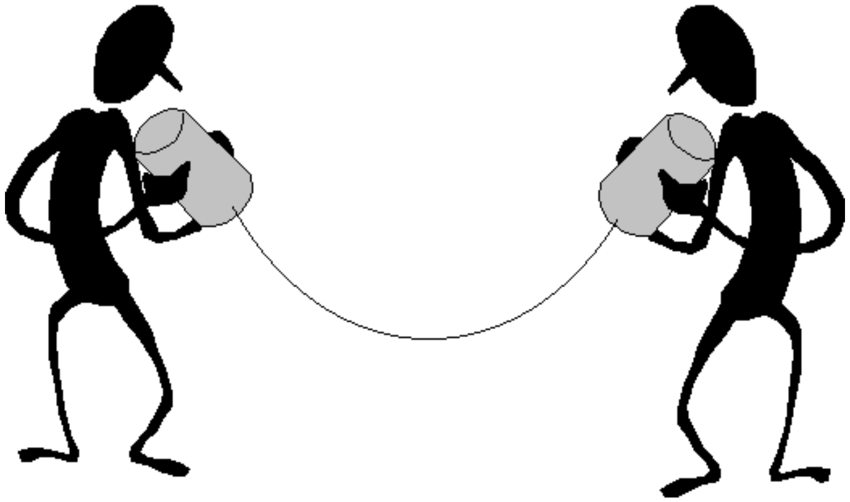
- **Goal**: communicate information to a receiver *in bits*
- Ex: as bikes go past, communicate the maker of each bike



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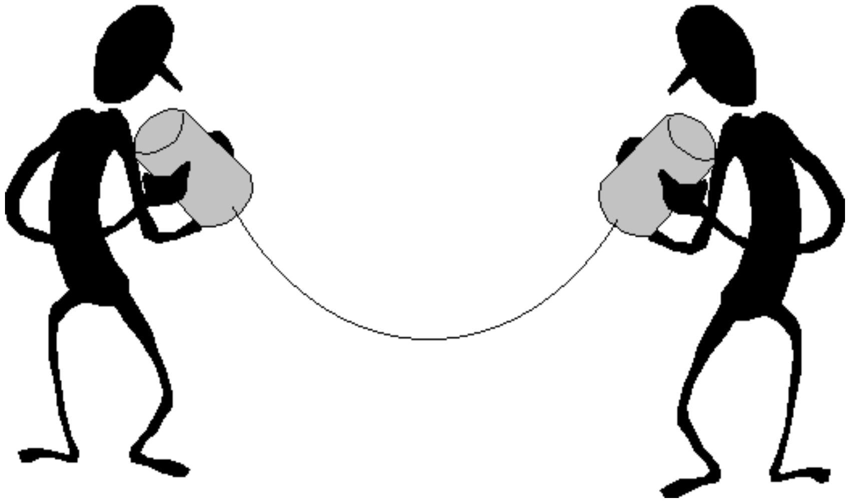

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type	code
Trek	11
Specialized	10
Cervelo	01
Serrota	00

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- Now, some bikes are rarer than others…
  - **Cervelo** is a rarer specialty bike.
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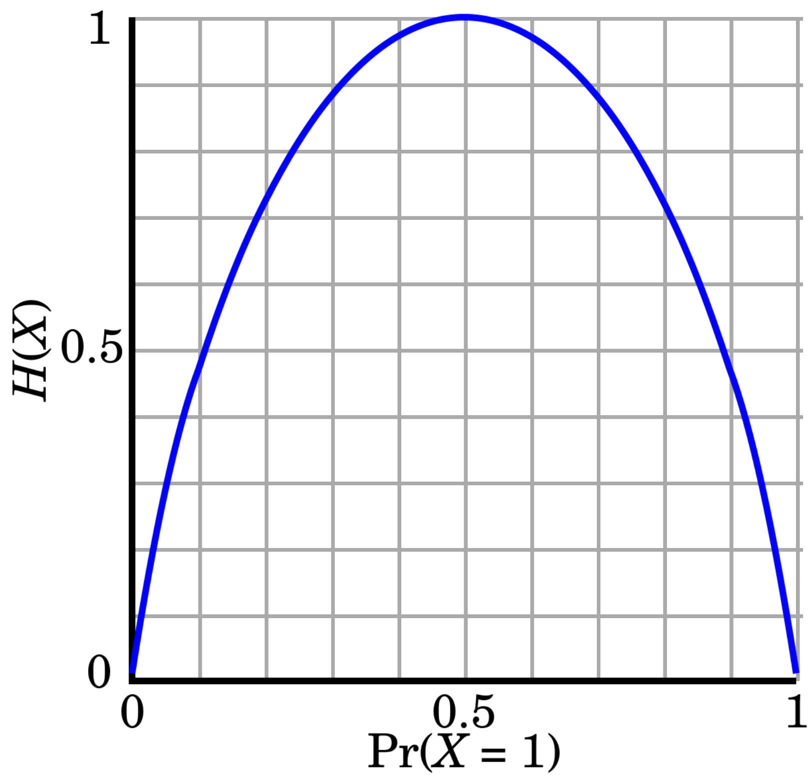

Information Theory: Conditional Entropy

$$H(Y|X) = \sum_{x \in \mathcal{X}} \Pr(X = x) H(Y|X = x)$$

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$H(Y|X=black) = -0.5 \log(0.5) - 0.25 \log(0.25) - 0.25 \log(0.25) - 0 = 1.5$

$H(Y|X=white) = -0.5 \log(0.5) - 0.25 \log(0.25) - 0 - 0.25 \log(0.25) = 1.5$

$H(Y|X) = 0.5 * H(Y|X=black) + 0.5 * H(Y|X=white) = 1.5$

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I(Y:X) = H(Y) – H(Y|X) = 1.75 – 1.5 = 0.25

DT Learning: Back to Splits

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Want to choose split S that maximizes

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- Equivalent to maximally reducing the entropy of Y conditioned on a split S

DT Learning: InfoGain Example

Simple binary classification (**play tennis**?) with 4 features.

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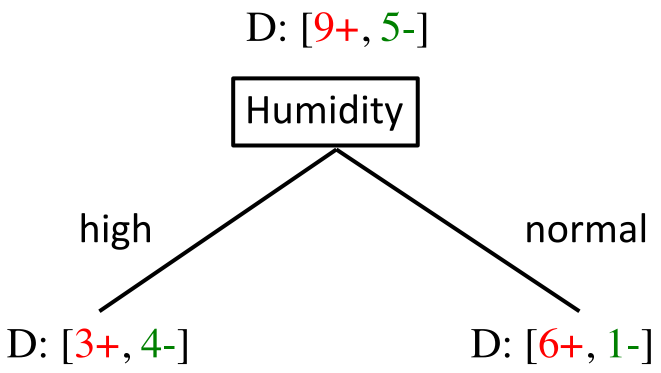
PlayTennis: training examples

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

DT Learning: InfoGain For One Split

- What is the information gain of splitting on Humidity?



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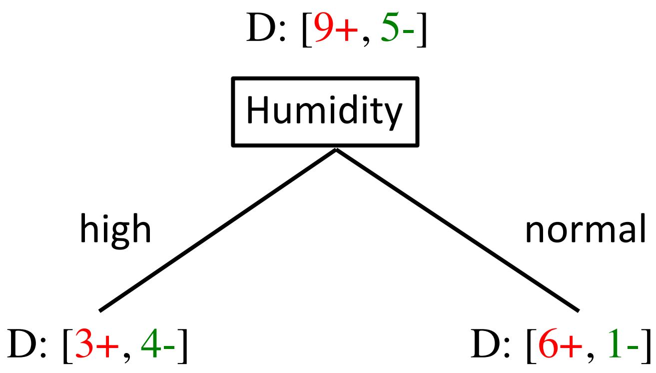

$$H_D(Y) = -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right) = 0.940$$

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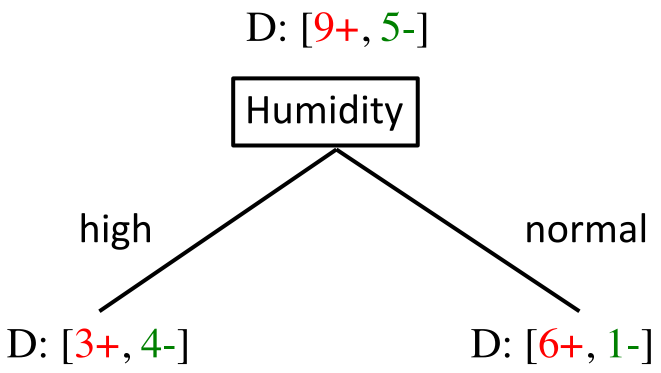

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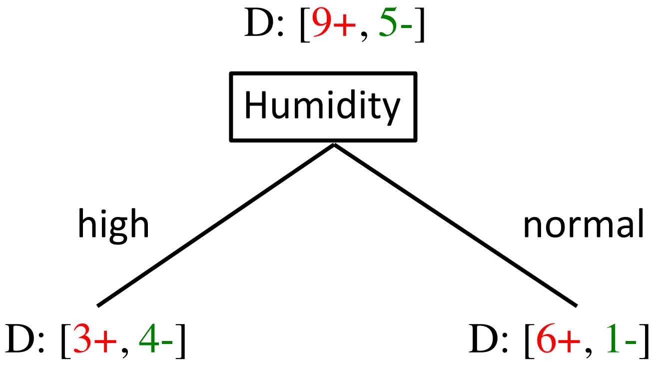

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$$H_D(Y \mid \text{normal}) = -\frac{6}{7}\log_2\left(\frac{6}{7}\right) - \frac{1}{7}\log_2\left(\frac{1}{7}\right)$$
$$= 0.592$$

DT Learning: InfoGain For One Split

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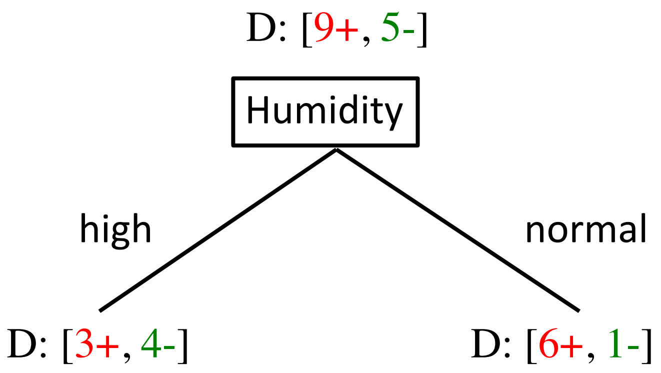

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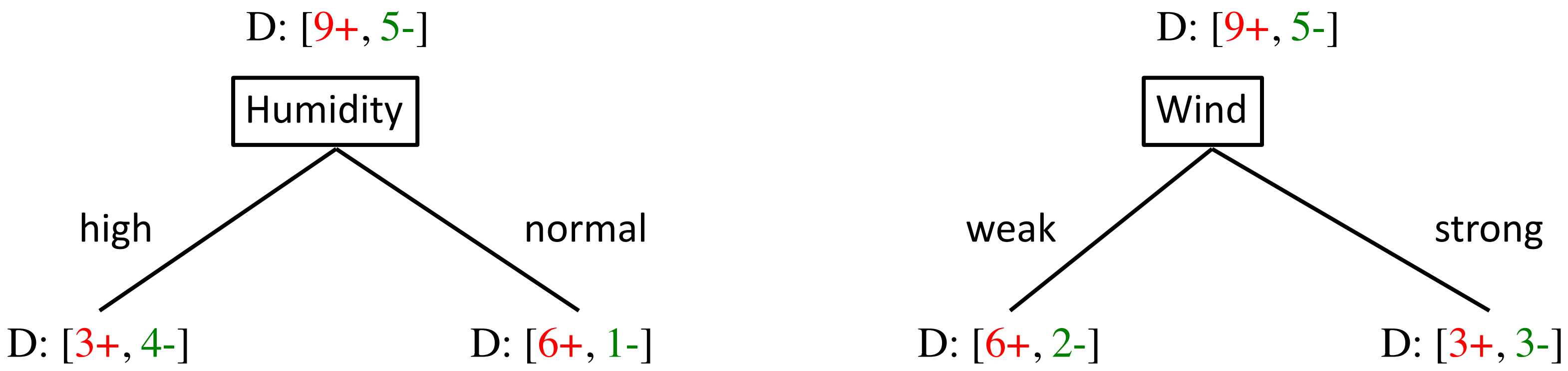
$$\begin{aligned}\text{InfoGain}(D, \text{Humidity}) &= H_D(Y) - H_D(Y \mid \text{Humidity}) \\ &= 0.940 - \left[\frac{7}{14}(0.985) + \frac{7}{14}(0.592)\right] \\ &= 0.151\end{aligned}$$

DT Learning: Comparing Split InfoGains

- Is it better to split on **Humidity** or **Wind**?



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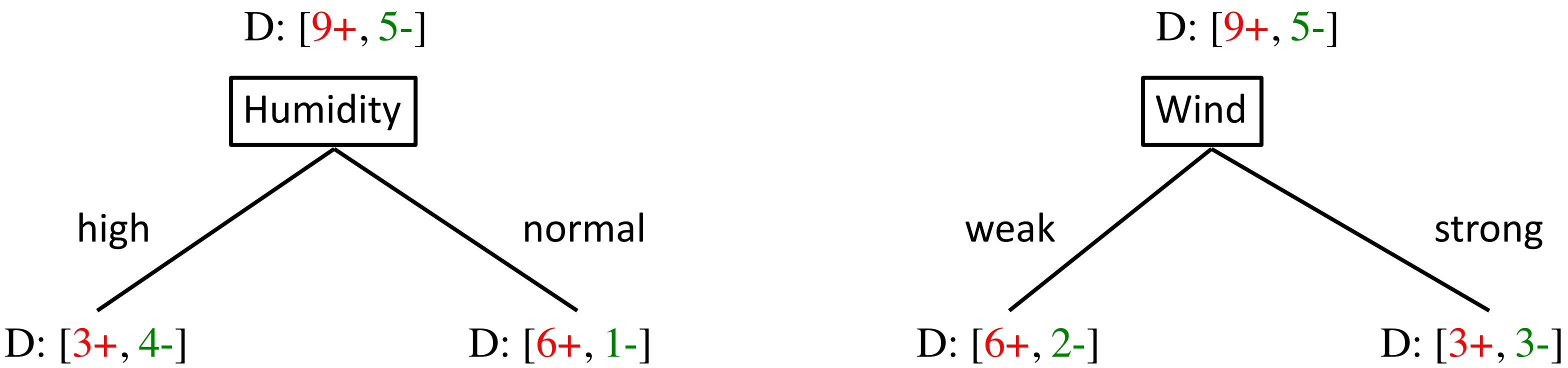

$$H_D(Y \mid \text{weak}) = 0.811$$

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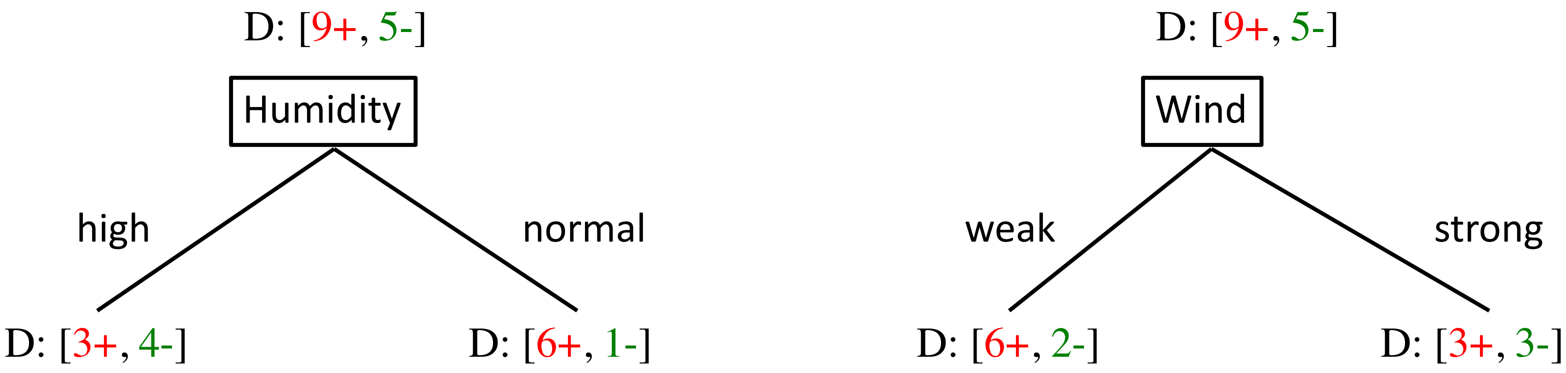

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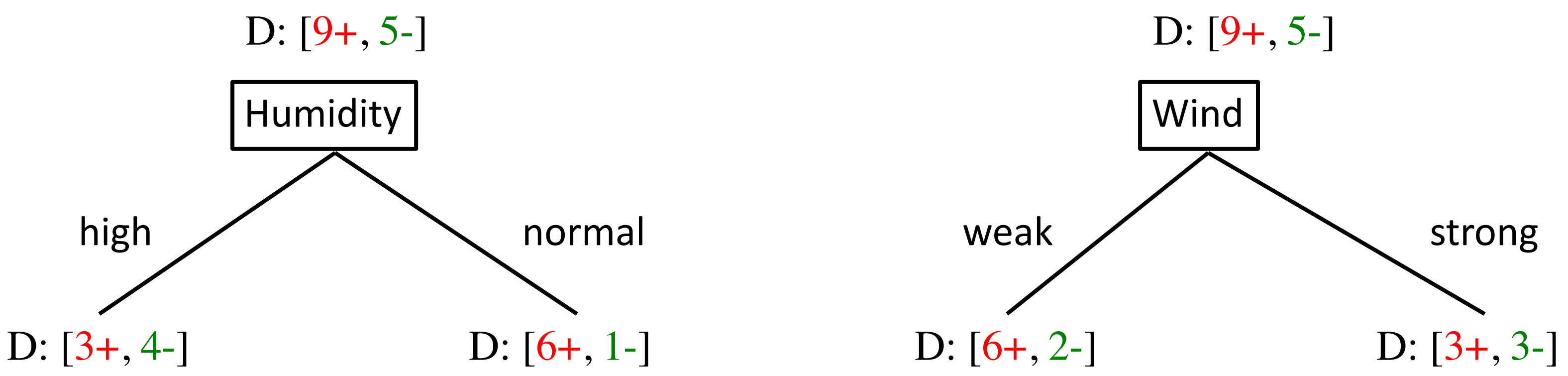

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✔

$$\begin{aligned}\text{InfoGain}(D, \text{Humidity}) &= 0.940 - \left[\frac{7}{14}(0.985) + \frac{7}{14}(0.592)\right] \\ &= 0.151\end{aligned}$$

$$\begin{aligned}\text{InfoGain}(D, \text{Wind}) &= 0.940 - \left[\frac{8}{14}(0.811) + \frac{6}{14}(1.0)\right] \\ &= 0.048\end{aligned}$$

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- Use **GainRatio**: normalize information gain by entropy

$$\text{GainRatio}(D, S) = \frac{\text{InfoGain}(D,S)}{H_D(S)} = \frac{H_D(Y) - H_D(Y|S)}{H_D(S)}$$

Homework: What is a good stopping criteria?

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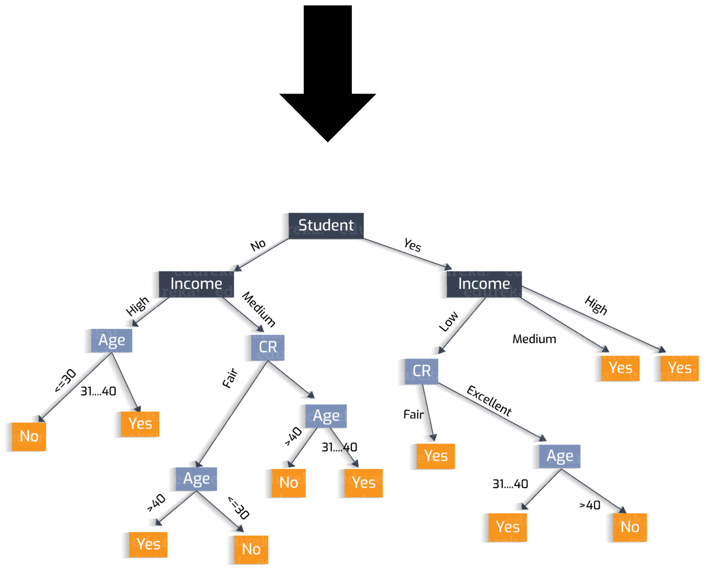

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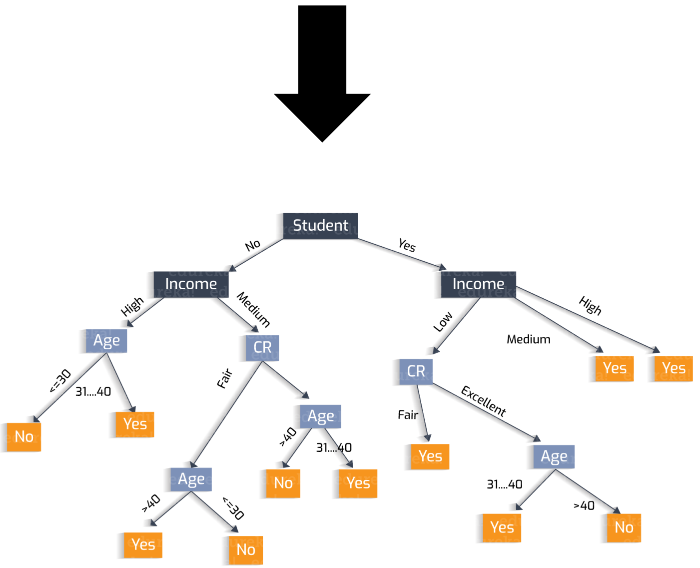

MakeSubtree(set of training instances D)

C = **DetermineCandidateSplits**(D)

if **stopping criteria** is met

make a leaf node N

determine class label for N

else

make an internal node N

S = **FindBestSplit**(D, C)

for each group k of S

D_k = subset of training data in group k

k^{th} child of N = MakeSubtree(D_k)

return subtree rooted at N

Inductive Bias

- Recall: ***Inductive bias***: assumptions a learner uses to predict y_i for a previously unseen instance $\boldsymbol{x}_i$
- Two components
  - *hypothesis space bias*: determines the models that can be represented
  - *preference bias*: specifies a preference ordering within the space of models

learner	**hypothesis space bias**	**preference bias**
Decision trees	trees with single-feature, axis-parallel splits	small trees identified by greedy search
k-NN	Decomposition of space determined by nearest neighbors	Instances in neighborhood belong to same class

Q3-1: Which of the following statements are True?

1. In a decision tree, once you split using one feature, you cannot split again using the same feature.
2. We should split along all features to create a decision tree.
3. We should keep splitting the tree until there is only one data point left at each leaf node.

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They are all false!

Today’s Learning Outcomes

- **After today’s lecture:**
  - You will be able to explain how the k-nearest neighbor’s algorithm classifies unseen instances.
  - You will be able to explain the concept of an inductive bias.
  - You will be able to explain how a decision tree classifies instances.

Thanks Everyone!

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, Pedro Domingos, Jerry Zhu, Yingyu Liang, Volodymyr Kuleshov