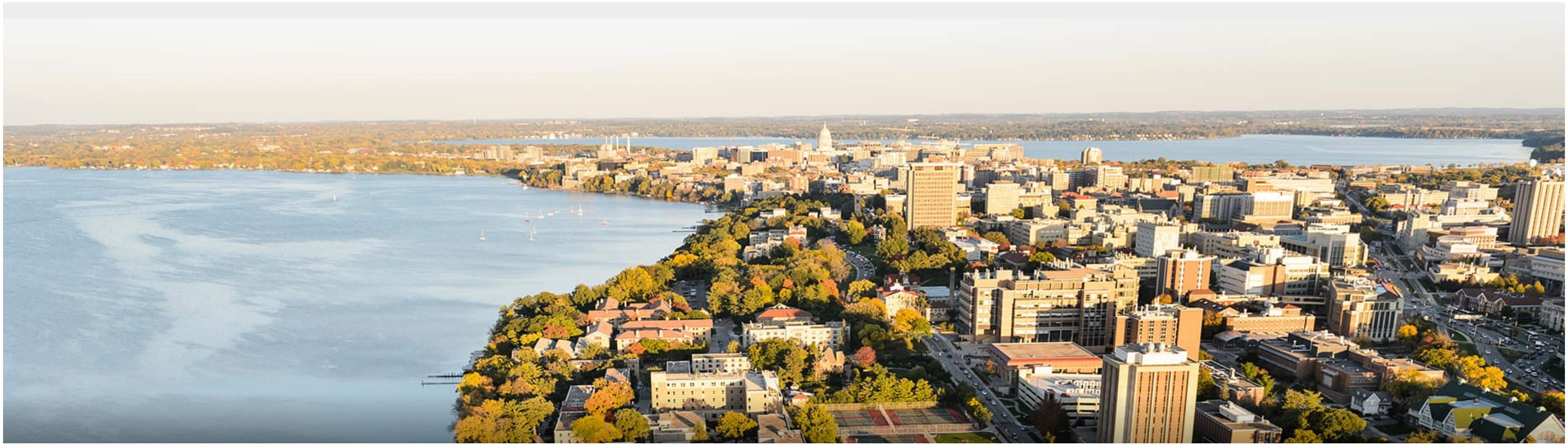

CS 760: Machine Learning
Supervised Learning I

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9/15/2021

Announcements

- Class roadmap:

Thursday Sept. 15	Supervised Learning I
Tuesday Sept. 20	Supervised Learning II
Thursday Sept. 22	Evaluation
Tuesday Sept. 27	Regression I
Thursday Sept. 29	Regression II

All Supervised Learning

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

- Set of possible instances $\mathcal{X}$
- Unknown *target function* $f : \mathcal{X} \rightarrow \mathcal{Y}$
- Set of *models* (a.k.a. *hypotheses*): $\mathcal{H} = \{h | h : \mathcal{X} \rightarrow \mathcal{Y}\}$

Get

- Training set of instances for unknown target function,

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

safe

poisonous

safe

Supervised Learning: Objects

Three types of sets

- Input space, output space, hypothesis class

$$\mathcal{X}, \mathcal{Y}, \mathcal{H}$$

- **Examples**:
  - Input space: feature vectors $\mathcal{X} \subseteq \mathbb{R}^d$

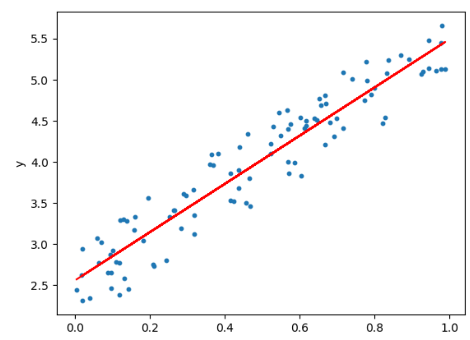
  - Output space:
    - **Binary** $\mathcal{Y} = \{-1, +1\}$ safe poisonous
    - **Continuous** $\mathcal{Y} \subseteq \mathbb{R}$ 13.23°

Output space: Classification vs. Regression

Choices of $\mathcal{Y}$ have special names:

- Discrete: "**classification**". The elements of $\mathcal{Y}$ are **classes**
  - Note: doesn't have to be binary

- Continuous: "**regression**"
  - Example: linear regression



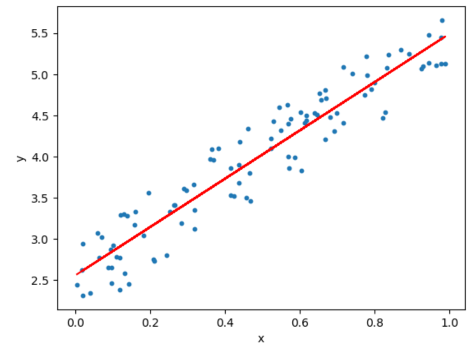
- There are other types…

Hypothesis class

We talked about $\mathcal{X}, \mathcal{Y}$ what about $\mathcal{H}$?

- Pick specific class of models. Ex: **linear models**:

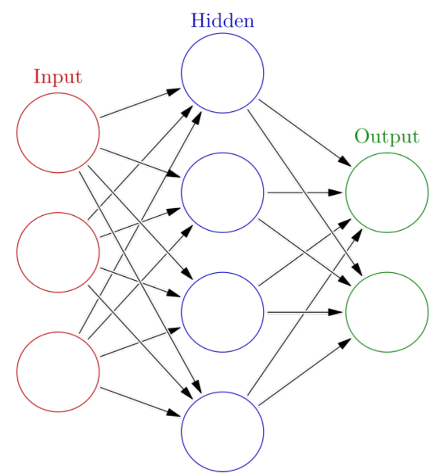
$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d$$



- Ex: **feedforward neural networks**

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

- **Parameters:** θs, Ws.



Wikipedia

SL: Training & Generalization

Goal: model *h* that best approximates *f*

- One way: empirical risk minimization (ERM)

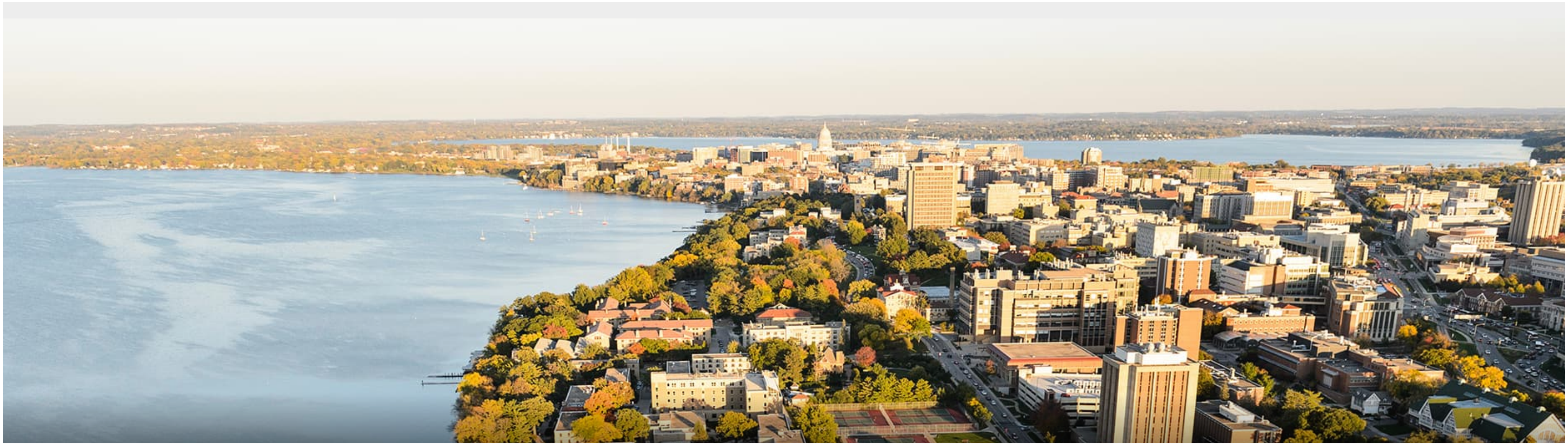
$$\hat{f} = \arg\min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}))$$

Model prediction

Hypothesis Class

Loss function (how far are we)?

- Generalization?



Break & Questions

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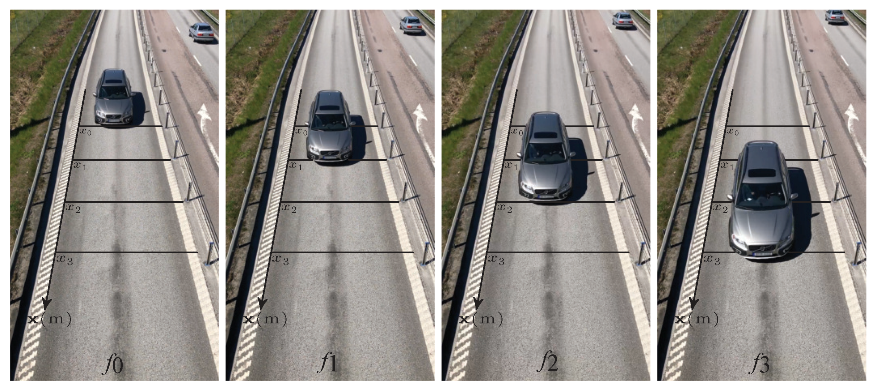
Nearest Neighbors: Idea

Basic idea: “nearby” feature vectors more likely have the same label

- **Example**: classify car/no car
  - All features same, except location of car

- What does “nearby” mean?



1-Nearest Neighbors: Algorithm

Training/learning: given

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

Do nothing. ("**lazy learner**").

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

1-Nearest Neighbors: Algorithm

Training/learning: given

safe

poisonous

x

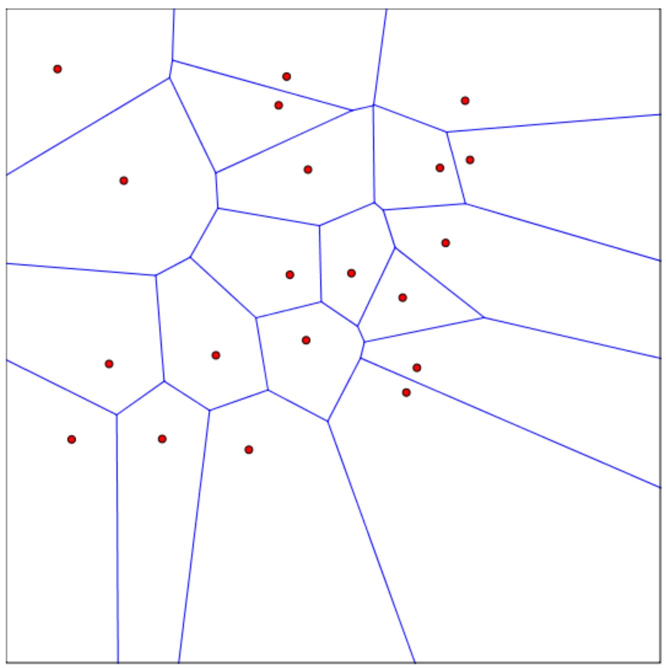
Prediction: for x, find nearest training point $x^{(j)}$

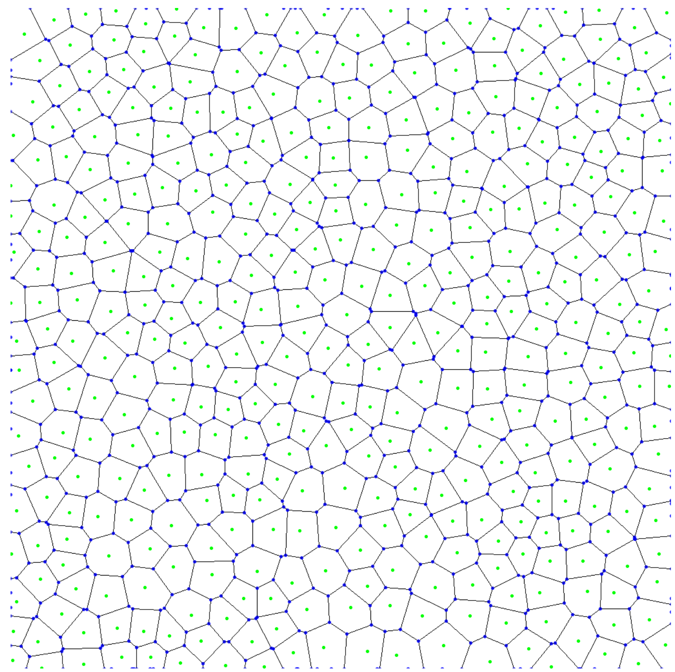
Return $y^{(j)}$ **poisonous**

1NN: Decision Regions

Defined by "**Voronoi Diagram**"

- Each cell contains points closer to a particular training point





k-Nearest Neighbors: Classification

Training/learning: given

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

Prediction: for x , find ***k*** most similar training points

Return plurality class

$$\hat{y} \leftarrow \arg\max_{v \in \mathcal{Y}} \sum_{i=1}^{k} \delta(v, y^{(i)})$$

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

k-Nearest Neighbors: Distances

Discrete features: Hamming distance

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

Continuous features:

- Euclidean distance:

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

- L1 (Manhattan) dist.:

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

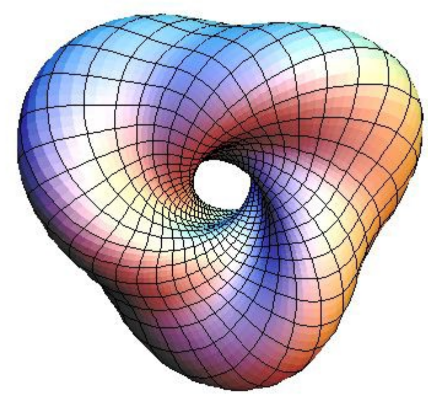
k-Nearest Neighbors: Mixed Distances

Might have features of both types

- Sum two types of distances components

- Might need **normalization**,
  - E.g., $\max_{i,a}\{x_a^{(i)}\} = 1$. Fix range, or ensure some distribution.

- Many other choices of distance.



k-Nearest Neighbors: Standardization

Typical in data science applications. Recipe:

- Compute empirical mean/stddev for a feature (in train set)

$$\mu_a = \frac{1}{n}\sum_{i=1}^{n} x_a^{(i)} \qquad\qquad \sigma_a = \left(\frac{1}{n}\sum_{i=1}^{n}(x_a^{(i)} - \mu_i)^2\right)^{\frac{1}{2}}$$

- Standardize features:
  - Do the same for test points!

$$\tilde{x}_a^{(j)} = \frac{x_a^{(j)} - \mu_a}{\sigma_a}$$

k-Nearest Neighbors: Regression

Training/learning: given

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

Prediction: for x , find ***k*** most similar training points

Return

$$\hat{y} = \frac{1}{k} \sum_{i=1}^{k} y^{(i)}$$

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

k-Nearest Neighbors: Variations

Could contribute to predictions via a weighted distance

- All k no longer equally contribute
- Classification / regression

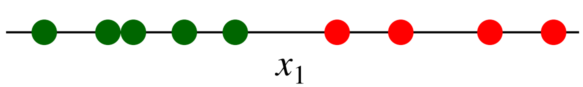
$$\hat{y} \leftarrow \arg\max_{v \in \mathcal{Y}} \sum_{i=1}^{k} \frac{1}{d(x, x^{(i)})^2} \delta(v, y^{(i)})$$

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

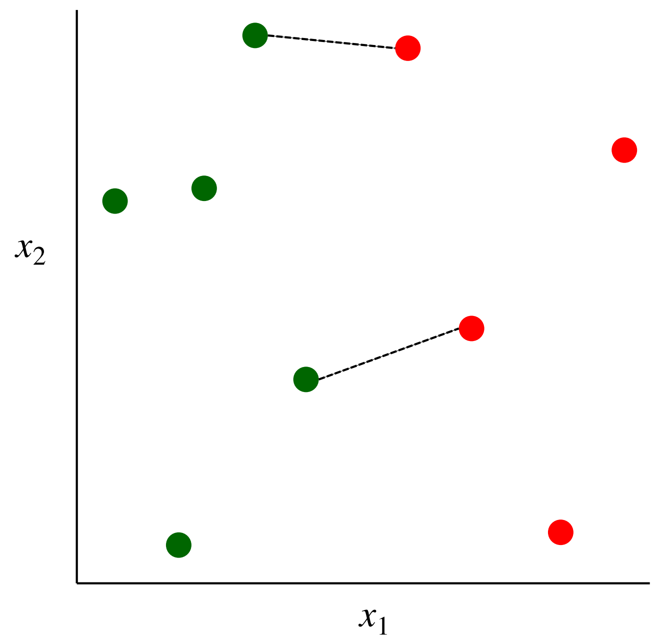
Dealing with **Irrelevant Features**

One relevant feature x_1

1-NN rule classifies each instance correctly



Effect of an irrelevant feature x_2 on distances and nearest neighbors



Locally Weighted Regression

- Intuitively, want to weight features differently
  - Locally weighted regression: kNN variation doing this

- Instead of standard kNN return value, do

$$f(x) = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

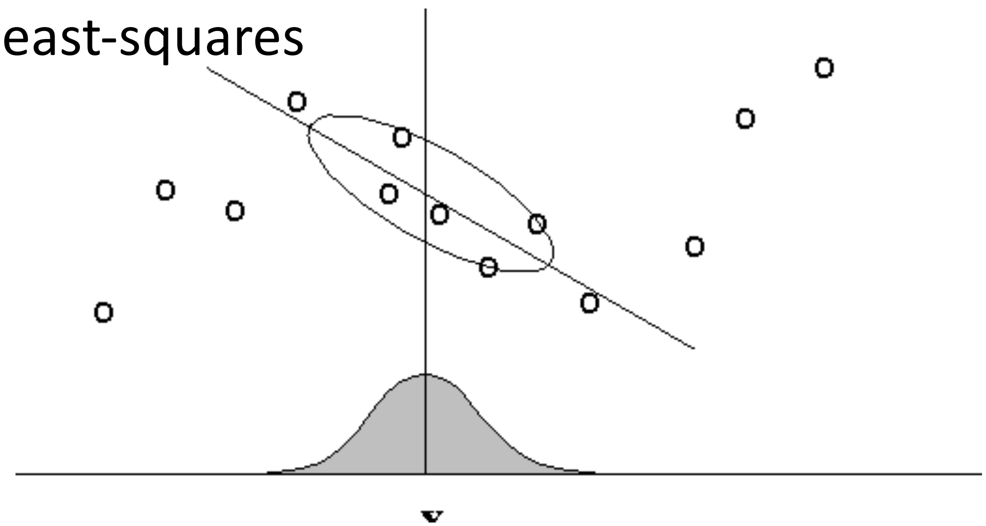
- Look familiar? **Linear prediction**
  - How do the neighbors come into play?

Locally Weighted Regression

- Need the **weights**
  - For each prediction x, minimize the loss

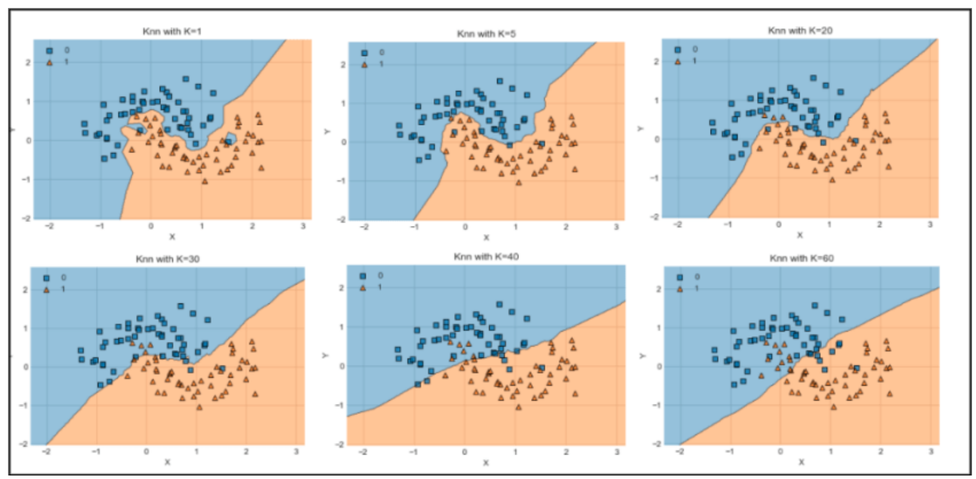
$$E(x) = \sum_{i=1}^{k} (f(x^{(i)}) - y^{(i)})^2$$

- In other words, **combination** of least-squares linear regression with kNN.



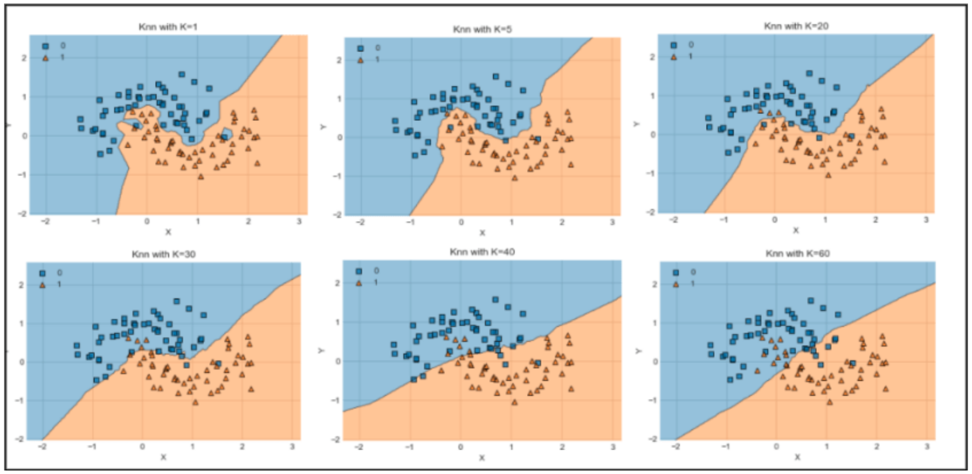
Instance-Based Learning: Strengths

- Simple to implement
- No training!
- Easily done online
- Robust to noisy data (for enough samples)
- Often good in practice!



Instance-Based Learning: Weaknesses

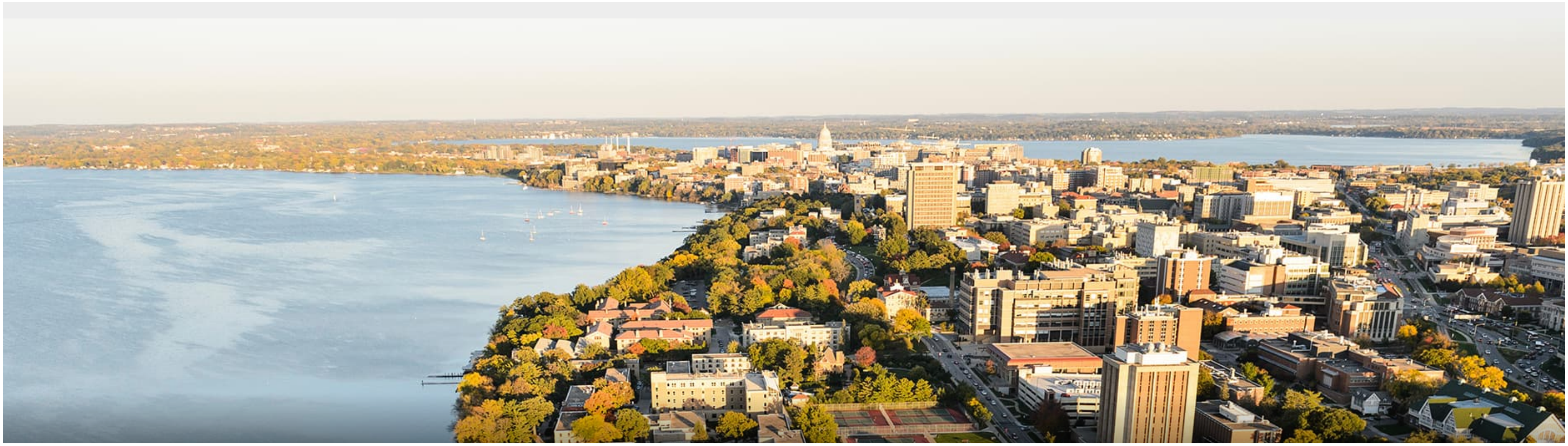
- Sensitive to range of values
- Sensitive to irrelevant + correlated features
  - Can try to solve via variations. More later
- Prediction stage can be expensive
- No “model” to examine



Inductive Bias

- ***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
k-NN	Voronoi decomposition 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 3NN 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	-

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

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

x	y	label
0	0	+
1	0	+
2	0	+
2	2	+
0	1	-
0	2	-
1	2	-
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 weight is **NOT** appropriate? Let p be the test data point and x_i {i = 1: N} be training data points.

1. $w_i = d(p, x_i)^{½}$
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.

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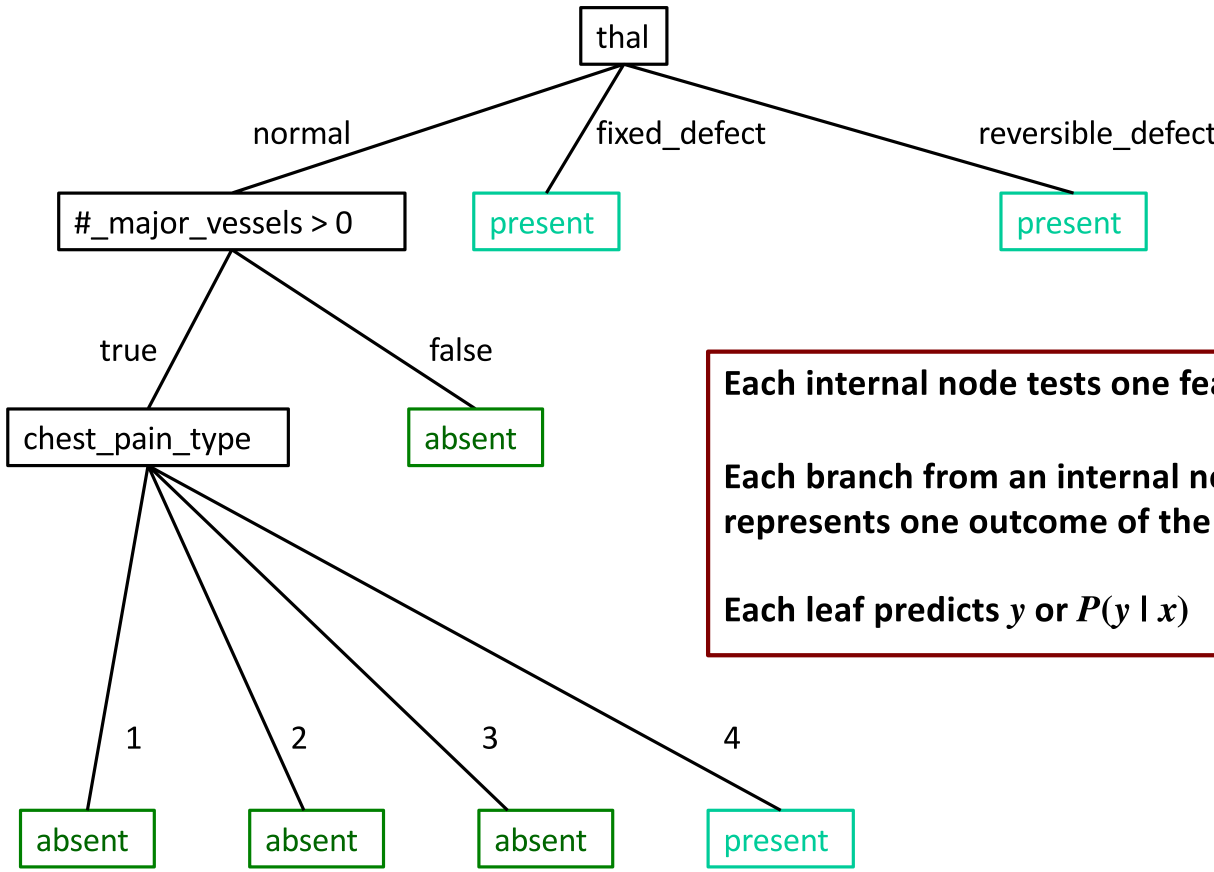
Decision Trees: Heart Disease Example



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 $P(y \mid x)$

Decision Trees: Logical Formulas

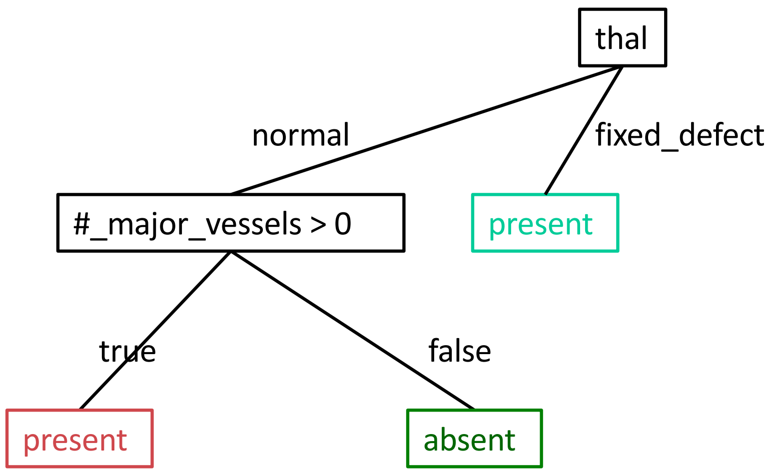
- Suppose $X_1 \ldots X_5$ are Boolean features, and Y is also Boolean
  - How would you represent the following with decision trees?

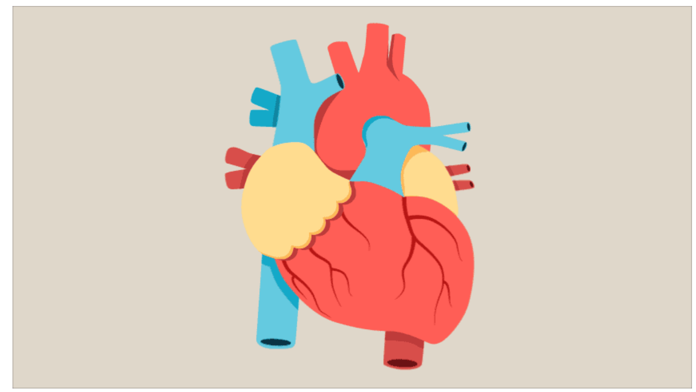
$$Y = X_2 X_5 \quad (\text{i.e.}, Y = X_2 \wedge X_5)$$

$$Y = X_2 \vee X_5$$

$$Y = X_2 X_5 \vee X_3 \neg X_1$$

Decision Trees: Textual Description





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)
```

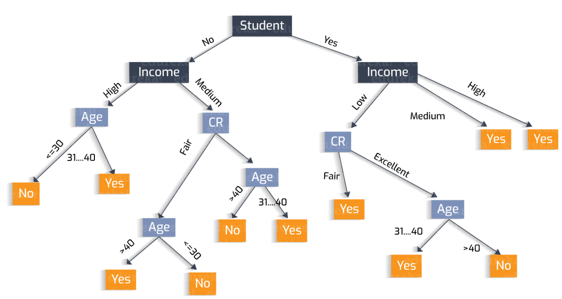
if odor=almond, predict edible

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

Decision Trees: Learning

- **Learning Algorithm**:

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



MakeSubtree(set of training instances D)

 C = DetermineCandidateSplits(D)

 if stopping criteria met

  make a leaf node N

  determine class label/probabilities for N

 else

  make an internal node N

  S = FindBestSplit(D, C)

  for each outcome k of S

   D_k = subset of instances that have outcome k

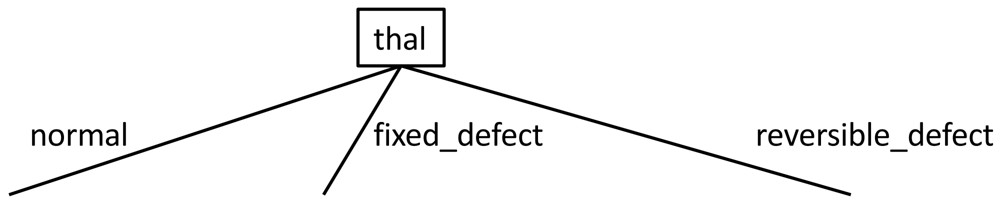
   k^{th} child of N = MakeSubtree(D_k)

 return subtree rooted at N

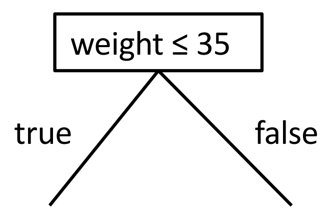
DT Learning: Candidate Splits

First, need to determine how to **split features**

- Splits on nominal features have one branch per value



- Splits on numeric features use a threshold/interval

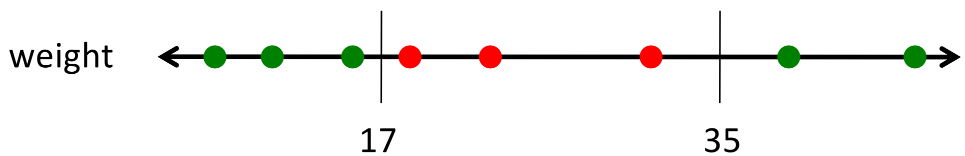


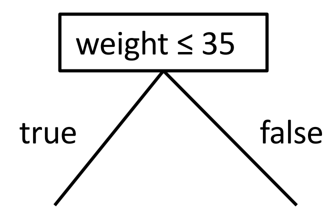
ID3, C4.5

DT Learning: Numeric Feature Splits

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

S = partition instances in D into sets $s_1 \ldots s_V$ where the instances in each set have the same value for X_i

let v_j denote the value of X_i for set s_j

sort the sets in S using v_j as the key for each s_j

for each pair of adjacent sets s_j, s_{j+1} in sorted S

if s_j and s_{j+1} contain a pair of instances with different class labels

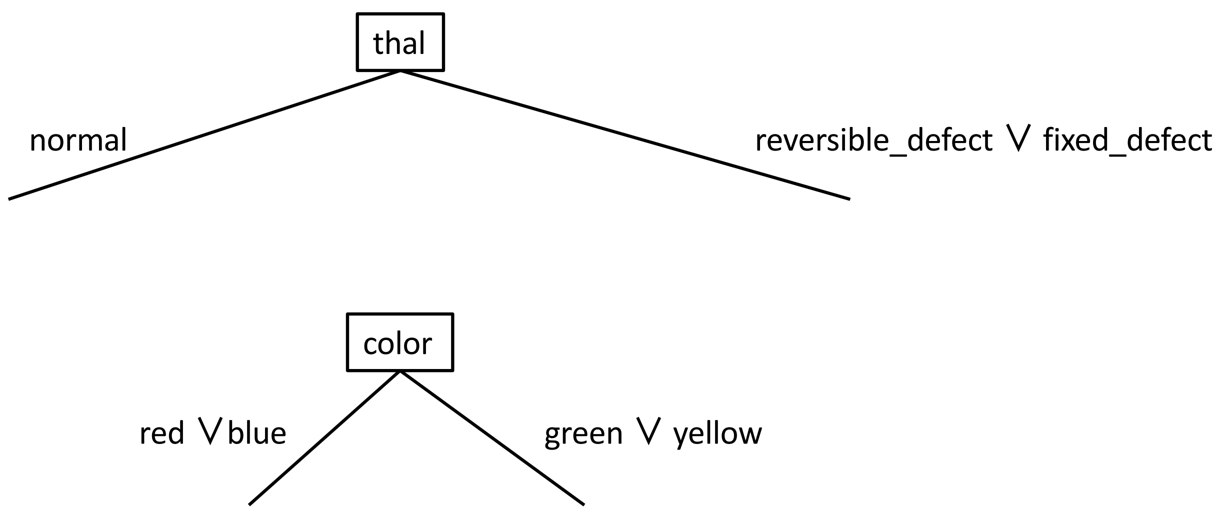
// assume we're using midpoints for splits

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 (CART does this)



DT Learning: Finding the Best Splits

How to we select the best feature to split on at each step?

- **Hypothesis**: simplest tree that classifies the training instances accurately will generalize

Occam's razor

- "Nunquam ponenda est pluralitis sin necesitate"
- "Entities should not be multiplied beyond necessity"
- "when you have two competing theories that make the same predictions, the simpler one is the better"

DT Learning: Finding the Best Splits

Occam's razor

- "Nunquam ponenda est pluralitis sin necesitate"
- "Entities should not be multiplied beyond necessity"
- "when you have two competing theories that make the same predictions, the simpler one is the better"

- **Ptolemy** (~1000 years earlier)
- "We consider it a good principle to explain the phenomena by the simplest hypothesis possible."

Ptolemy

DT Learning: Finding the Best Splits

How to we select the best feature to split on at each step?

- **Hypothesis**: simplest tree that classifies the training instances accurately will generalize

Why is Occam’s razor a **reasonable heuristic?**

- There are fewer short models (i.e. small trees) than long ones
- A short model is unlikely to fit the training data well by chance
- A long model is more likely to fit the training data well coincidentally

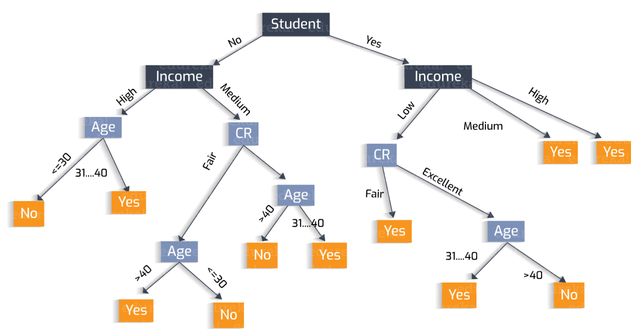
DT Learning: Finding Optimal Splits?

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

- **NO! This is an NP-hard problem**

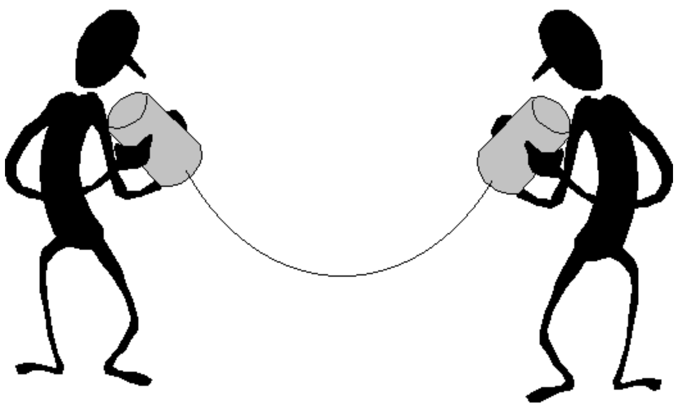
  [Hyafil & Rivest, *Information Processing Letters, 1976]*

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



Information Theory: Super-Quick Intro

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



Information Theory: Encoding

- Could yell out the names of the manufacturers…
  - Suppose there are 4: **Trek**, **Specialized**, **Cervelo**, **Serrota**

- Inefficient… since there's just 4, we could **encode** them
  - # of bits: 2 per communication

type	code
Trek	11
Specialized	10
Cervelo	01
Serrota	00

Information Theory: Encoding

- Now, some bikes are rarer than others…
  - **Cervelo** is a rarer specialty bike.
  - We could **save some bits**… make more popular messages fewer bits, rarer ones more bits
  - Note: this is **on average**

- Expected # bits: **1.75**

$$-\sum_{y \in \mathcal{Y}} P(y) \log_2 P(y)$$

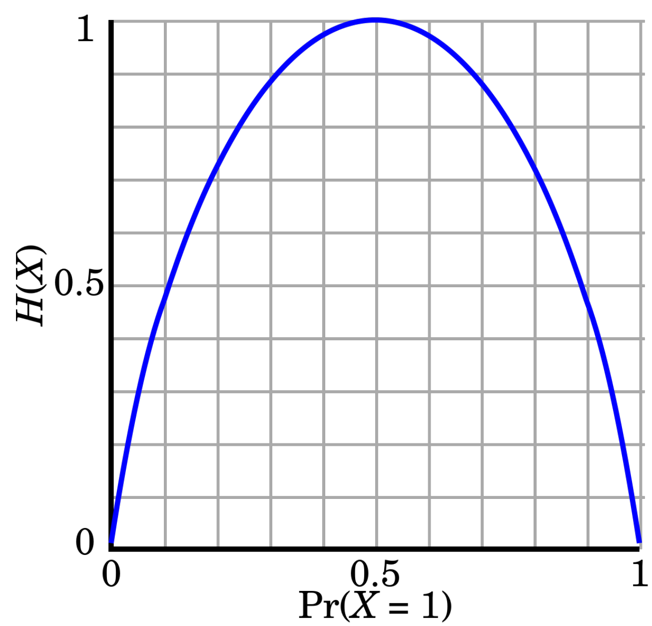
Type/probability	# bits	code
$P(\text{Trek}) = 0.5$	1	1
$P(\text{Specialized}) = 0.25$	2	01
$P(\text{Cervelo}) = 0.125$	3	001
$P(\text{Serrota}) = 0.125$	3	000

Information Theory: Entropy

- Measure of uncertainty for random variables/distributions

- **Expected number of bits** required to communicate the value of the variable

$$H(Y) = -\sum_{y \in \mathcal{Y}} P(y) \log_2 P(y)$$



Information Theory: Conditional Entropy

- Suppose we know *X*. **CE**: how much uncertainty left in *Y*?

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

- Here,

$$H(Y|X = x) = -\sum_{y \in \mathcal{Y}} P(Y = y|X = x) \log_2 P(Y = y|X = x)$$

- What is it if Y=X?
- What if Y is **independent** of X?

Information Theory: Conditional Entropy

- Example. *Y* is still the bike maker, *X* is color.

Y=Type/X=Color	Black	White
Trek	0.25	0.25
Specialized	0.125	0.125
Cervelo	0.125	0
Serrota	0	0.125

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

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

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

Information Theory: Mutual Information

- Similar comparison between R.V.s:

$$I(Y;X) = H(Y) - H(Y|X)$$

- How much uncertainty of Y that X can reduce.

Y=Type/X=Color	Black	White
Trek	0.25	0.25
Specialized	0.125	0.125
Cervelo	0.125	0
Serrota	0	0.125

$$I(Y;X) = H(Y) - H(Y|X) = 1.75 - 1.5 = 0.25$$

DT Learning: Back to Splits

Want to choose split S that maximizes

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

ie, mutual information.

- Note: D denotes that this is the **empirical** entropy
  - We don't know the real distribution of *Y*, just have our dataset

- Equivalent to maximally reduces conditional entropy of Y

DT Learning: InfoGain Example

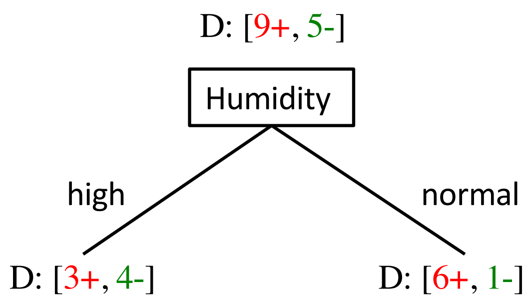
Simple binary classification (**play tennis**?) with 4 features.

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's the information gain of splitting on Humidity?



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

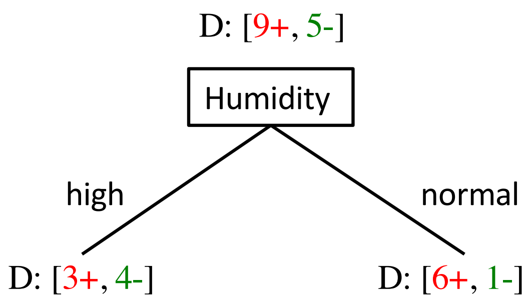
$$H_D(Y \mid \text{high}) = -\frac{3}{7}\log_2\left(\frac{3}{7}\right) - \frac{4}{7}\log_2\left(\frac{4}{7}\right)$$
$$= 0.985$$

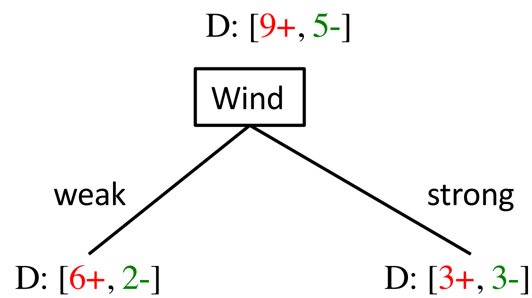
$$H_D(Y \mid \text{normal}) = -\frac{6}{7}\log_2\left(\frac{6}{7}\right) - \frac{1}{7}\log_2\left(\frac{1}{7}\right)$$
$$= 0.592$$

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

DT Learning: Comparing Split InfoGains

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





$H_D(Y \mid \text{weak}) = 0.811$ $\quad$ $H_D(Y \mid \text{strong}) = 1.0$

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

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

DT Learning: InfoGain Limitations

- InfoGain is biased towards tests with many outcomes
  - A feature that uniquely identifies each instance
  - Splitting on it results in many branches, each of which is "pure" (has instances of only one class)
  - **Maximal** information gain!

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

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

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
ID3 decision tree	trees with single-feature, axis-parallel splits	small trees identified by greedy search
k-NN	Voronoi decomposition determined by nearest neighbors	instances in neighborhood belong to same class

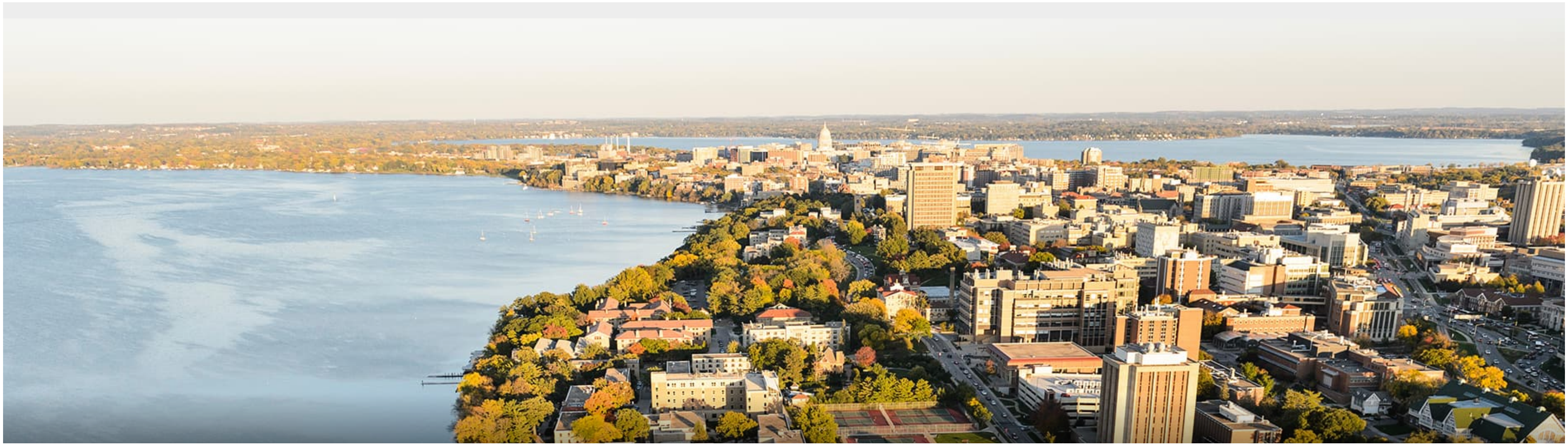
Q3-1: How many distinct (binary classification) decision trees are possible with *4* Boolean attributes? Here distinct means representing different functions.

1. 2^4
2. 2^8
3. 2^{16}
4. 2^{32}

Q3-1: How many distinct (binary classification) decision trees are possible with *4* Boolean attributes? Here distinct means representing different functions.

1. 2^4
2. 2^8
3. 2^{16}
4. 2^{32}

#distinct decision trees
= #distinct Boolean functions
= #functions of 2^4 = 16 inputs, binary label for each input
= $\mathbf{2^{16}}$



Thanks Everyone!

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