As you login

1. Rename yourself in Zoom to *pre*-pend your house number
   - e.g. “0 – Pat Virtue”

2. Open Piazza (getting ready for polls)

3. Download preview slides from course website

4. Grab something to write with/on ☺

Announcements

Assignments

- HW1
  - Due Thu, 9/10, 11:59 pm (all times will be Pittsburgh time)
  - HW1 only – Extension request form – see Piazza
- HW2
  - Out after HW1 due
  - Due Mon, 9/21, 11:59 pm

Announcements

Participation

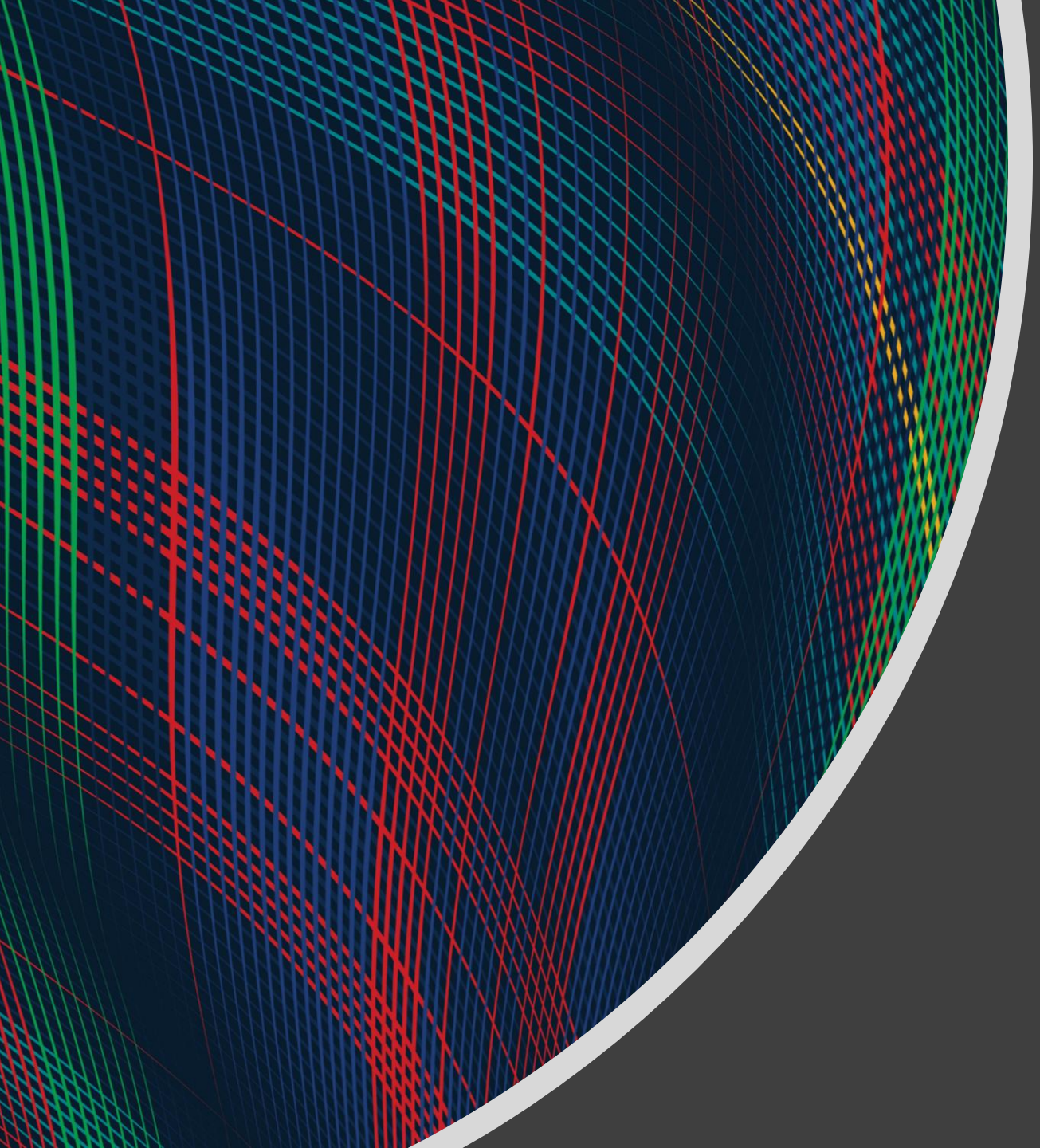
- Earn participation points for study group sessions
- See Piazza for details

OH by appointment

- Check OH Appointment Slots link on course webpage
- Private post on Piazza with appointment request

Breakout rooms

- Video on, unmute
- Introduce yourself if you haven’t already met



Introduction to Machine Learning

Decision Trees

Instructor: Pat Virtue

Plan

Last time

- Problem formulation (notation)
- Algorithm 0-2: Memorization, majority vote, decision stump

Today

- Decision trees
  - Recursive algorithm
  - Better splitting criteria (entropy, mutual information)

Next time

- Wrap up decision trees (overfitting, continuous features)
- Nearest neighbor methods

Decision Trees

A few tools

Majority vote:

$$\hat{y} = \operatorname{argmax}_c \frac{N_c}{N}$$

Classification error rate:

$$ErrorRate = \frac{1}{N}\sum_i \mathbb{I}\left(y^{(i)} \neq \hat{y}^{(i)}\right)$$

What fraction did we predict incorrectly

Expected value

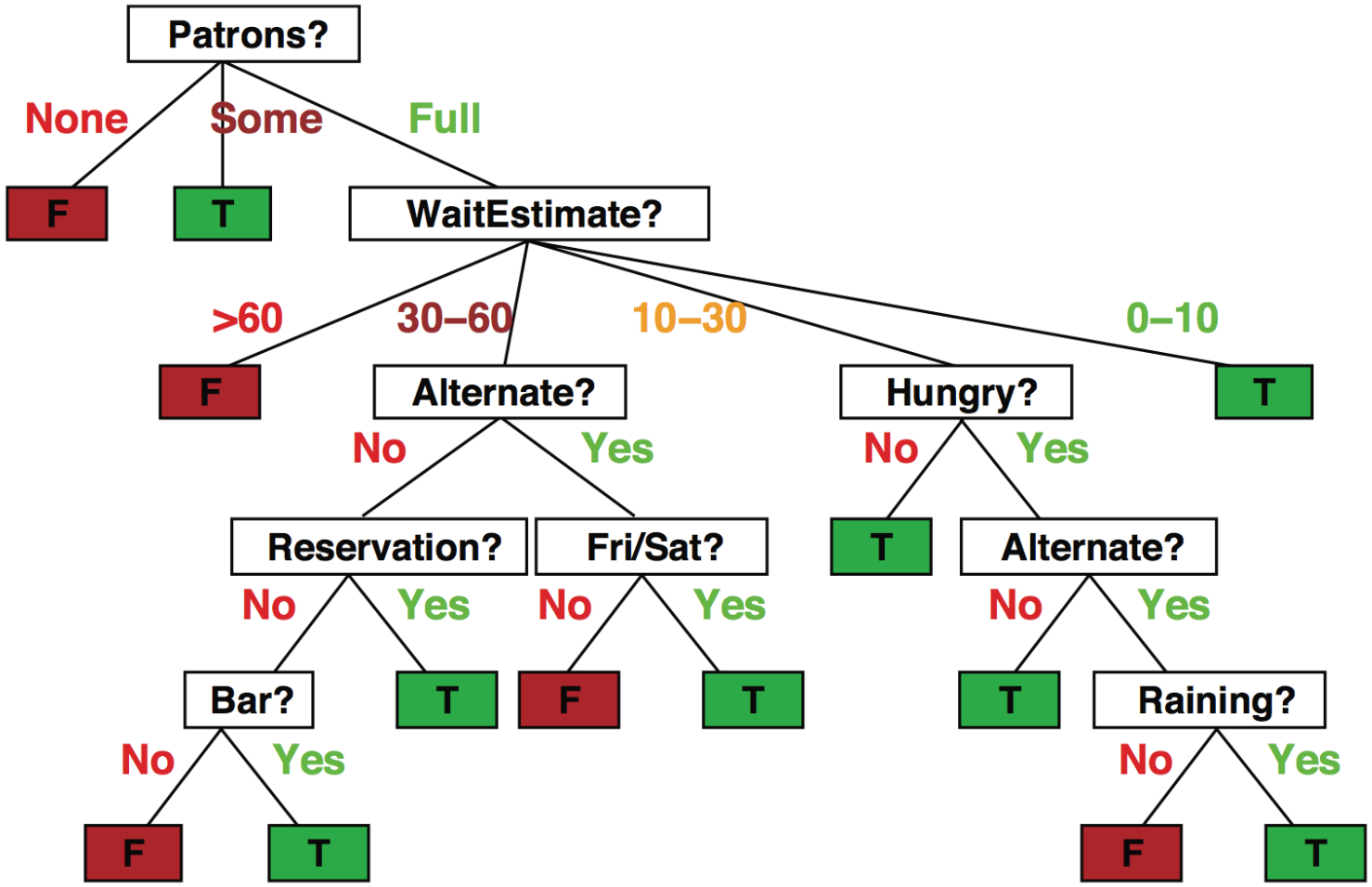
$$\mathbb{E}[f(X)] = \sum_{x \in \mathcal{X}} f(x)\, P(X = x) \quad \text{or} \quad \mathbb{E}[f(X)] = \int_{\mathcal{X}} f(x)\, p(x)\, dx$$

Decision trees

Popular representation for classifiers

- Even among humans!

I’ve just arrived at a restaurant: should I stay (and wait for a table) or go elsewhere?



Slide credit: ai.berkeley.edu

Decision trees

$x = [\text{Friday}, \text{full}, \text{no res}, 45, \text{rain} \ldots]$

$y = ?$

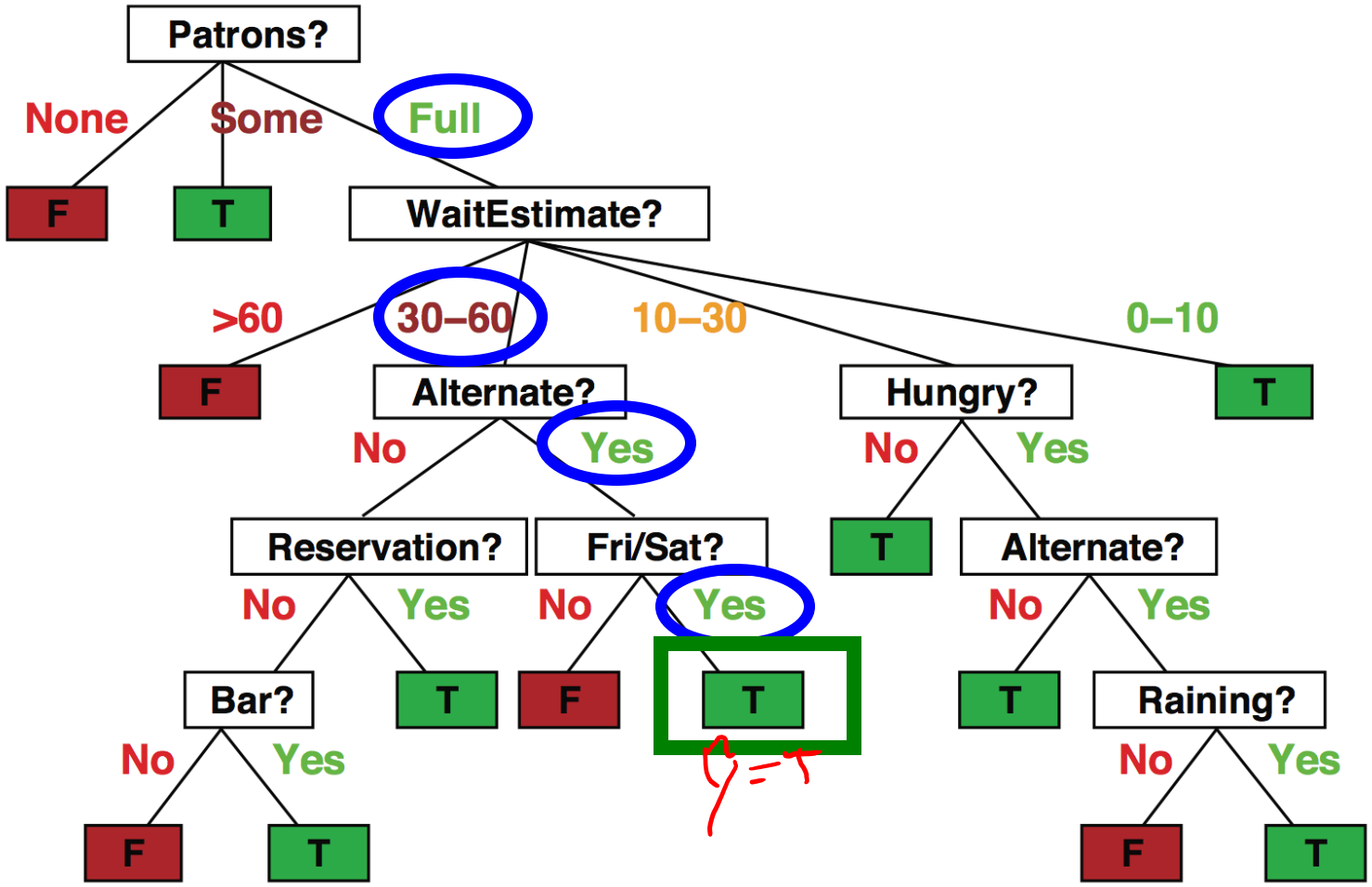
It's Friday night and you're hungry

You arrive at your favorite cheap but really cool happening burger place

It's full and you have no reservation but there is a bar

The host estimates a 45 minute wait

There are alternatives nearby but it's raining outside



Decision tree ***partitions*** the input space, assigns a label to each partition

Slide credit: ai.berkeley.edu

Problem Formulation

Medical Prediction

Y	X_1	X_2	X_3
Outcome	**Fetal Position**	**Fetal Distress**	**Previous C-sec**
Natural	Vertex	N	N
C-section	Breech	N	N
Natural	Vertex	Y	Y
C-section	Vertex	N	Y
Natural	Abnormal	N	N

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = [x_1, x_2, x_3]^T$$

$x_1 \in \{Vertex, Breech, Abn\}$
$x_2 \in \{Y, N\}$
$x_3 \in \{Y, N\}$

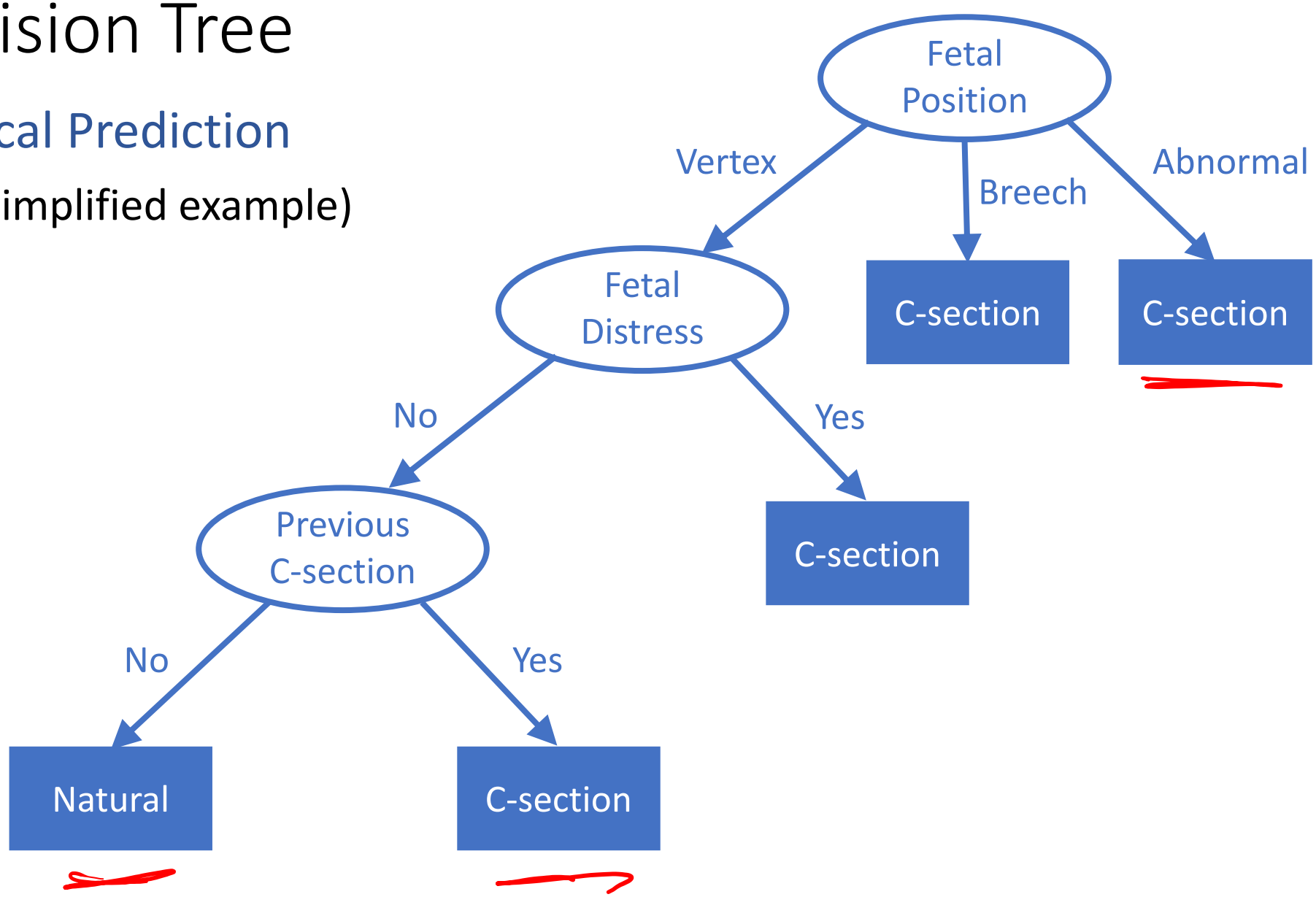
$y \in \{Csection, Natural\}$

$\hat{y} = h(\boldsymbol{x})$

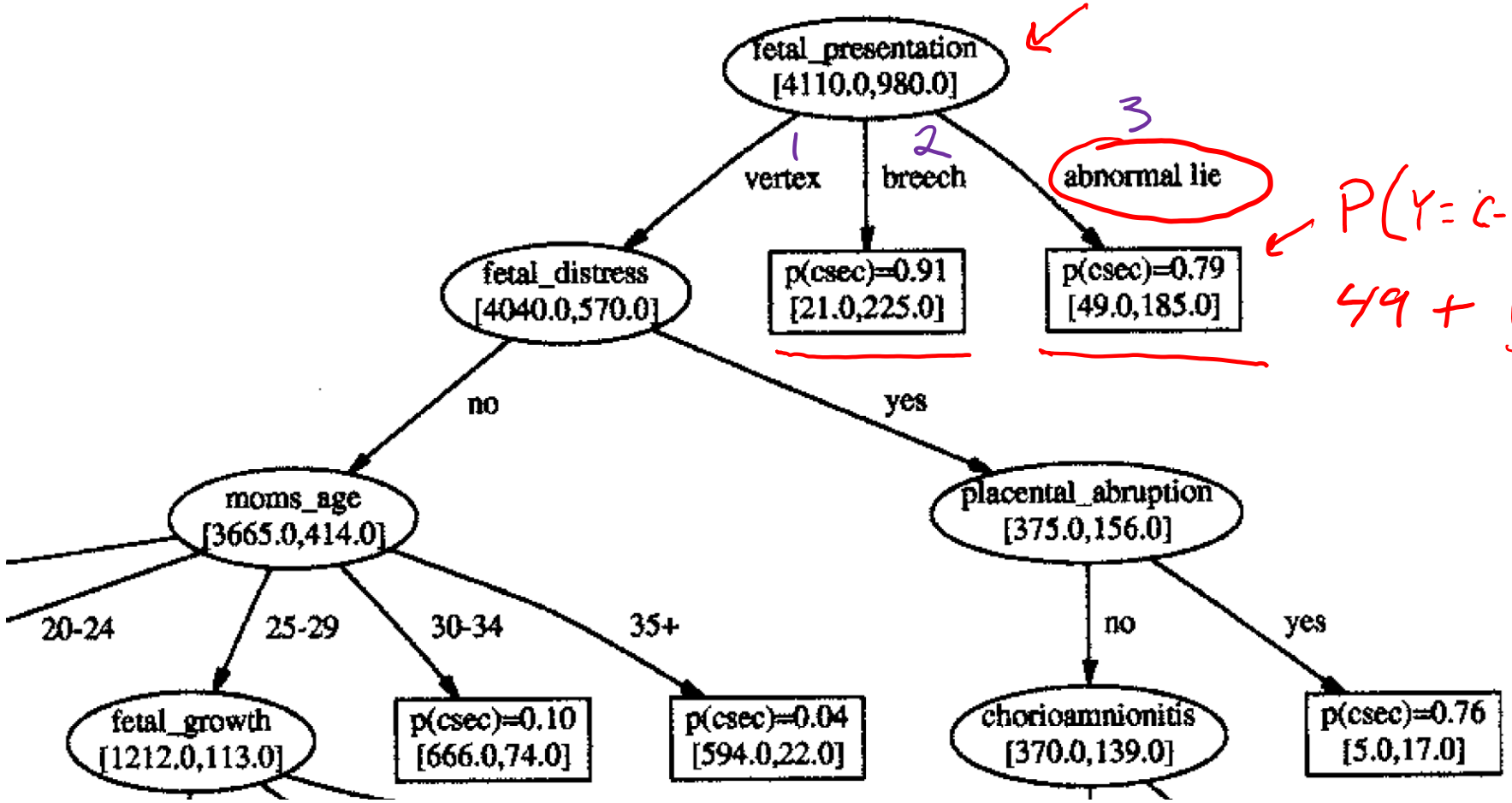
Decision Tree

Medical Prediction

(Oversimplified example)



Tree to Predict C-Section Risk



4110 + 980 −

$P(Y = \text{C-sec} \mid X) = 0.79$

49 + 185 −

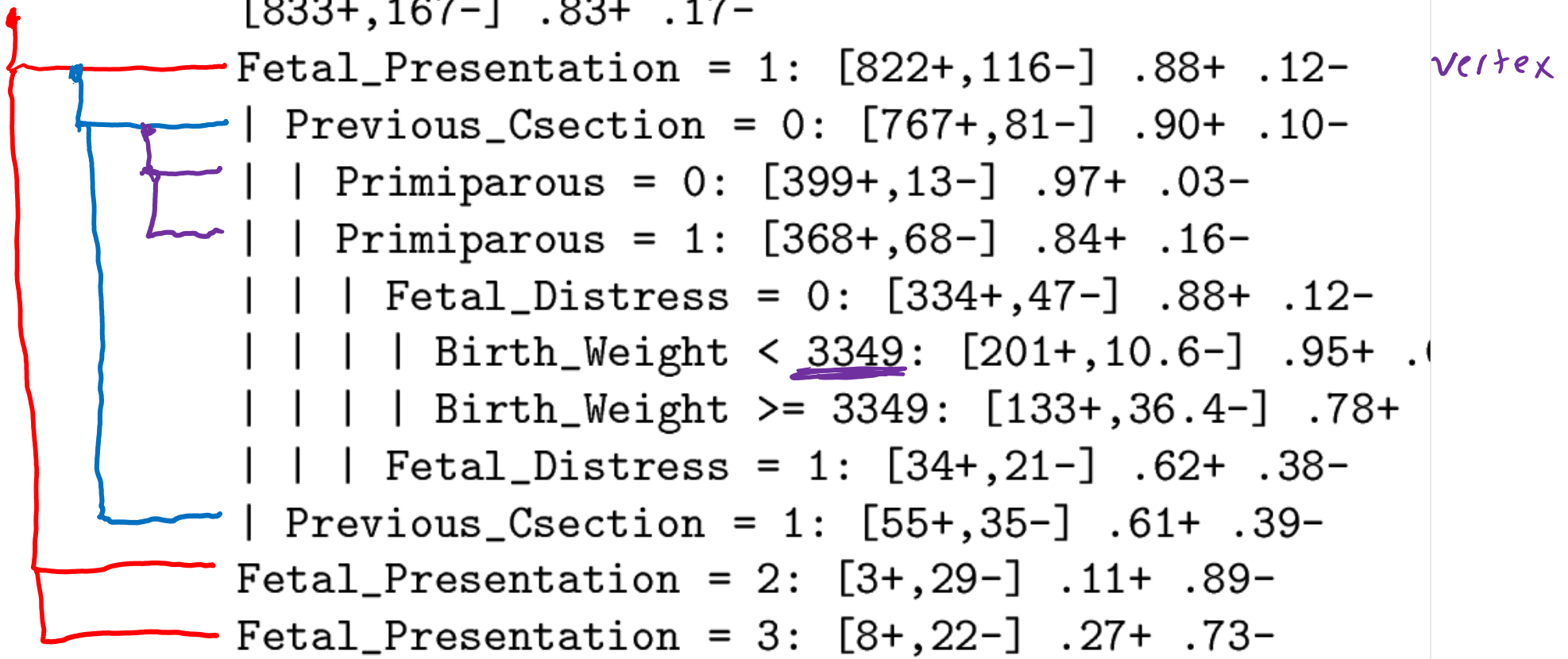
49 + 185

Sims, C.J., Meyn, L., Caruana, R., Rao, R.B., Mitchell, T. and Krohn, M.
American journal of obstetrics and gynecology, 2000

Tree to Predict C-Section Risk

Learned from medical records of 1000 women

Negative examples are C-sections



```
[833+,167-] .83+ .17-
Fetal_Presentation = 1: [822+,116-] .88+ .12-
| Previous_Csection = 0: [767+,81-] .90+ .10-
| | Primiparous = 0: [399+,13-] .97+ .03-
| | Primiparous = 1: [368+,68-] .84+ .16-
| | | Fetal_Distress = 0: [334+,47-] .88+ .12-
| | | | Birth_Weight < 3349: [201+,10.6-] .95+ .(
| | | | Birth_Weight >= 3349: [133+,36.4-] .78+
| | | Fetal_Distress = 1: [34+,21-] .62+ .38-
| Previous_Csection = 1: [55+,35-] .61+ .39-
Fetal_Presentation = 2: [3+,29-] .11+ .89-
Fetal_Presentation = 3: [8+,22-] .27+ .73-
```

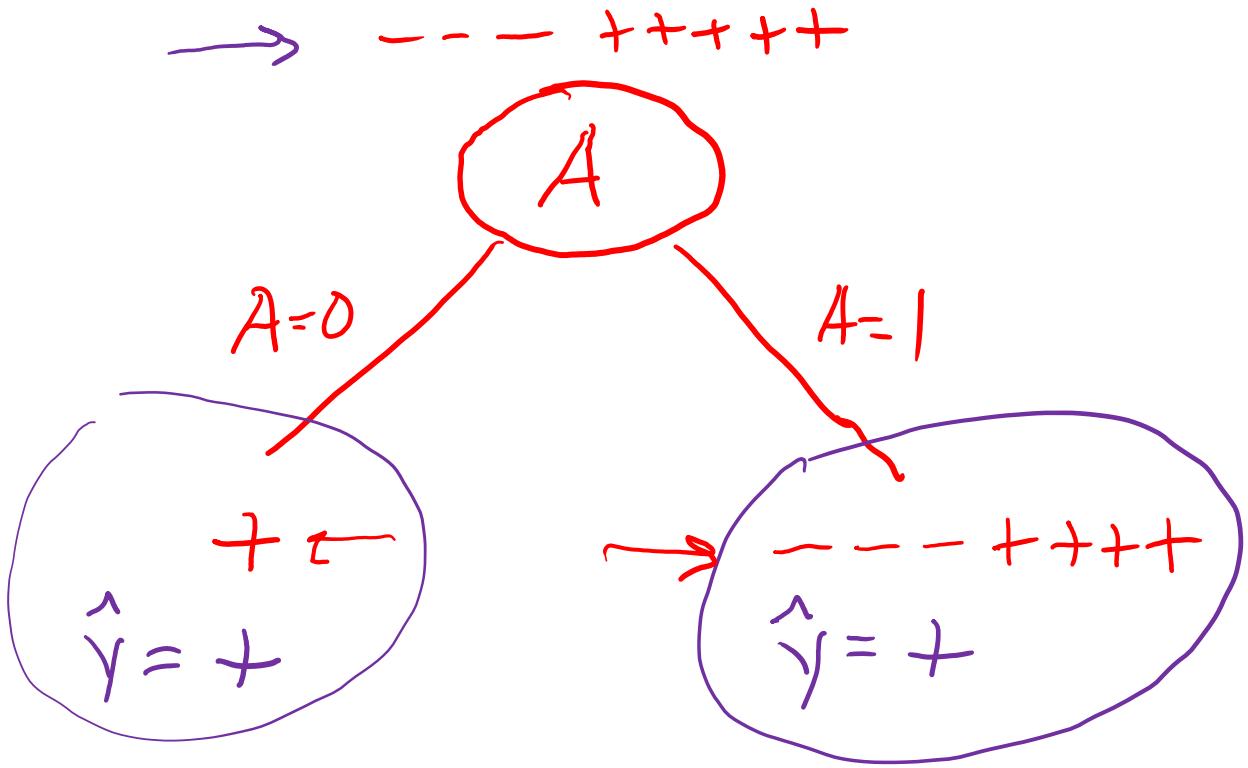
vertex

Slide credit: CMU MLD Tom Mitchell

Decision Stumps

Split data based on a single attribute

Majority vote at leaves



Dataset:

Output Y, Attributes A, B, C

Y	A	B	C
-	1	0	0
-	1	0	1
-	1	0	0
+	0	0	1
+	1	1	0
+	1	1	1
+	1	1	0
+	1	1	1

How could we implement training and prediction?

Algorithm 2: Decision stump algorithm

def train(D)

① pick an attribute X_m

② Divide dataset as

$$D^{(0)} = \{(\vec{x}, y) \in D \mid X_m = 0\}$$

$$D^{(1)} = \{(\vec{x}, y) \in D \mid X_m = 1\}$$

③ two votes

$$v^{(0)} = \text{majority}(D^{(0)})$$

$$v^{(1)} = \text{majority}(D^{(1)})$$

def h($\vec{x}$)

if $x_m = 0$

return $v^{(0)}$

if $x_m = 1$

return $v^{(1)}$

Slide credit: CMU MLD Matt Gormley

Decision Stumps

Splitting on which attribute {A, B, C} creates a decision stump with the lowest training error?

Dataset:

Output Y, Attributes A, B, C

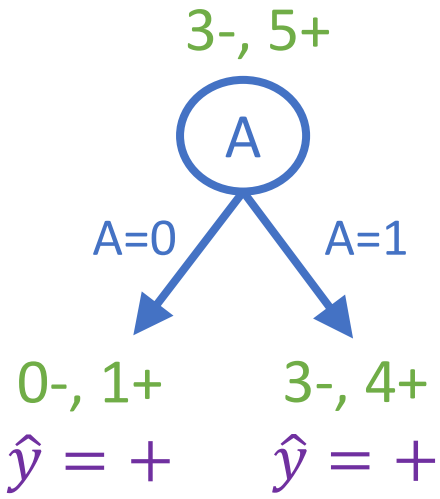
Y	A	B	C
-	1	0	0
-	1	0	1
-	1	0	0
+	0	0	1
+	1	1	0
+	1	1	1
+	1	1	0
+	1	1	1

Slide credit: CMU MLD Matt Gormley

Decision Stumps

Splitting on which attribute {A, B, C} creates a decision stump with the lowest training error?

Answer: B



Error: (0 + 3) / 8

= 3/8

Dataset:

Output Y, Attributes A, B, C

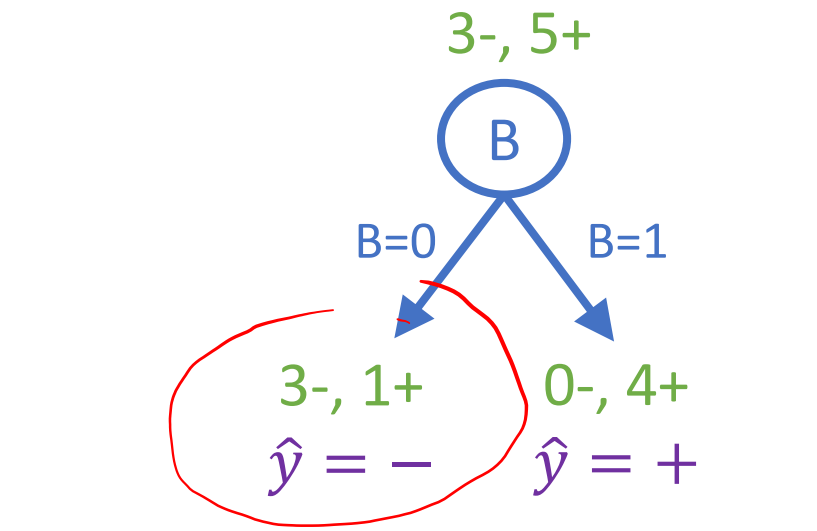
Y	A	B	C
-	1	0	0
-	1	0	1
-	1	0	0
+	0	0	1
+	1	1	0
+	1	1	1
+	1	1	0
+	1	1	1

Slide credit: CMU MLD Matt Gormley

Decision Stumps

Splitting on which attribute {A, B, C} creates a decision stump with the lowest training error?

Answer: B



Error: (1 + 0) / 8
= 1/8

Dataset:

Output Y, Attributes A, B, C

Y	A	B	C
-	1	0	0
-	1	0	1
-	1	0	0
+	0	0	1
+	1	1	0
+	1	1	1
+	1	1	0
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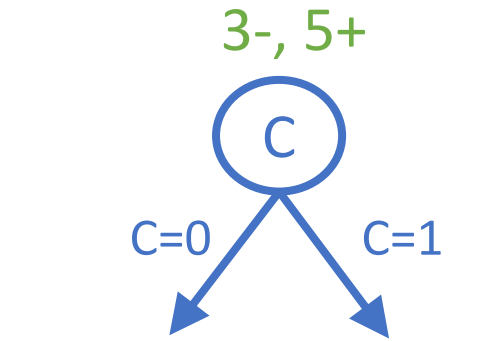
Slide credit: CMU MLD Matt Gormley

Decision Stumps

Splitting on which attribute {A, B, C} creates a decision stump with the lowest training error?

Answer: B



Error: (2 + 1) / 8
= 3/8

Dataset:

Output Y, Attributes A, B, C

Y	A	B	C
-	1	0	0
-	1	0	1
-	1	0	0
+	0	0	1
+	1	1	0
+	1	1	1
+	1	1	0
+	1	1	1

Slide credit: CMU MLD Matt Gormley

Building a Decision Tree

```
Function BuildTree(D,A)
    # D: dataset at current node, A: current set of attributes
    If empty(A) or all labels in D are the same
        # Leaf node
        class = most common class in D
    else
        # Internal node
        a ⇐ bestAttribute(D,A)
        LeftNode = BuildTree(D(a=1), A \ {a})
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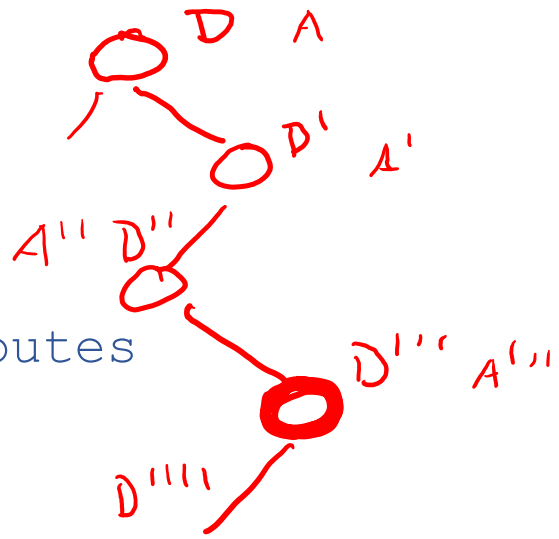
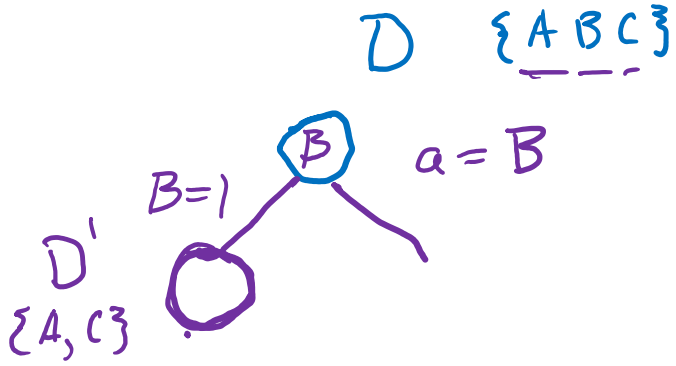
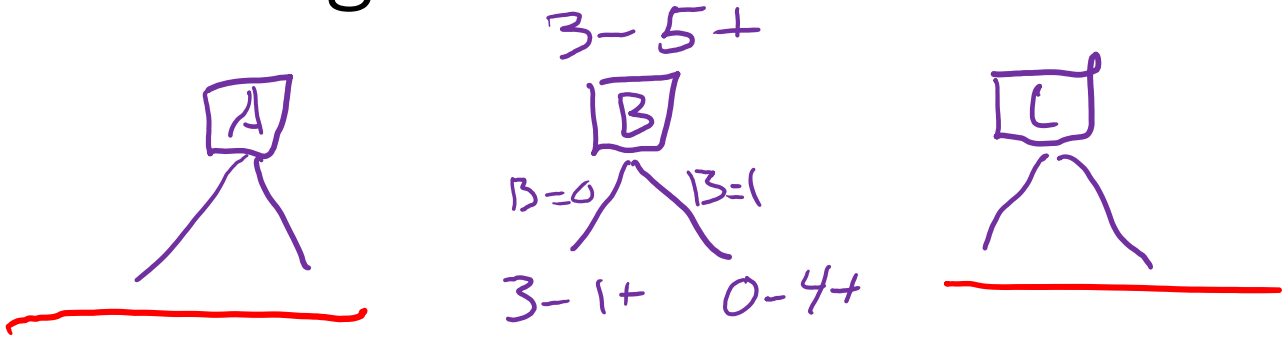


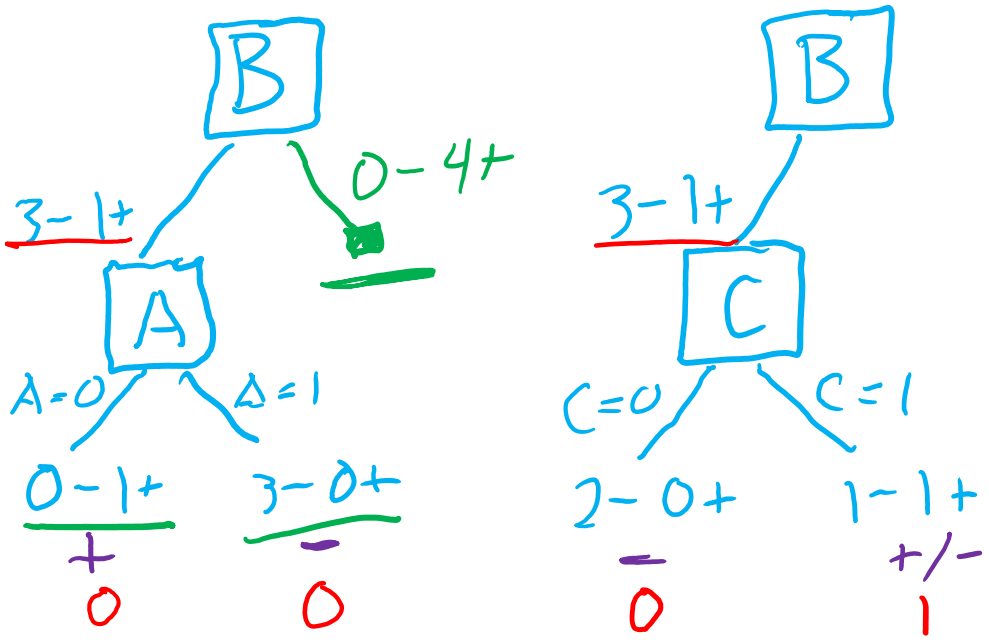
maj vote



Building a Decision Tree

Greedy





Dataset:

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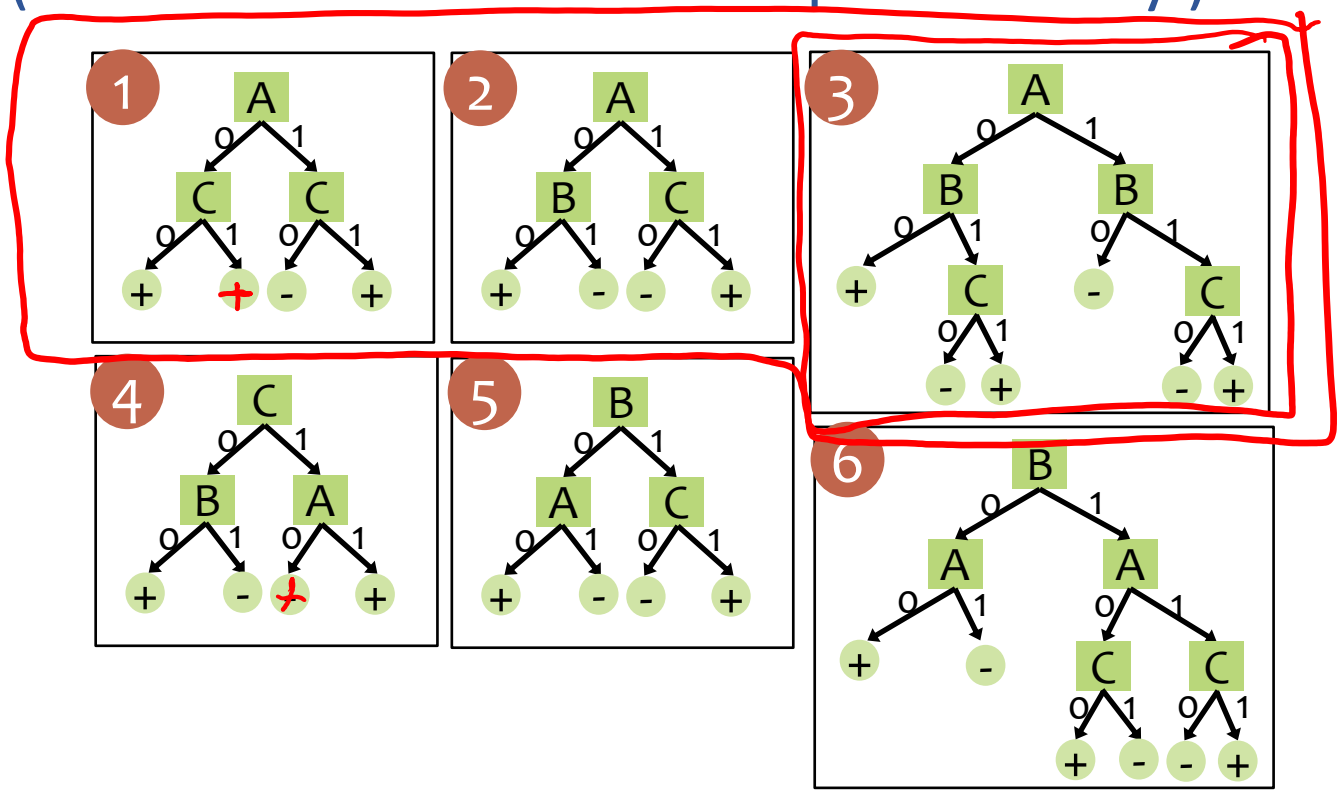
-	1	0	0
-	1	0	1
-	1	0	0
+	0	0	1
+	1	1	0
+	1	1	1
+	1	1	0
+	1	1	1

Piazza Poll 1

Which of the following trees would be learned by the decision tree learning algorithm using “error rate” as the splitting criterion?

(Assume ties are broken alphabetically.)



Dataset:

Output Y, Attributes A, B, C

Y	A	B	C
+	0	0	0
+	0	0	1
-	0	1	0
+	0	1	1
-	1	0	0
-	1	0	1
-	1	1	0
+	1	1	1

Slide credit: CMU MLD Matt Gormley

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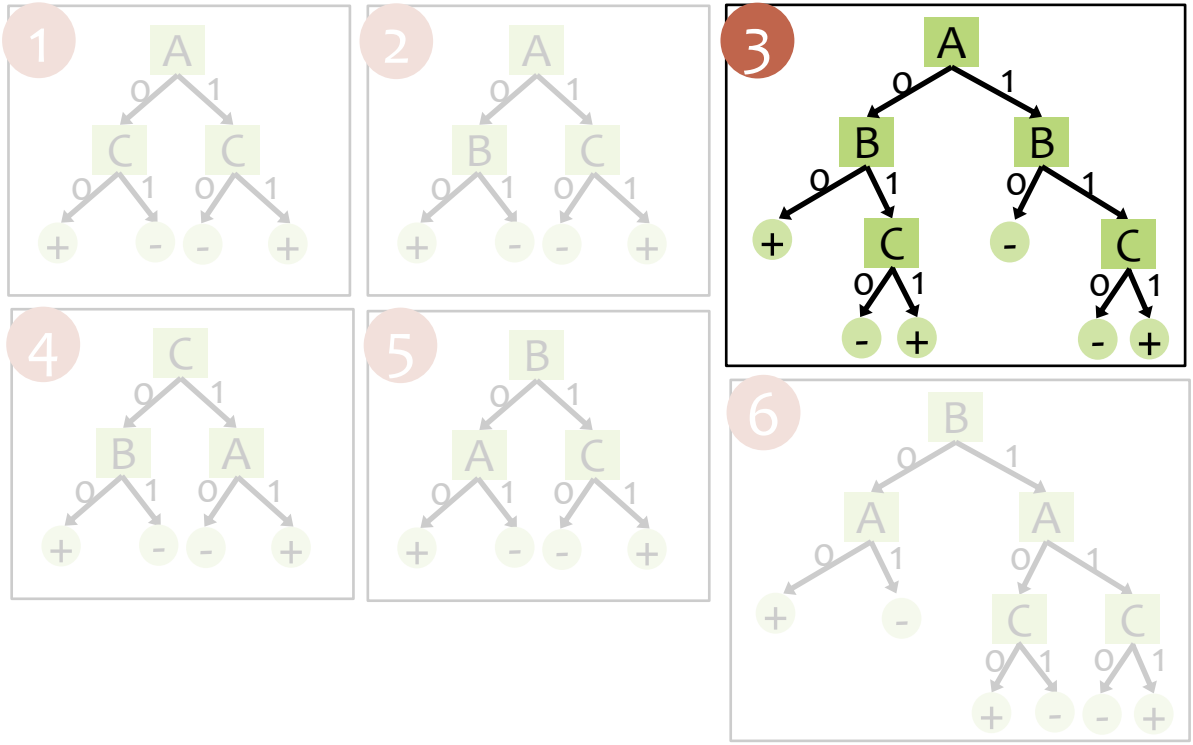

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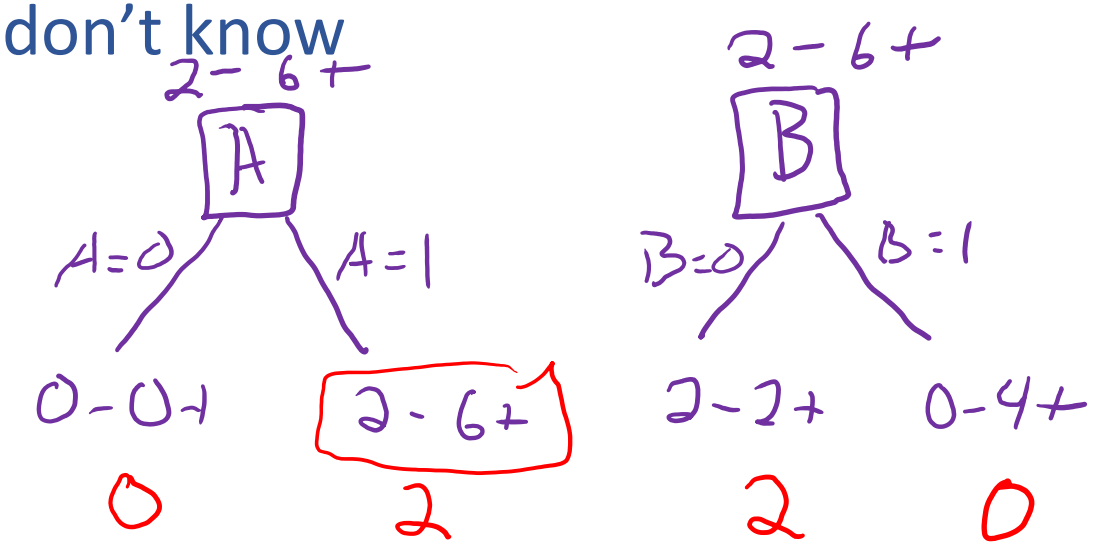
+	0	1	1
-	1	0	0
-	1	0	1
-	1	1	0
+	1	1	1

Slide credit: CMU MLD Matt Gormley

Piazza Poll 2

Which attribute {A, B} would error rate select for the next split?

1) A
2) B
3) A or B (tie)
4) I don't know



Dataset:

Output Y, Attributes A and B

Y	A	B
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

Slide credit: CMU MLD Matt Gormley

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        RightNode = BuildTree(D(a=0), A \ {a})
    end
end
```
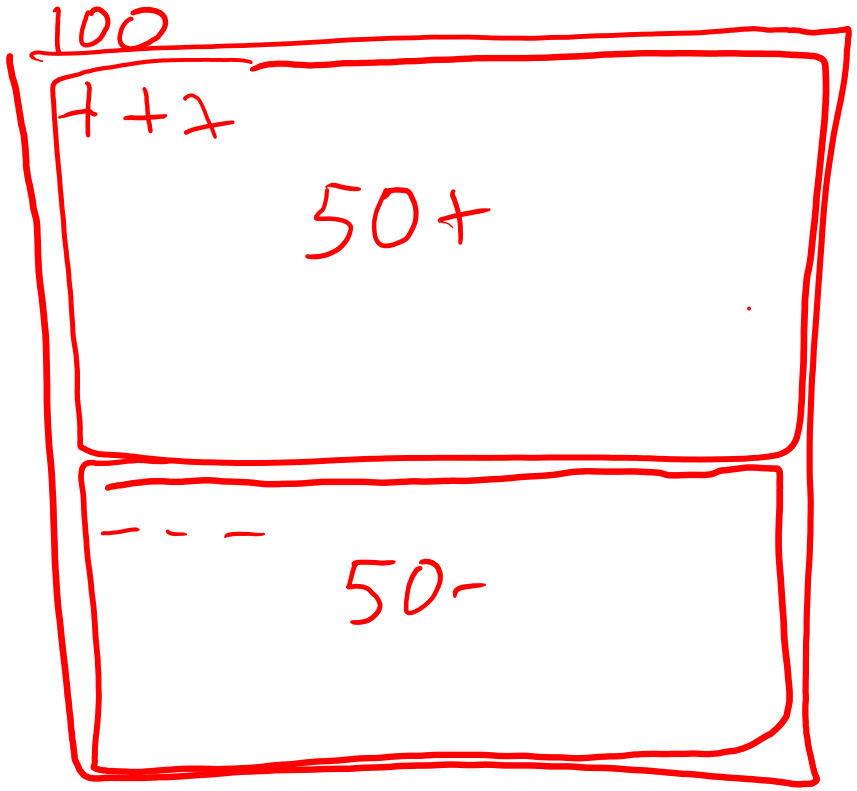
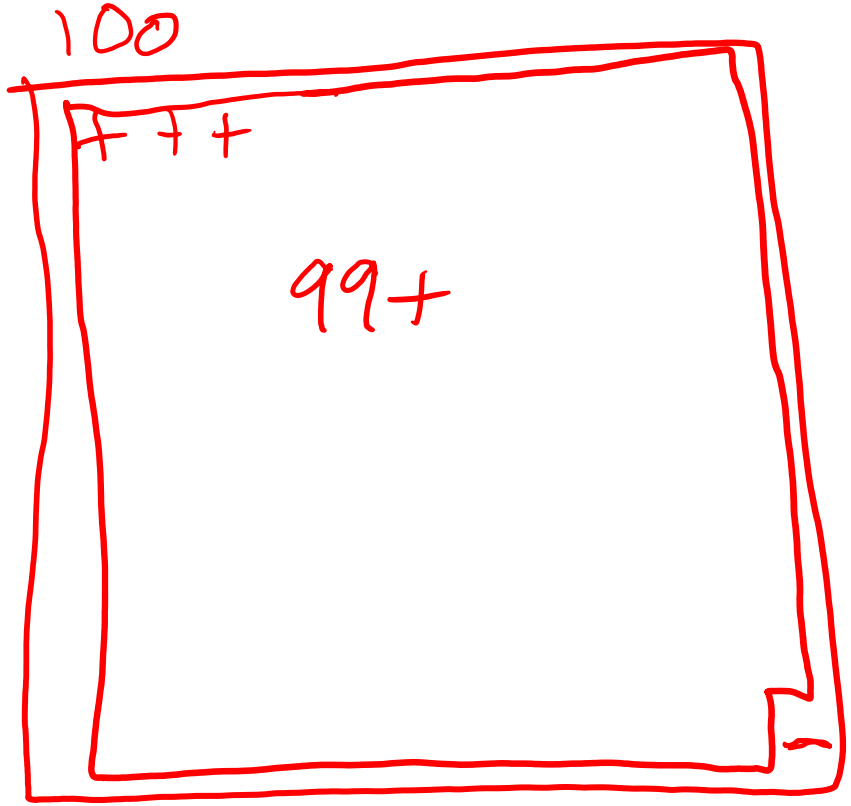

Gini, Mutual info, (Entropy)

Entropy

- Quantifies the amount of uncertainty associated with a specific probability distribution
- The higher the entropy, the less confident we are in the outcome





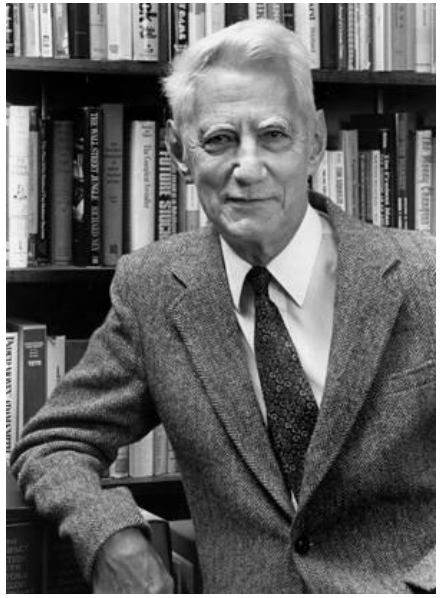
Entropy

- Quantifies the amount of uncertainty associated with a specific probability distribution
- The higher the entropy, the less confident we are in the outcome
- Definition

surprise

$$H(X) = \sum_x p(X = x) \log_2 \frac{1}{p(X = x)}$$

$$H(X) = -\sum_x p(X = x) \log_2 p(X = x)$$

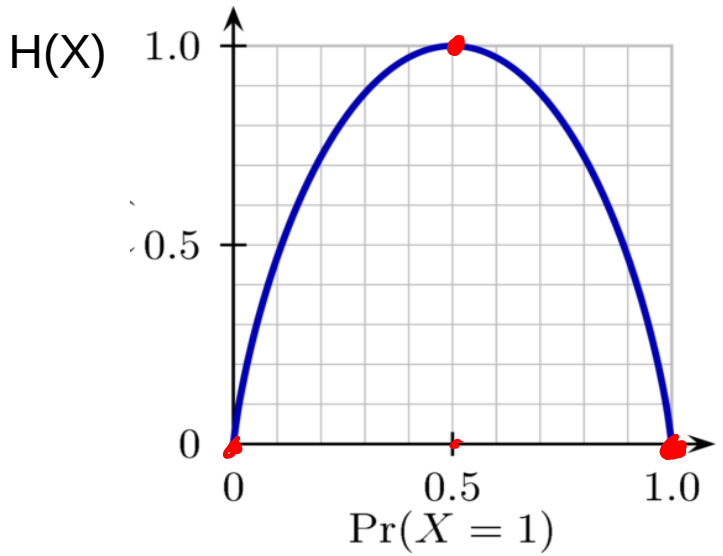


Claude Shannon (1916 – 2001), most of the work was done in Bell labs

Entropy

- Definition

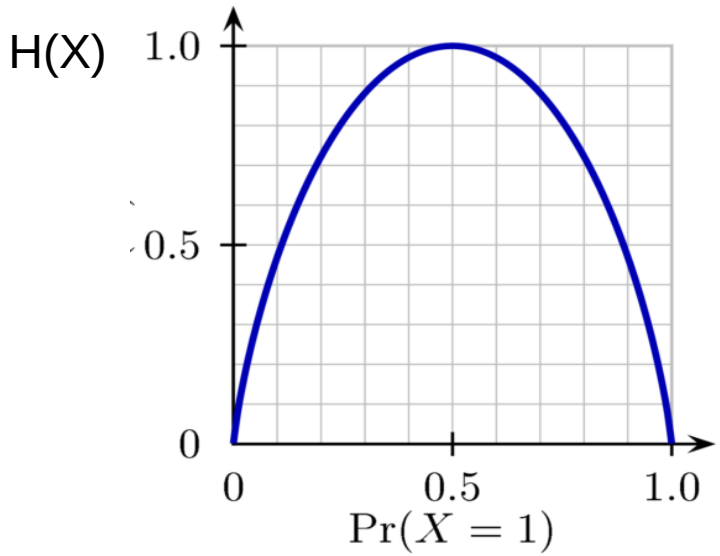
$$H(X) = -\sum_{x} p(X = x) \log_2 p(X = x)$$



- So, if P(X=1) = 1 then

- If P(X=1) = .5 then

Entropy



- Definition

$$H(X) = -\sum_{x} p(X = x) \log_2 p(X = x)$$

- So, if P(X=1) = 1 then

$$H(X) = -p(x = 1) \log_2 p(X = 1) - p(x = 0) \log_2 p(X = 0)$$
$$= -1 \log 1 - 0 \log 0 = 0$$

- If P(X=1) = .5 then

$$H(X) = -p(x = 1) \log_2 p(X = 1) - p(x = 0) \log_2 p(X = 0)$$
$$= -.5 \log_2 .5 - .5 \log_2 .5 = -\log_2 .5 = 1$$

Mutual Information

Let X be a random variable with $X \in \mathcal{X}$.
Let Y be a random variable with $Y \in \mathcal{Y}$.

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

Specific Conditional Entropy: $H(Y \mid X = x) = -\sum_{y \in \mathcal{Y}} P(Y = y \mid X = x) \log_2 P(Y = y \mid X = x)$

Conditional Entropy: $H(Y \mid X) = \sum_{x \in \mathcal{X}} P(X = x) H(Y \mid X = x)$

Mutual Information: $I(Y; X) = H(Y) - H(Y|X)$

- For a decision tree, we can use **mutual information** of the output class *Y* and some attribute *X* on which to split **as a splitting criterion**
- Given a dataset *D* of training examples, we can estimate the required probabilities as…

$$P(Y = y) = N_{Y=y}/N$$
$$P(X = x) = N_{X=x}/N$$
$$P(Y = y|X = x) = N_{Y=y,X=x}/N_{X=x}$$

where $N_{Y=y}$ is the number of examples for which $Y = y$ and so on.

Slide credit: CMU MLD Matt Gormley

Mutual Information

Let X be a random variable with $X \in \mathcal{X}$.
Let Y be a random variable with $Y \in \mathcal{Y}$.

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Conditional Entropy: $H(Y \mid X) = \sum_{x \in \mathcal{X}} P(X = x) H(Y \mid X = x)$

Mutual Information: $I(Y; X) = H(Y) - H(Y|X)$

- **Entropy** measures the **expected # of bits** to code one random draw from X**.**
- For a decision tree, we want to **reduce the entropy of the random variable we are trying to predict**!

Conditional entropy is the expected value of specific conditional entropy
$E_{P(X=x)}[H(Y \mid X = x)]$

Informally, we say that **mutual information** is a measure of the following:
If we know X, how much does this reduce our uncertainty about Y?

Slide credit: CMU MLD Matt Gormley

Piazza Poll 3

Which attribute {A, B} would **mutual information** select for the next split?

1) A
2) B
3) A or B (tie)
4) I don't know

Dataset:

Output Y, Attributes A and B

Y	A	B
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

Decision Tree Learning Example

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

Specific Conditional Entropy: $H(Y \mid X = x) = -\sum_{y \in \mathcal{Y}} P(Y = y \mid X = x) \log_2 P(Y = y \mid X = x)$

Conditional Entropy: $H(Y \mid X) = \sum_{x \in \mathcal{X}} P(X = x) H(Y \mid X = x)$

Mutual Information: $I(Y; X) = H(Y) - H(Y|X)$

Y	A	B
-	1	0
-	1	0
+	1	0
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+	1	1
+	1	1
+	1	1

Slide credit: CMU MLD Matt Gormley

Decision Tree Learning Example

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

Specific Conditional Entropy: $H(Y \mid X = x) = -\sum_{y \in \mathcal{Y}} P(Y = y \mid X = x) \log_2 P(Y = y \mid X = x)$

Conditional Entropy: $H(Y \mid X) = \sum_{x \in \mathcal{X}} P(X = x) H(Y \mid X = x)$

Mutual Information: $I(Y; X) = H(Y) - H(Y|X)$

Y	A	B
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

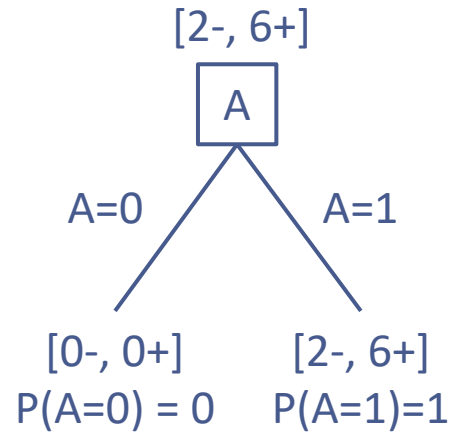
$$H(Y) = -\left[\frac{2}{8}\log_2\frac{2}{8} + \frac{6}{8}\log_2\frac{6}{8}\right]$$

$$H(Y \mid A = 0) = undefined$$

$$H(Y \mid A = 1) = -\left[\frac{2}{8}\log_2\frac{2}{8} + \frac{6}{8}\log_2\frac{6}{8}\right] = H(Y)$$

$$H(Y \mid A) = P(A = 0)H(Y \mid A = 0) + P(A = 1)H(Y \mid A = 1)$$
$$= 0 + H(Y \mid A = 1)$$
$$= H(Y)$$

$$I(Y; A) = H(Y) - H(Y \mid A) = 0$$



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Decision Tree Learning Example

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

Specific Conditional Entropy: $H(Y \mid X = x) = -\sum_{y \in \mathcal{Y}} P(Y = y \mid X = x) \log_2 P(Y = y \mid X = x)$

Conditional Entropy: $H(Y \mid X) = \sum_{x \in \mathcal{X}} P(X = x) H(Y \mid X = x)$

Mutual Information: $I(Y; X) = H(Y) - H(Y|X)$

Y	A	B
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

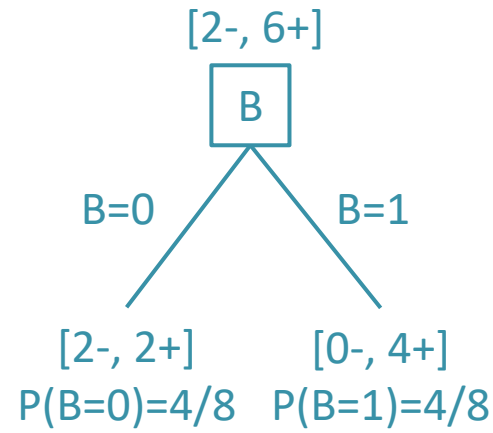
$$H(Y) = -\left[\frac{2}{8}\log_2\frac{2}{8} + \frac{6}{8}\log_2\frac{6}{8}\right]$$

$$H(Y \mid B = 0) = -\left[\frac{2}{4}\log_2\frac{2}{4} + \frac{2}{4}\log_2\frac{2}{4}\right]$$
$$H(Y \mid B = 1) = -[0 \log_2 0 + 1 \log_2 1] = 0$$

$$H(Y \mid B) = P(B = 0)H(Y \mid B = 0) + P(B = 1)H(Y \mid B = 1)$$
$$= \frac{4}{8}H(Y \mid B = 0) + \frac{4}{8} \cdot 0$$

$$I(Y; B) = H(Y) - H(Y \mid B) > 0$$

$I(Y; B)$ ends up being greater than $I(Y; A) = 0$, so we split on B



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Mutual Information Notation

We use mutual information in the context of before and after a split, regardless of where that split is in the tree.

$$I(Y; X) = H(Y) - H(Y \mid X)$$