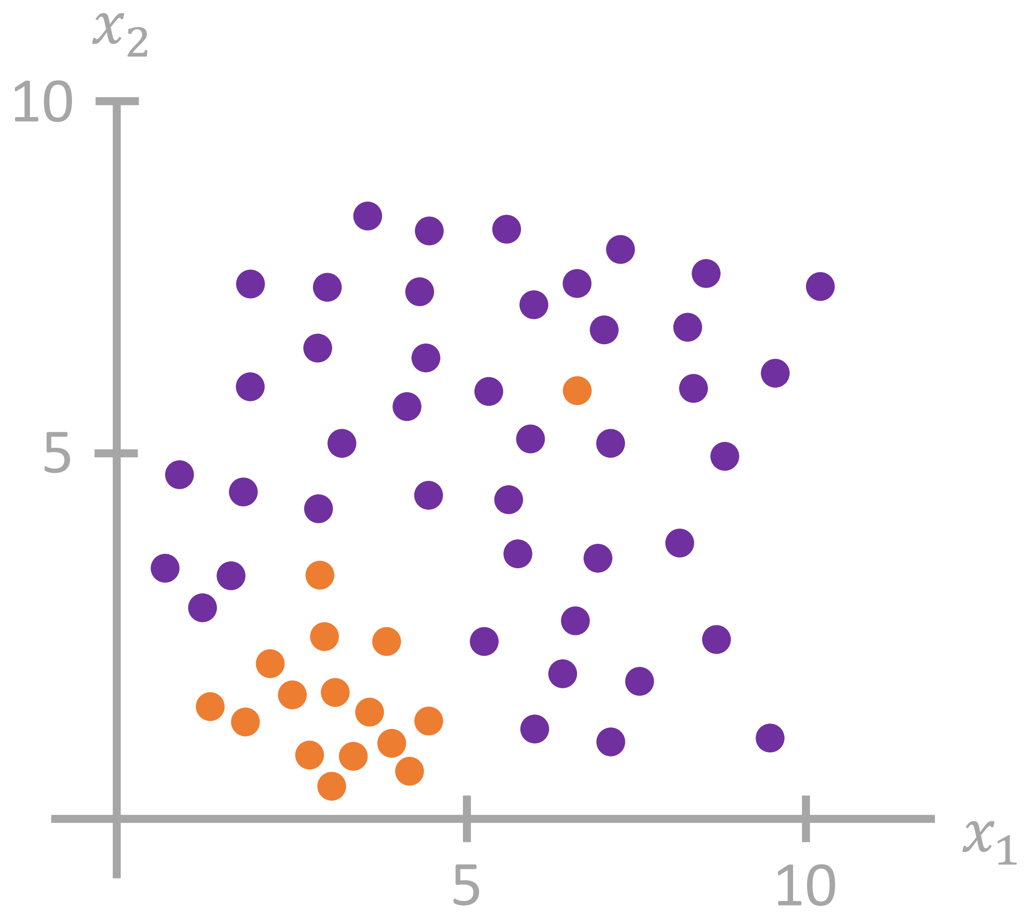
Warm-up as you walk in: Worksheet

Consider input features $\mathbf{x} \in \mathbb{R}^2$.

Draw a reasonable decision tree.



10-315
Introduction to ML

Decision Trees

Instructor: Pat Virtue

Outline: Decision Trees

Motivation

Pre-reading Content

- Example decision trees for classification tasks
- Majority vote and classification error rate
- Decision stumps

Decision Boundaries

Building Decision Trees

- Splitting criteria: Entropy and Mutual Information
- Stopping criteria

Decision Trees

Why are we talking about decision trees?

Explainability

- Decision trees can be incredibly useful as they can more easily be interpreted and altered by humans than other ML algorithms

Basis of very powerful set of techniques: Random Forests

- Random forests train many simple decision trees (ML topic: ensemble learning)
- While powerful, random forests unfortunately have poor explainablility

Pre-reading Content

Problem Formulation

Medical Prediction

Outcome (y)	Fetal Position (x_1)	Fetal Distress (x_2)	Previous C-sec (x_3)
Natural	Vertex	N	N
C-section	Breech	N	N
Natural	Vertex	Y	Y
C-section	Vertex	N	Y
Natural	Abnormal	N	N

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

$x_1 \in \{Vertex, Breech, Abn\}$

$x_2 \in \{Y, N\}$

$x_3 \in \{Y, N\}$

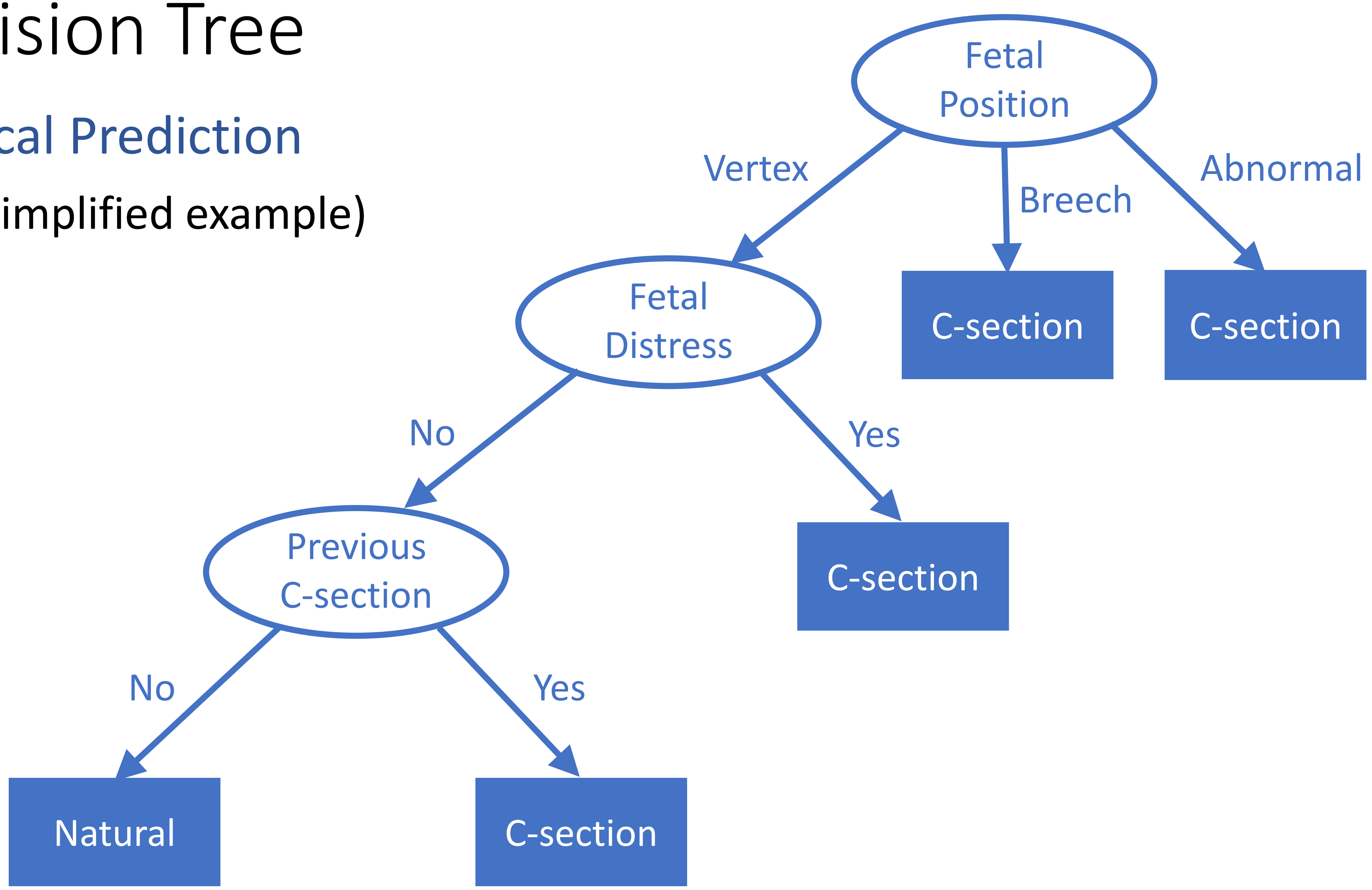
$y \in \{Csection, Natural\}$

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

Decision Tree

Medical Prediction

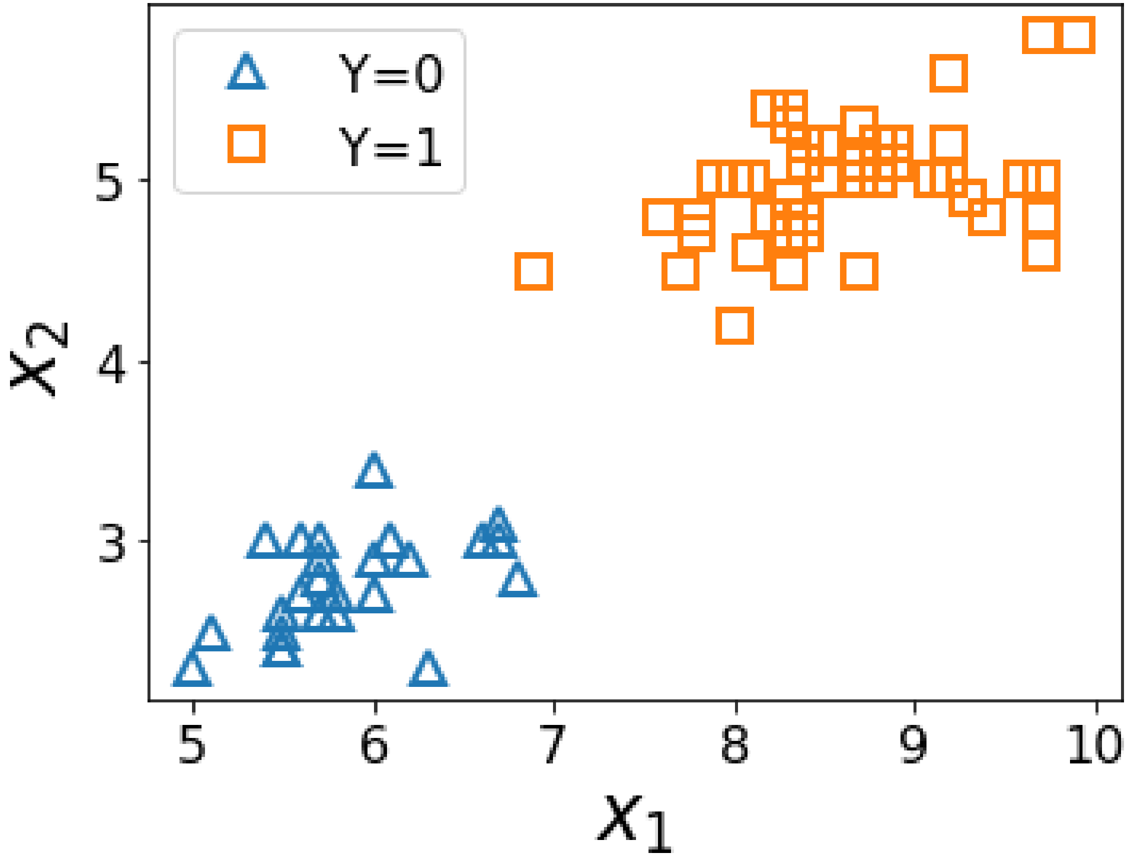
(Oversimplified example)



ML Task: Classification

Predict species label from first two input measurements

$$h(\mathbf{x}) \rightarrow \hat{y}$$



Species	Sepal Length	Sepal Width
0	4.3	3.0
0	4.9	3.6
0	5.3	3.7
1	4.9	2.4
1	5.7	2.8
1	6.3	3.3

Images and full dataset: https://en.wikipedia.org/wiki/Iris_flower_data_set

Decision Trees

Species	Sepal Length	Sepal Width	Petal Length	Petal Width
0	4.3	3.0	1.1	0.1
0	4.9	3.6	1.4	0.1
0	5.3	3.7	1.5	0.2
1	4.9	2.4	3.3	1.0
1	5.7	2.8	4.1	1.3
1	6.3	3.3	4.7	1.6
2	5.9	3.0	5.1	1.8

A few tools

Majority vote:

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

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 Stumps

Split data based on a single attribute

Majority vote at leaves

Dataset:

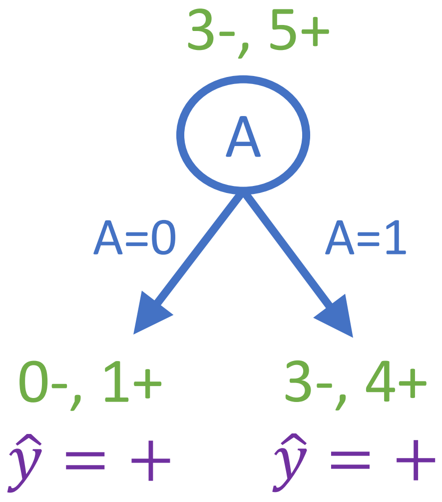
Output Y, Attributes A, B, C

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

Decision Stumps

Split data based on a single attribute

Majority vote at leaves



Error: (0 + 3) / 8

= 3/8

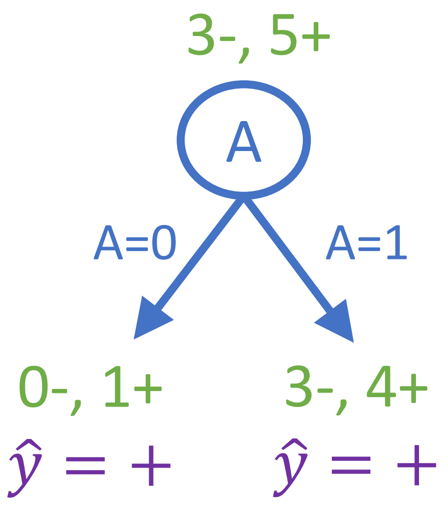
Dataset:

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

Poll (not used)

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



Error: (0 + 3) / 8

= 3/8

Dataset:

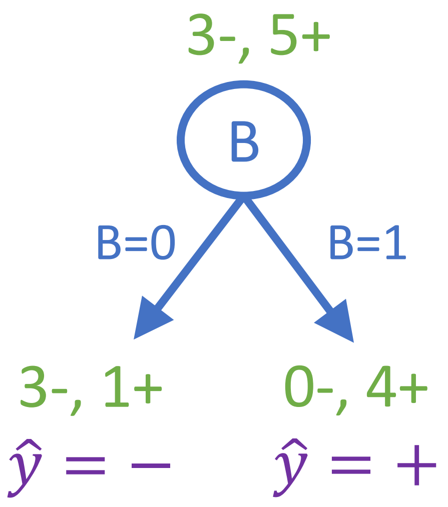
Output Y, Attributes A, B, C

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

Poll (not used)

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

Answer: B



Error: $(\ 1 \quad + \quad 0\ )\ /\ 8$

$= 1/8$

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
+	1	1	1

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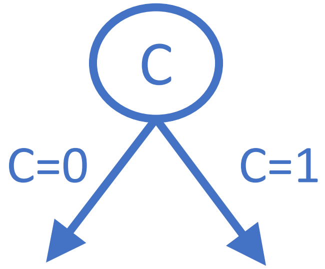
Poll (not used)

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

Answer: B

3-, 5+



2-, 2+ 1-, 3+

$\hat{y} = +/-$ $\hat{y} = +$

Error: (2 + 1) / 8

= 3/8

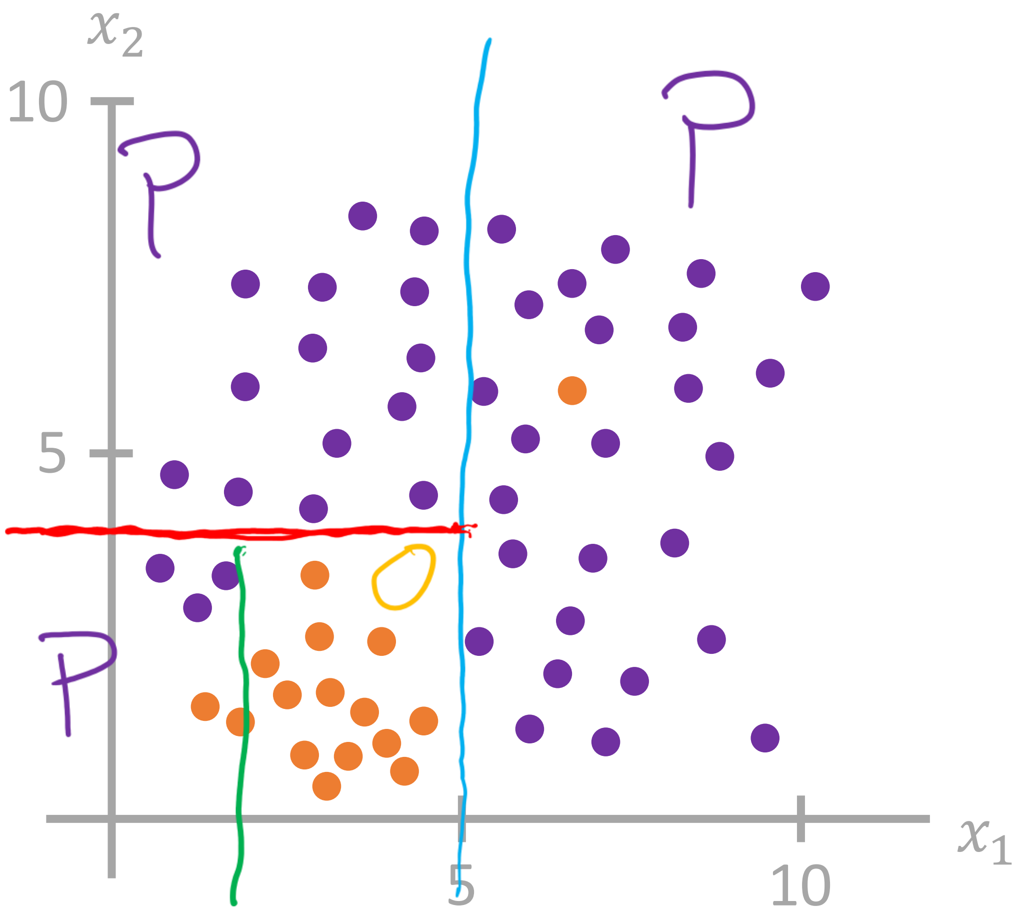
Dataset:

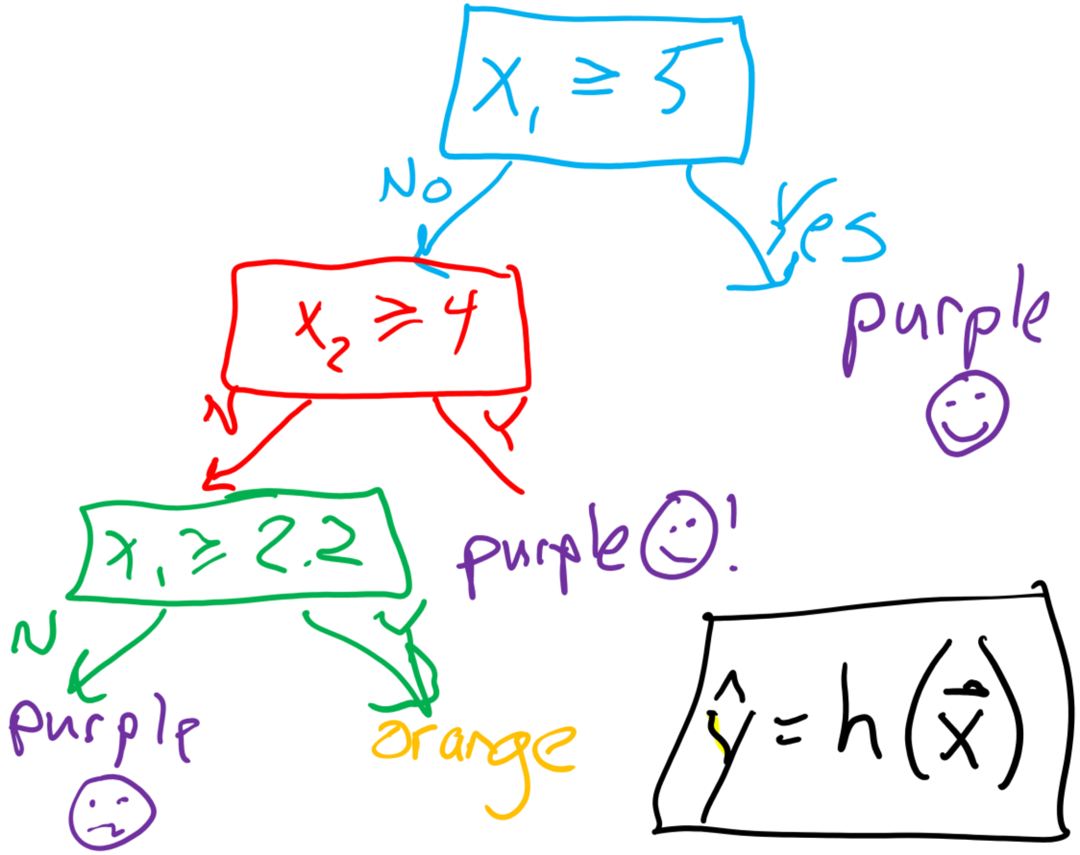
Output Y, Attributes A, B, C

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

Decision Boundaries

Decision boundaries are the locations in the input space that separate regions where input points **x** are classified as different classes.





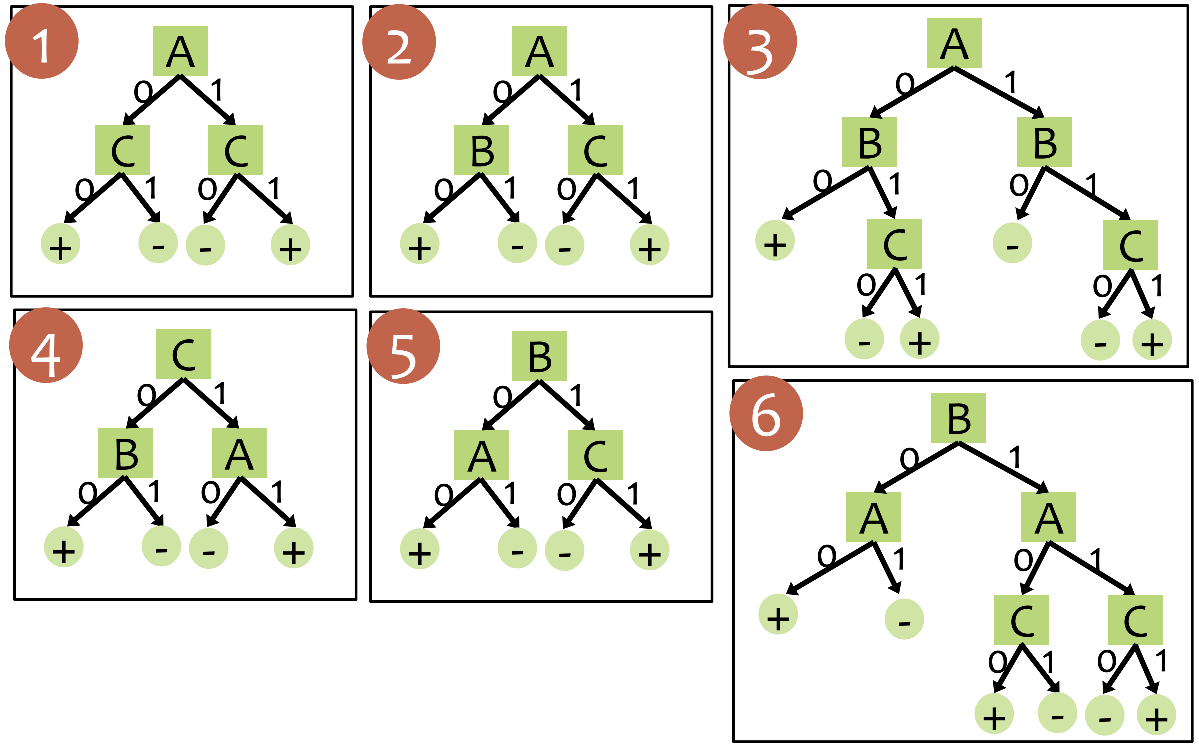
Building a Decision Tree

```
Function BuildTree(D, Attributes)
    # D: dataset at current node
    # Attributes : current set of attributes

    # TODO Base Case



    else
        # Internal node
        X ⇐ bestAttribute(D, Attributes)
        LeftNode = BuildTree(D(X=1), Attributes \ {X})
        RightNode = BuildTree(D(X=0), Attributes \ {X})
    end
end
```

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, Features x_A, x_B, x_C

Y	X_A	X_B	X_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

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Poll 1

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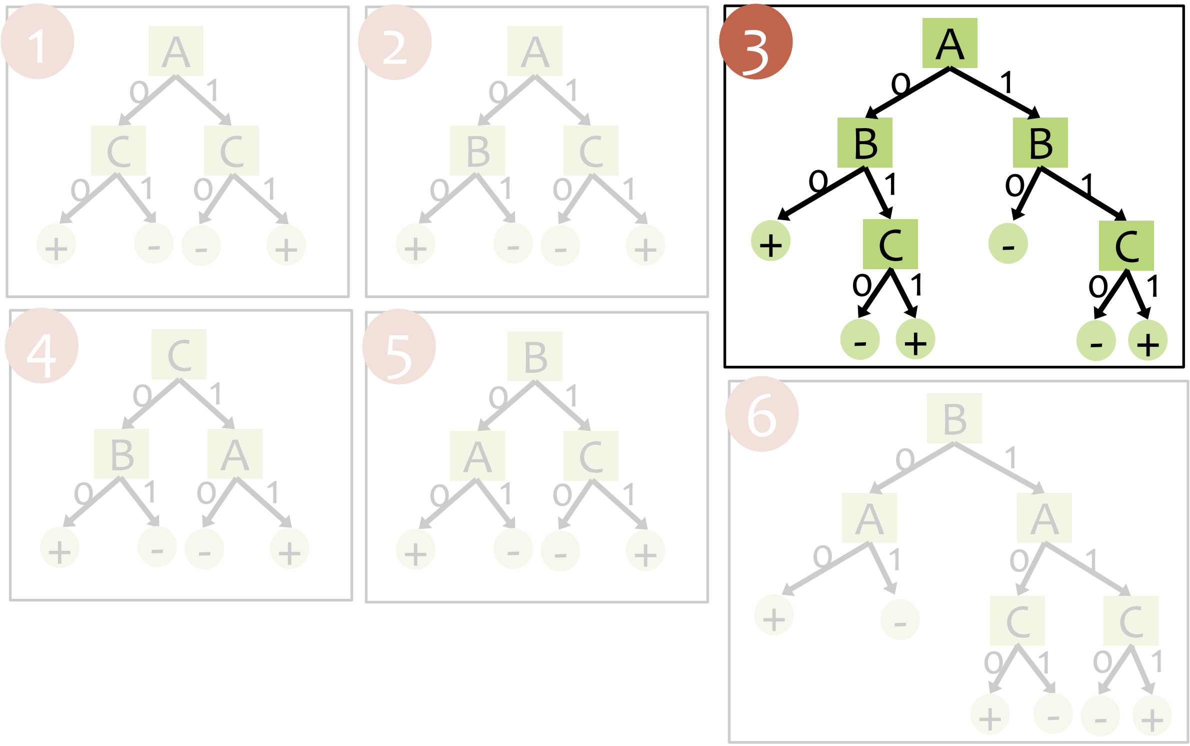

Dataset:

Output Y, Features x_A, x_B, x_C

Y	X_A	X_B	X_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

Poll 2

How many errors do each of the two decision stumps make on the training set?

Dataset:

Output Y, Features A and B

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

Building a Decision Tree

```
Function BuildTree(D, Attributes)
    # D: dataset at current node
    # Attributes : current set of attributes

    # TODO Base Case



    else
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        X ⇐ bestAttribute(D, Attributes)
        LeftNode = BuildTree(D(X=1), Attributes \ {X})
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    end
end
```
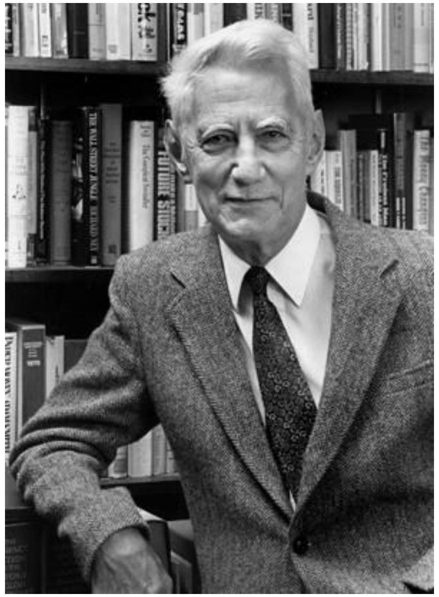

Entropy

Surprisal



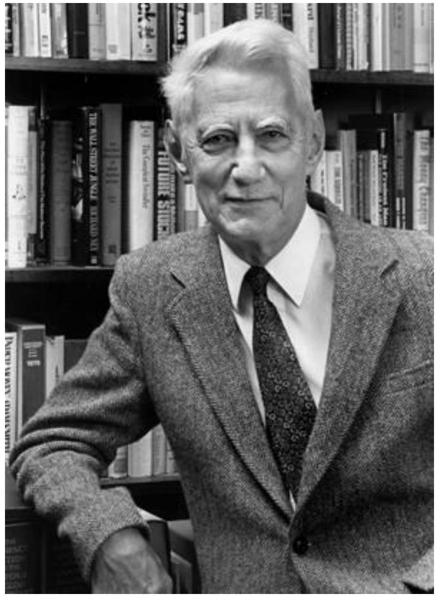
Claude Shannon (1916 – 2001), most of the work was done in Bell labs

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

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

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



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

Conditional Entropy

Entropy Definition

$$H(Y) = \sum_y p(Y = y) \log_2 \frac{1}{p(Y=y)}$$

$$H(Y) = -\sum_y p(Y = y) \log_2 p(Y = y)$$

Conditional Entropy

Entropy after splitting on a particular feature

- Must consider expected value over both branches!

Conditional Entropy

Entropy Definition

$H(Y) = \sum_y p(Y = y) \log_2 \frac{1}{p(Y=y)}$

$H(Y) = -\sum_y p(Y = y) \log_2 p(Y = y)$

Conditional Entropy

Entropy after splitting on a particular feature

- Must consider expected value over both branches!

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

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.

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

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

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

- 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.

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

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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?

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Splitting with Mutual Information

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
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

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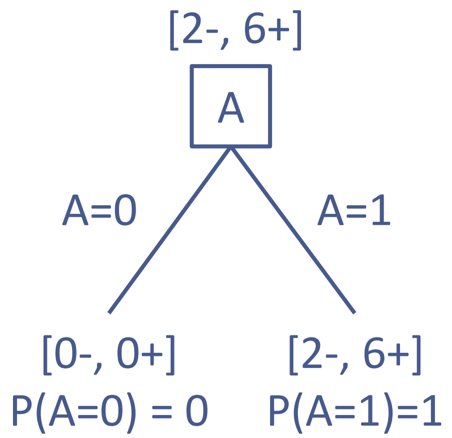
Mutual Information: $I(Y; X) = H(Y) - H(Y|X)$

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

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

$$H(Y \mid A = 0) = undefined$$
$$H(Y \mid A = 1) = -\left[\frac{2}{8}\log_2\frac{2}{8} + \frac{6}{8}\log_2\frac{6}{8}\right] = H(Y)$$

$$\begin{aligned} H(Y \mid A) &= P(A = 0)H(Y \mid A = 0) + P(A = 1)H(Y \mid A = 1) \\ &= 0 + H(Y \mid A = 1) \\ &= H(Y) \end{aligned}$$
$$I(Y; A) = H(Y) - H(Y \mid A) = 0$$



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Decision Tree Learning Example

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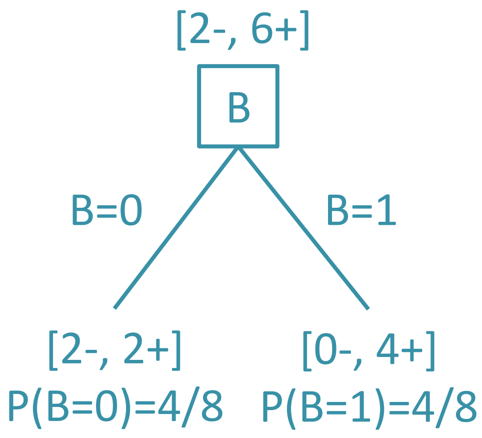
Y	A	B
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1



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

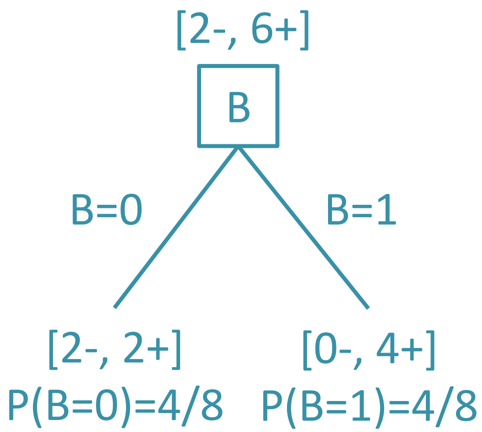
Mutual Information: $I(Y; X) = H(Y) - H(Y|X)$

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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Building a Decision Tree

How do we choose the best feature?

A **splitting criterion** is a function that measures how good or useful splitting on a particular feature is *for a specified dataset*

Insight: use the feature that optimizes the splitting criterion current decision

Potential splitting criteria:

- Training error rate (minimize)
- Gini impurity (minimize) → CART algorithm
- Mutual information (maximize) → ID3 algorithm

Slide credit: CMU MLD Henry Chai

Are decision trees algorithms optimal?

Well, what do we mean by optimal?

Considering all possible decision trees (i.e., trees splitting on one feature per node),

will the ID3 algorithm (each split maximizes mutual information; stopping when mutual information is zero)…

produce the smallest decision tree that has lowest classification training error?

No, they aren’t optimal

Decision trees are greedy algorithms, i.e., they make the best local decision without considering longer term possibilities.

- Better trees are possible, but it takes too long to search all combinations

Recall: Building a Decision Tree

```
Function BuildTree(D, Attributes)
    # D: dataset at current node
    # Attributes : current set of attributes

    # TODO Base Case



    else
        # Internal node
        X ⇐ bestAttribute(D, Attributes)
        LeftNode = BuildTree(D(X=1), Attributes \ {X})
        RightNode = BuildTree(D(X=0), Attributes \ {X})
    end
end
```

Stopping Criteria

When do we stop (base case)?

When leaves are “pure”, i.e., output values are all the same

- Likely to overfit

Limit

- Tree depth
- Total number of leaves
- Splitting criteria threshold, e.g. splitting criteria <= τ
- Minimum number of datapoints in a leaf

Sopping Criteria

But how do we choose all of those limits?!?

Answer: Model selection

Model selection is the process to choose the “best” among a set of (trained) models

Decision Trees: Pros & Cons

Pros

- Interpretable
- Efficient (computational cost and storage)
- Can be used for classification and regression tasks
- Compatible with categorical and real-valued features

Cons

- Greedy: each split only considers the immediate impact
  - Not guaranteed to find the smallest (fewest number of splits) tree that achieves a training error rate of 0.
- Liable to overfit!