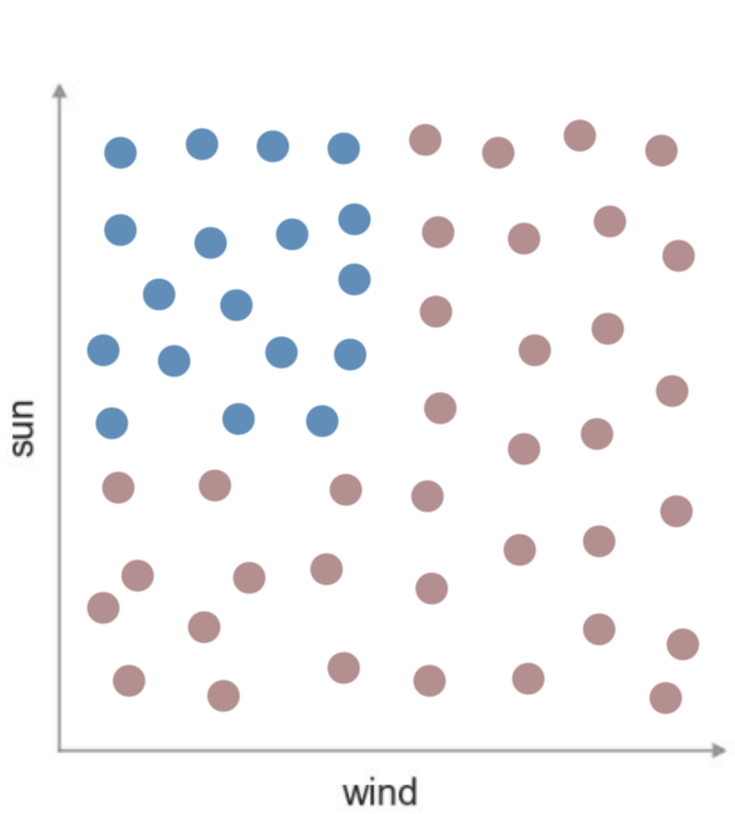
Decision Trees

- Decision Trees allow us to come up with nonlinear-ish decision boundaries via a union of simple linear boundaries
- Decision Trees are basis for many popular learning algorithms
- Two of the Top 10 Data Mining Algorithms (as voted by IEEE International Conference on Data Mining in 2006) are Decision Trees

Simple Example

Decide whether you should play tennis

Decision trees allow you to ask multiple linear questions



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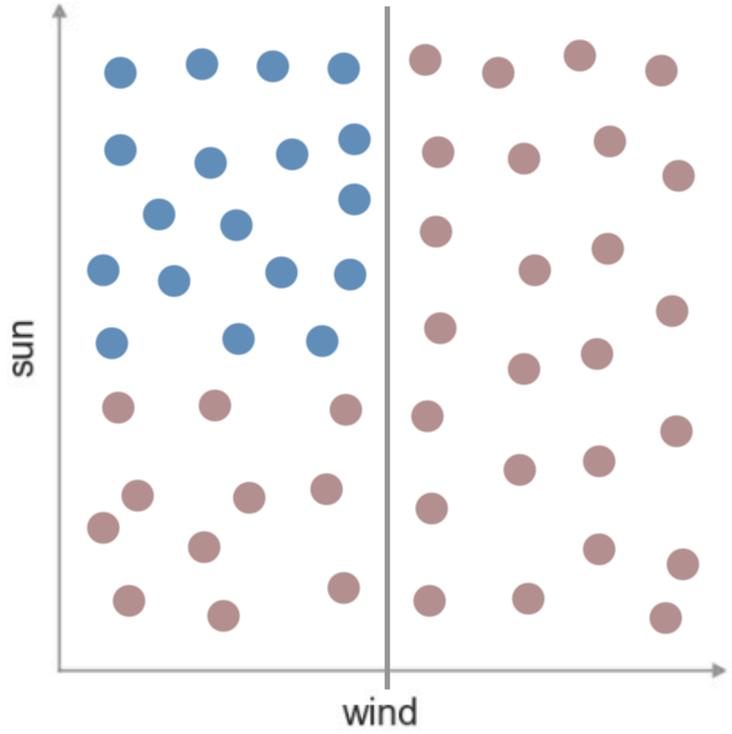

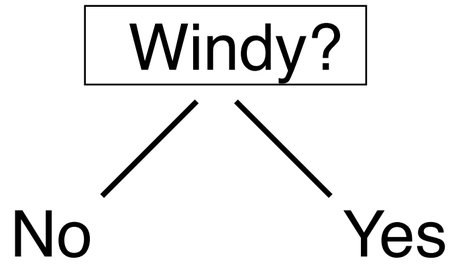

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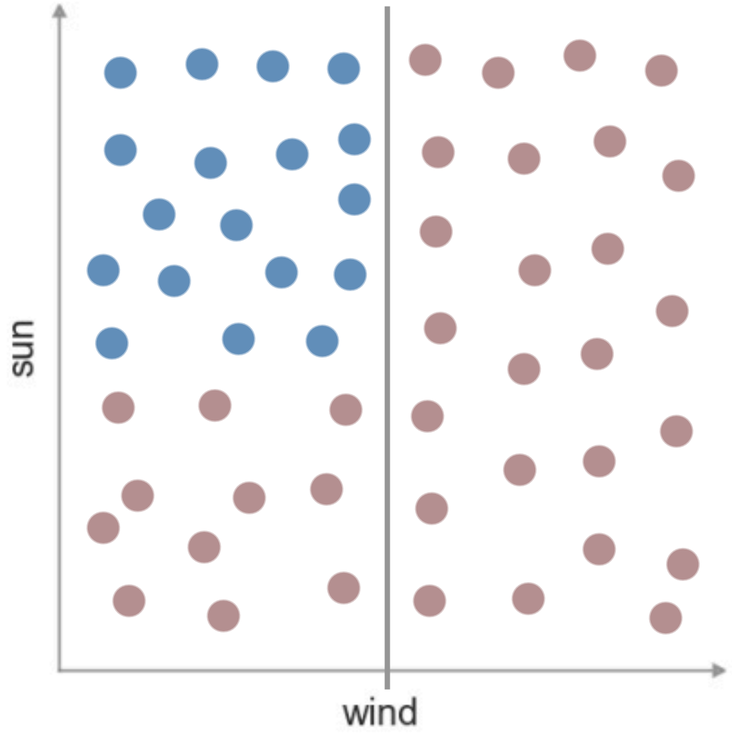

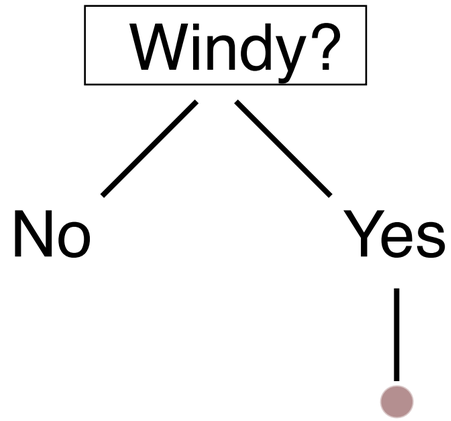

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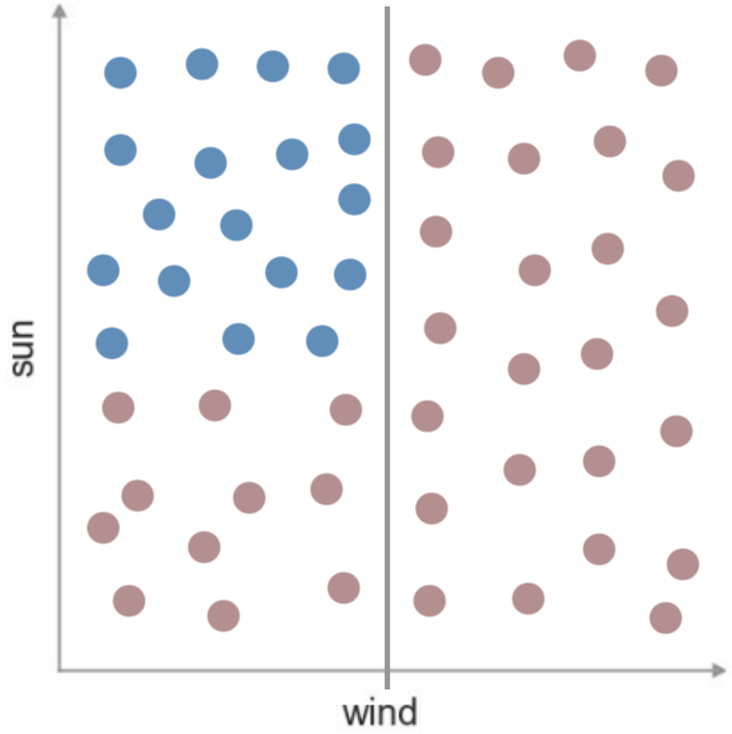

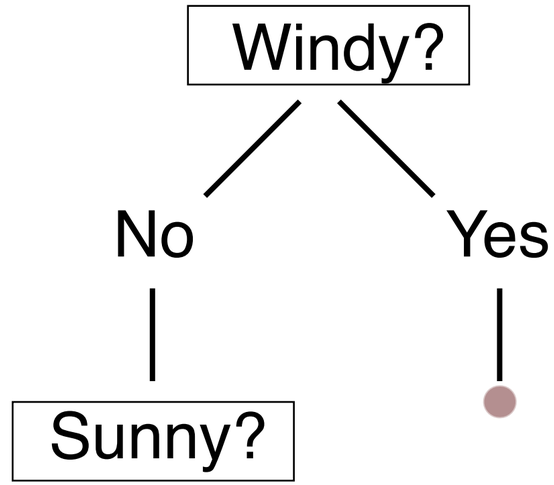

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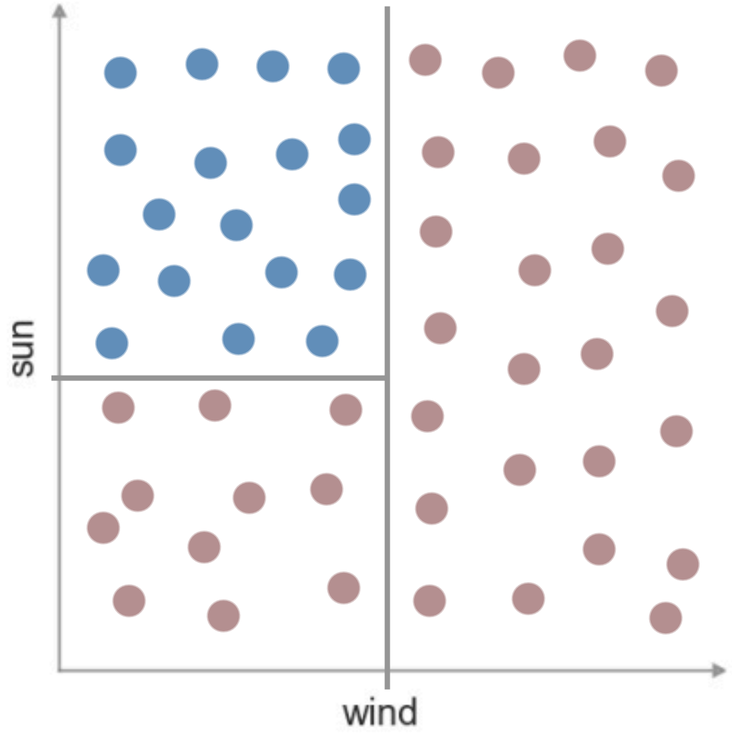

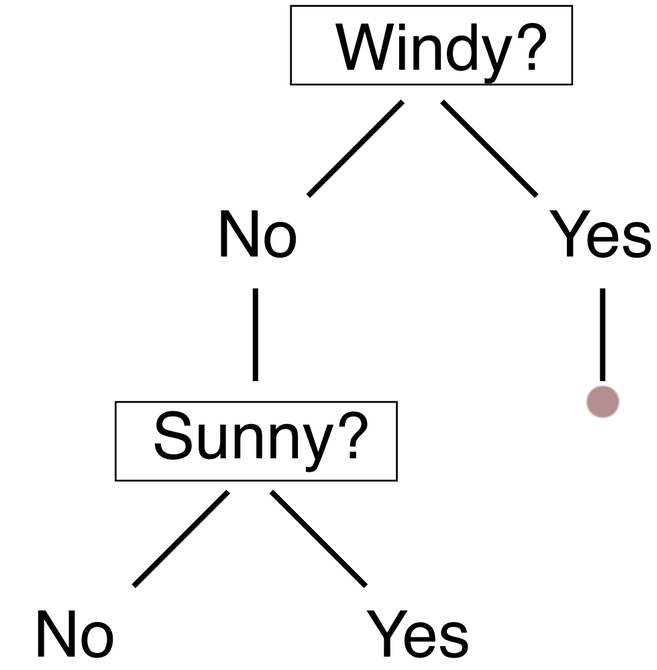

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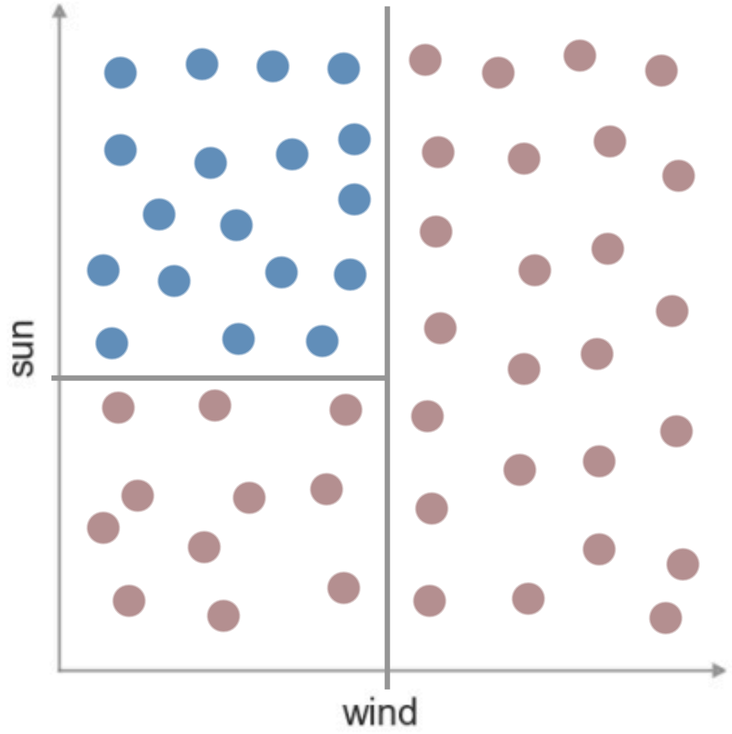
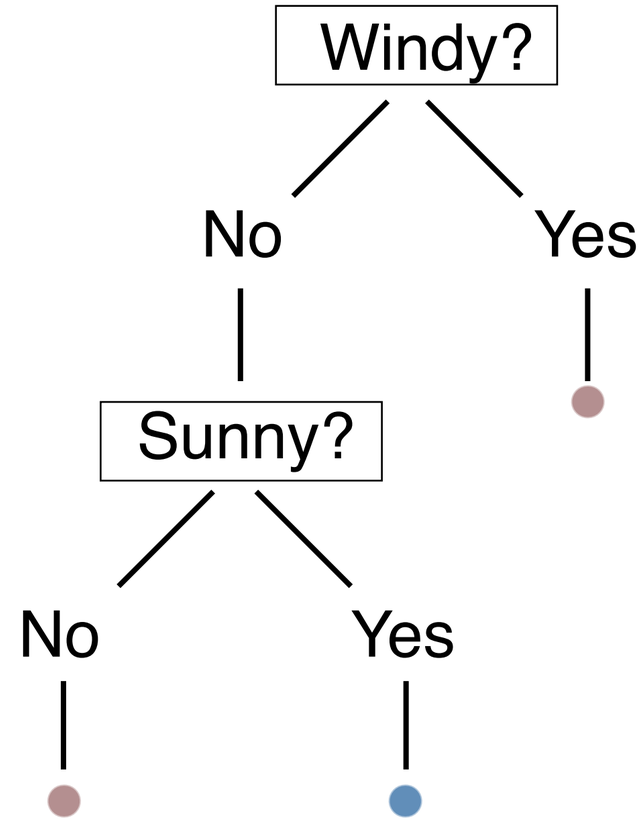
Decide whether you should play tennis

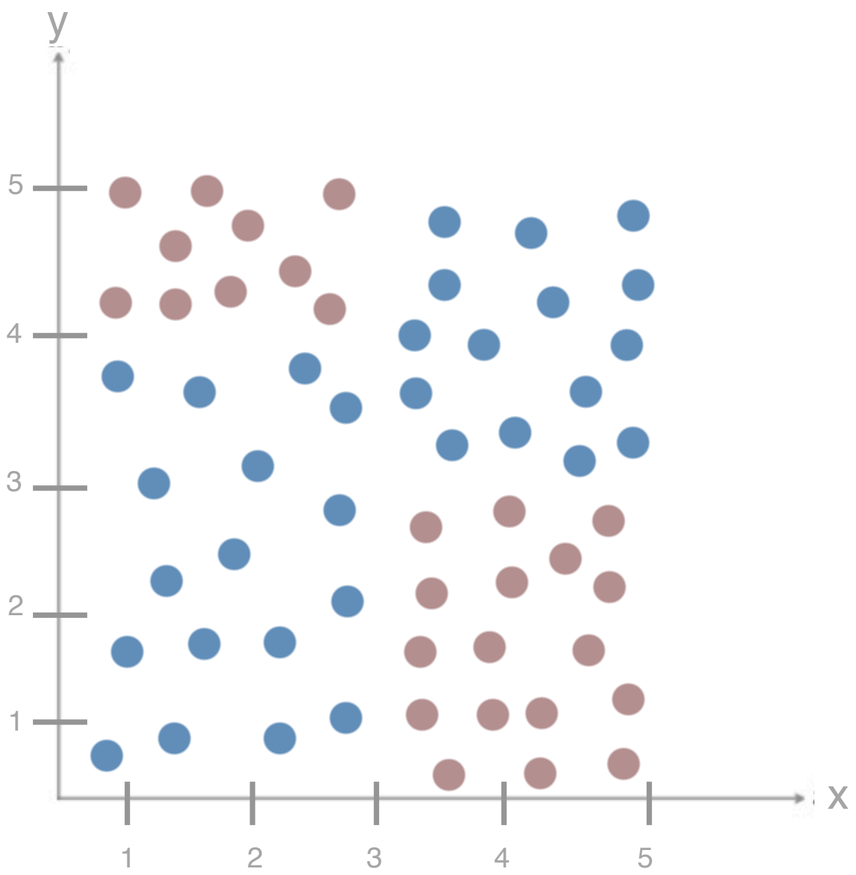
Decision trees allow you to ask multiple linear questions





Slightly Less Simple Example

Decision trees allow you to ask multiple linear questions



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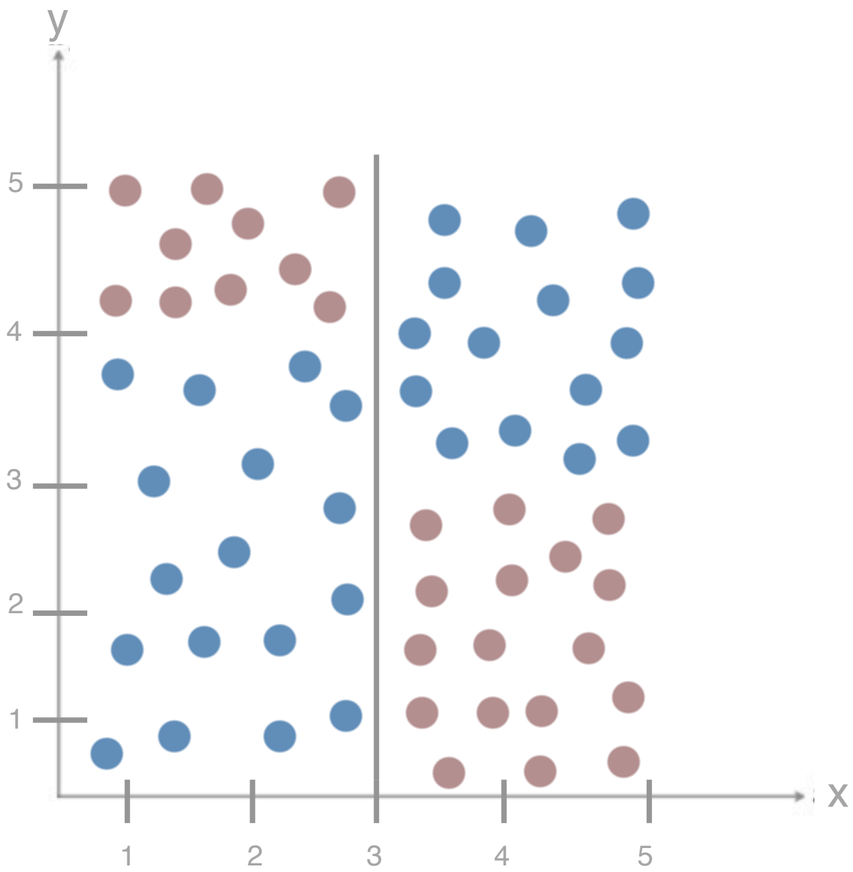
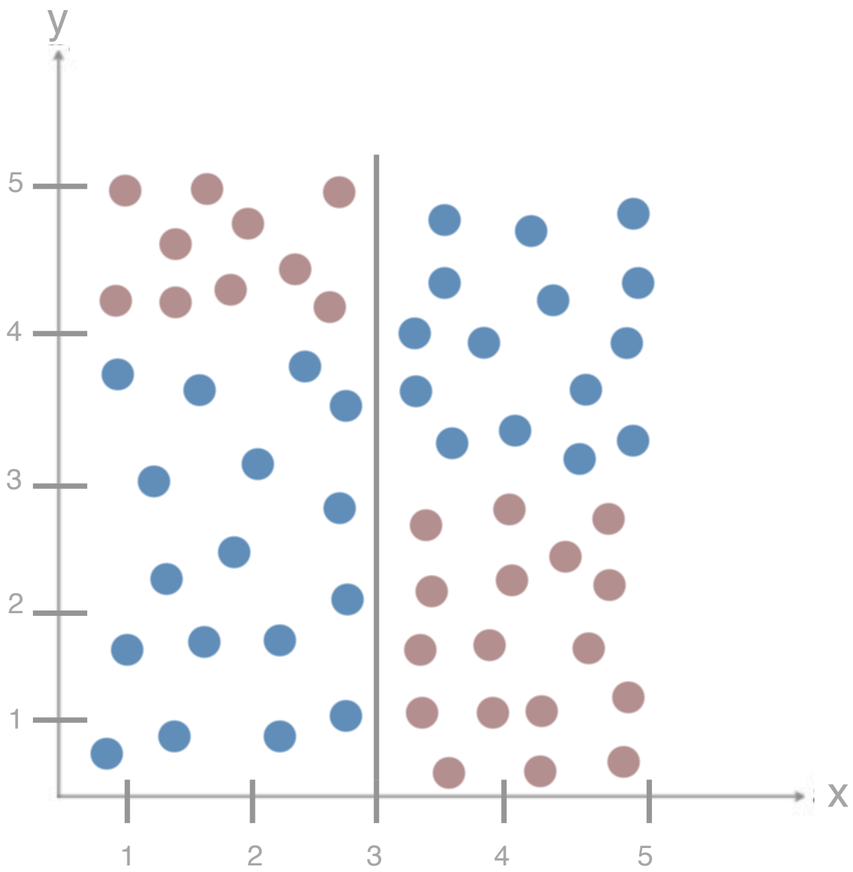
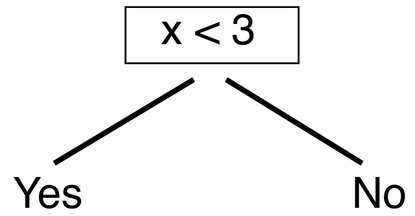


x < 3

Slightly Less Simple Example

Decision trees allow you to ask multiple linear questions





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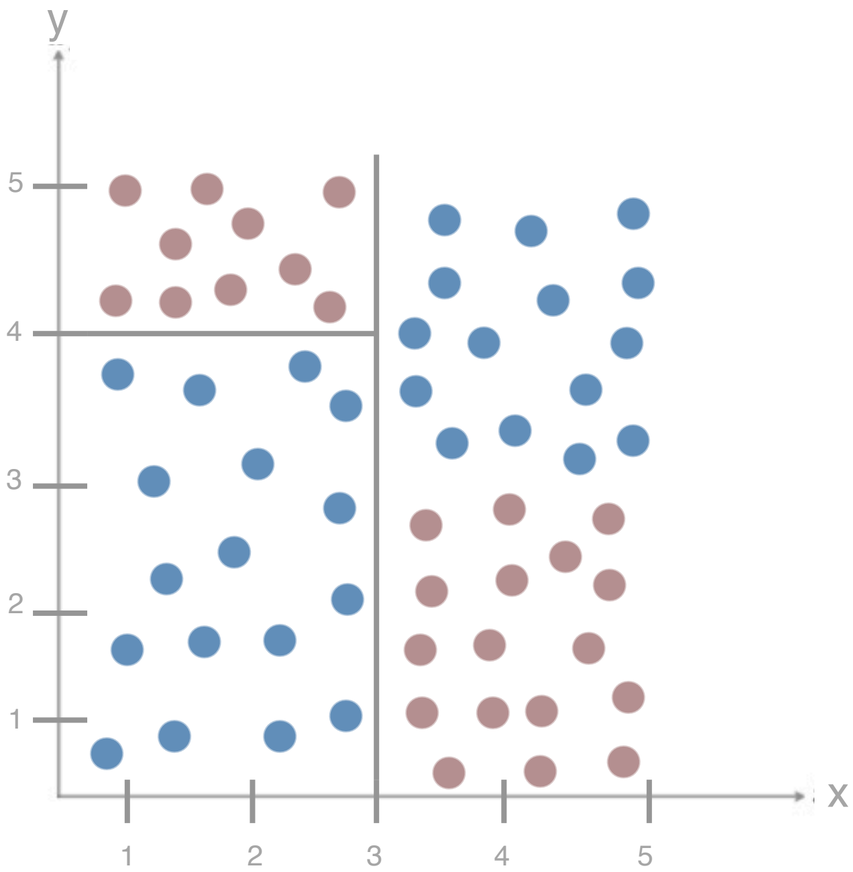

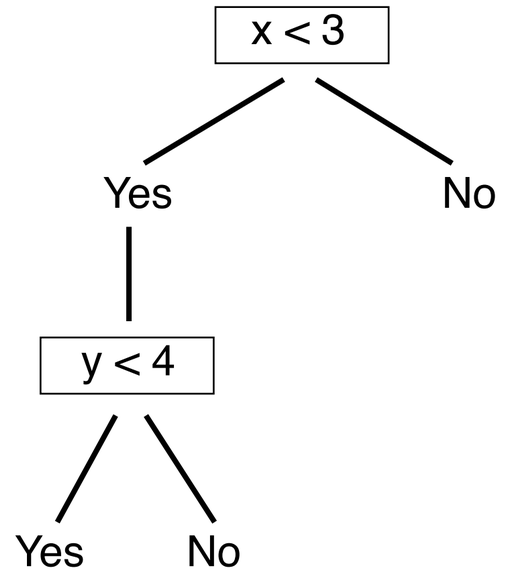

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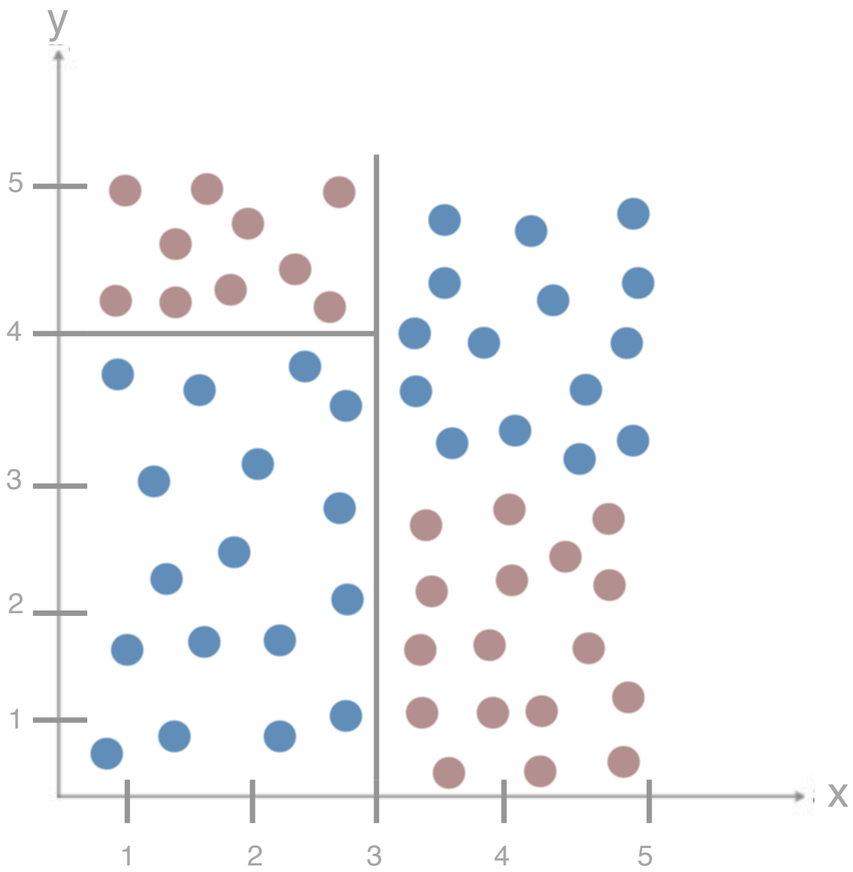

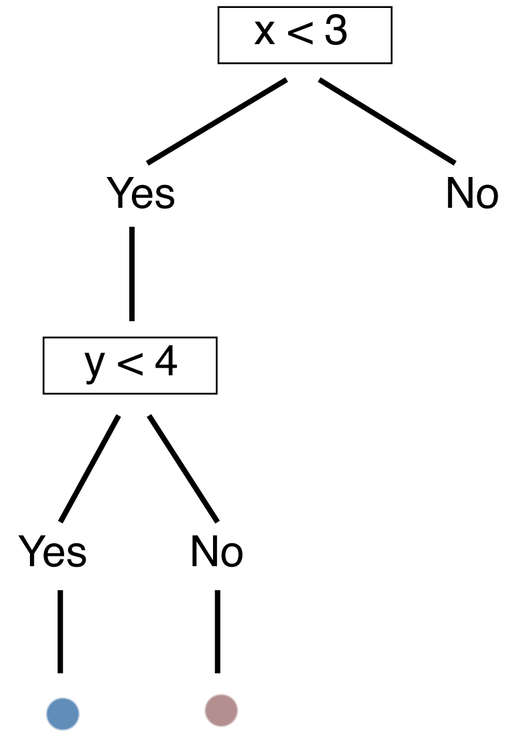

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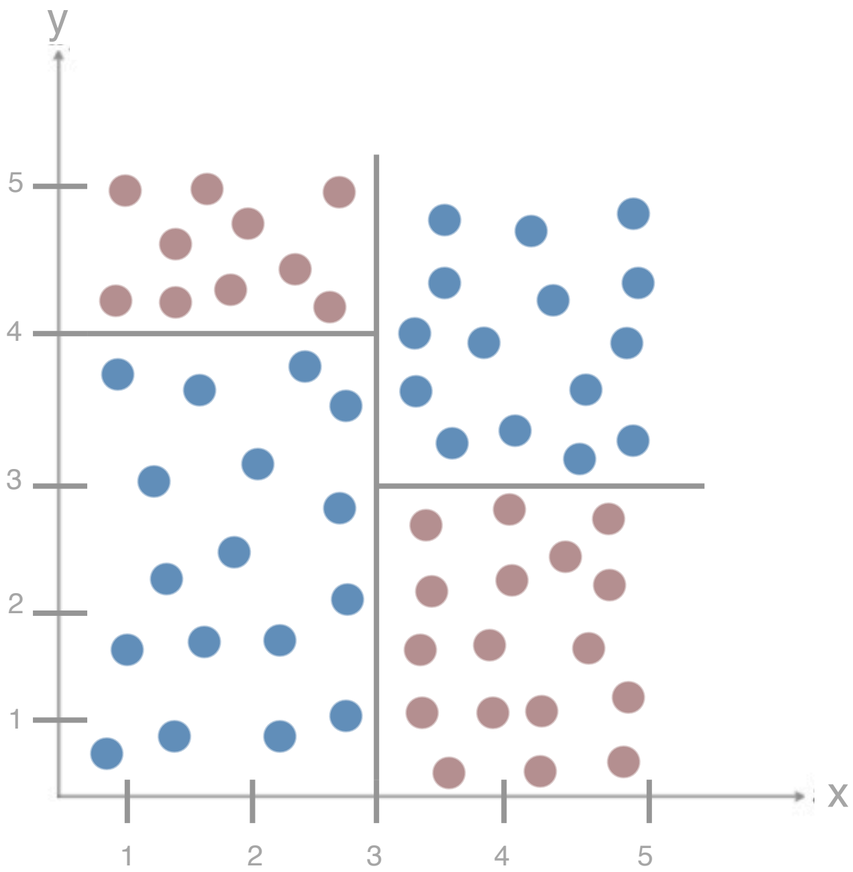

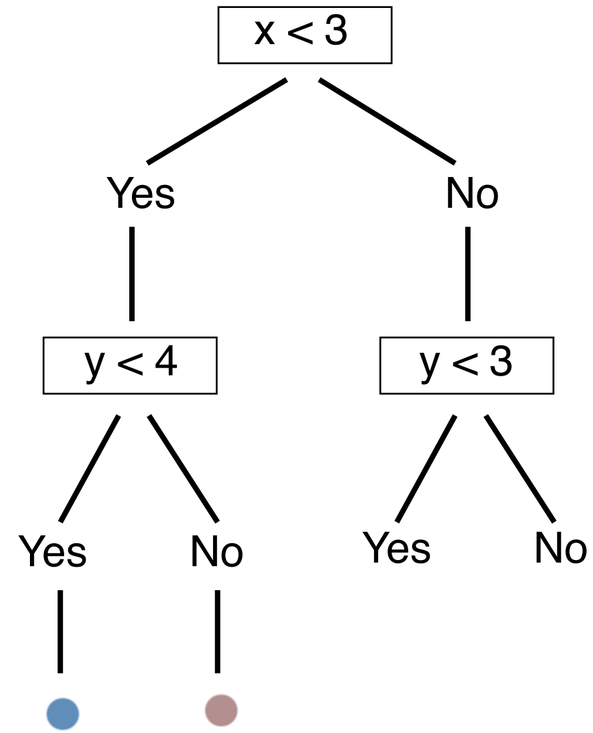

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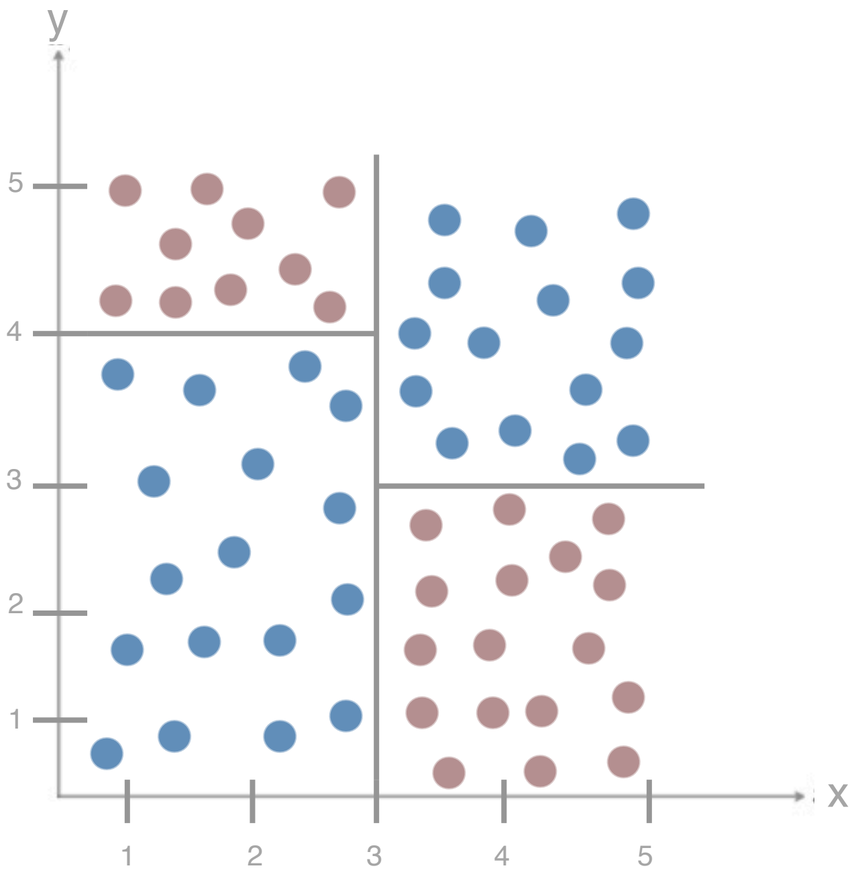
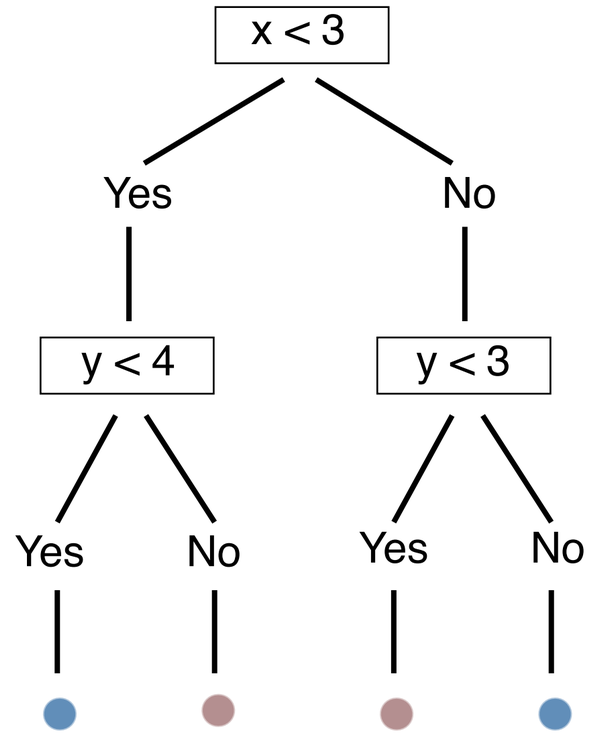
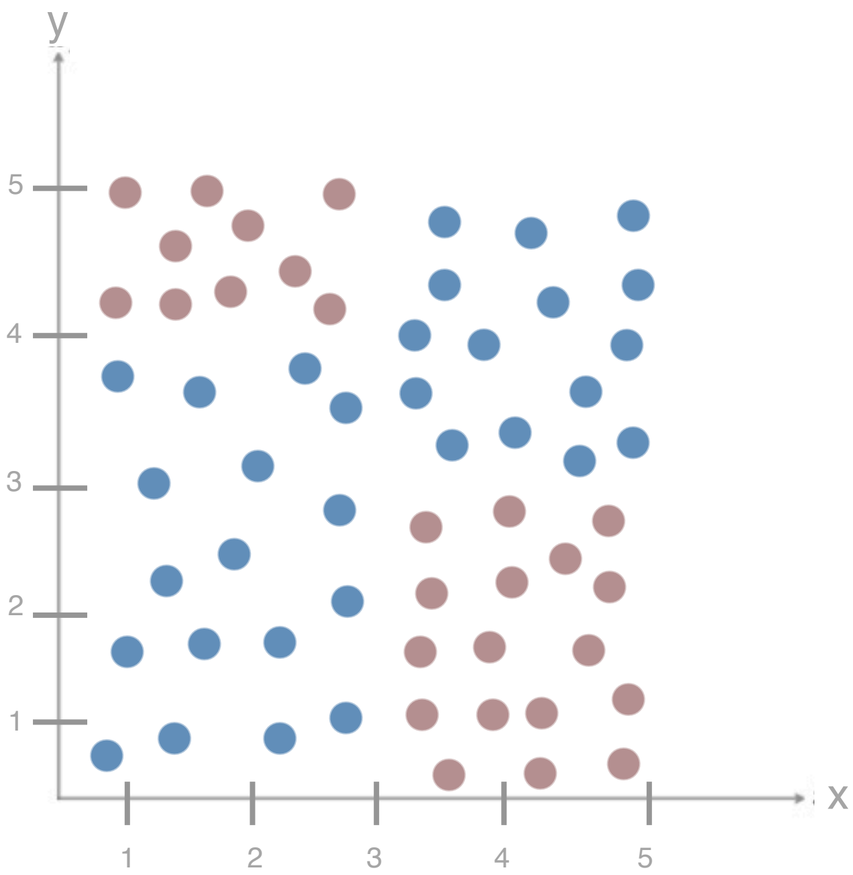




Slightly Less Simple Example

Notice that in this example we first split on x

What if we split on y first?



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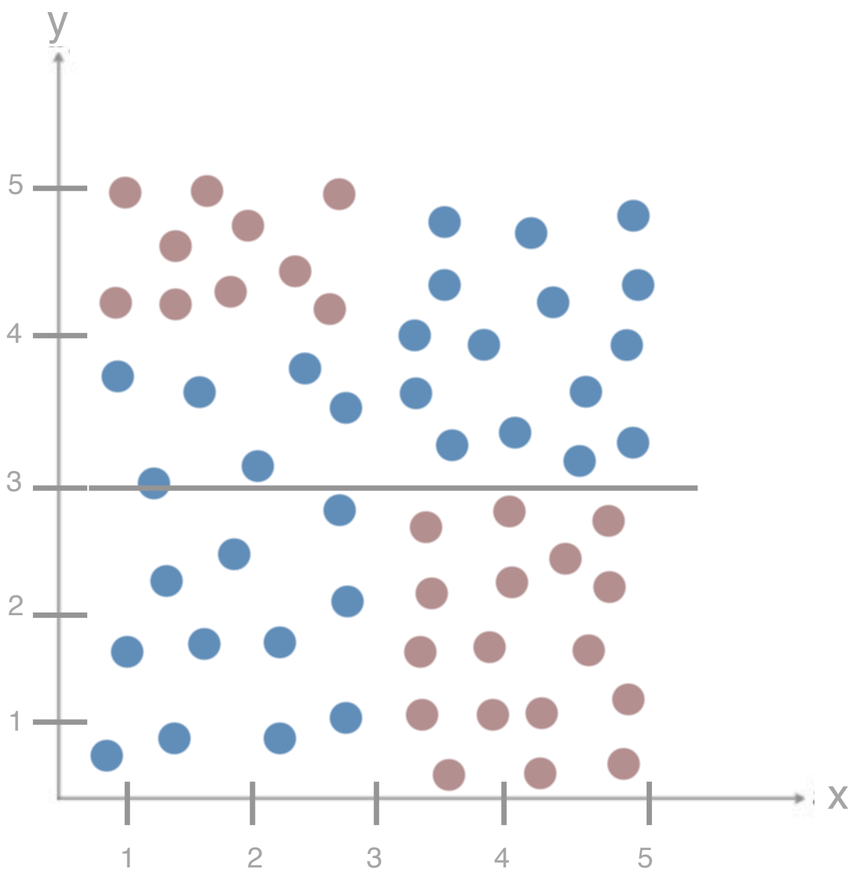

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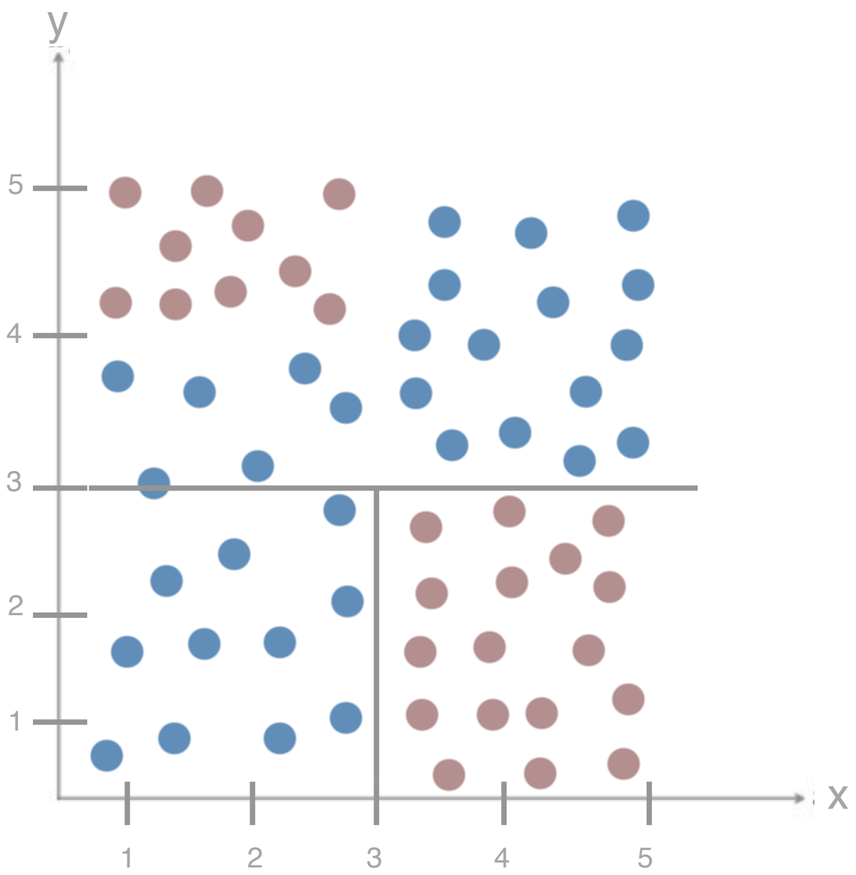

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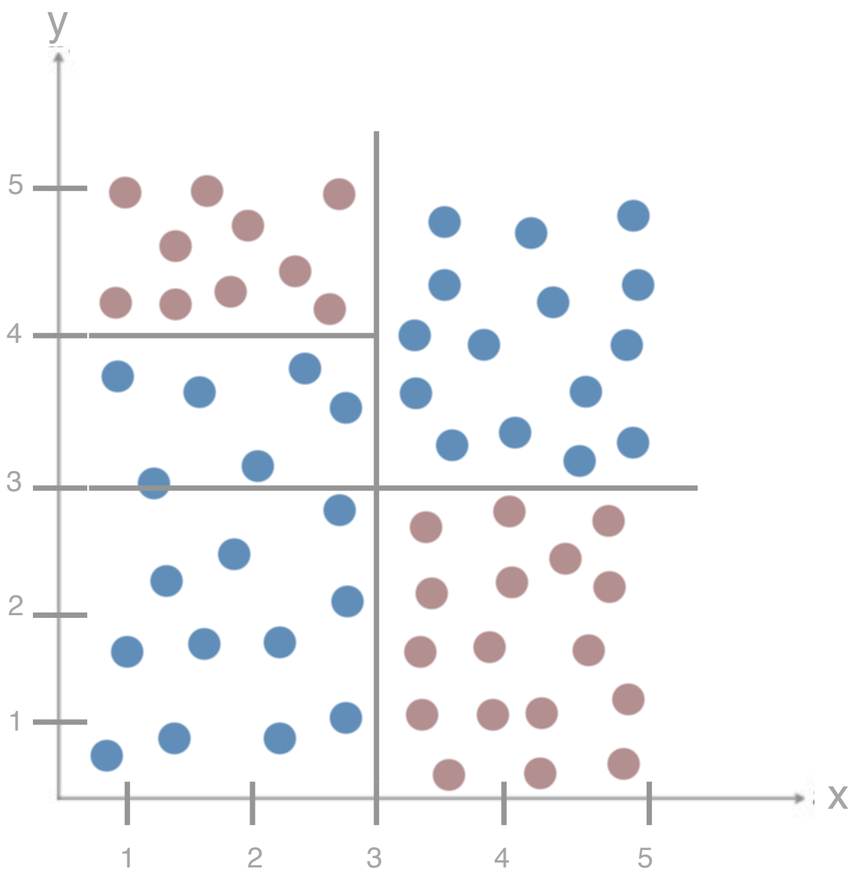

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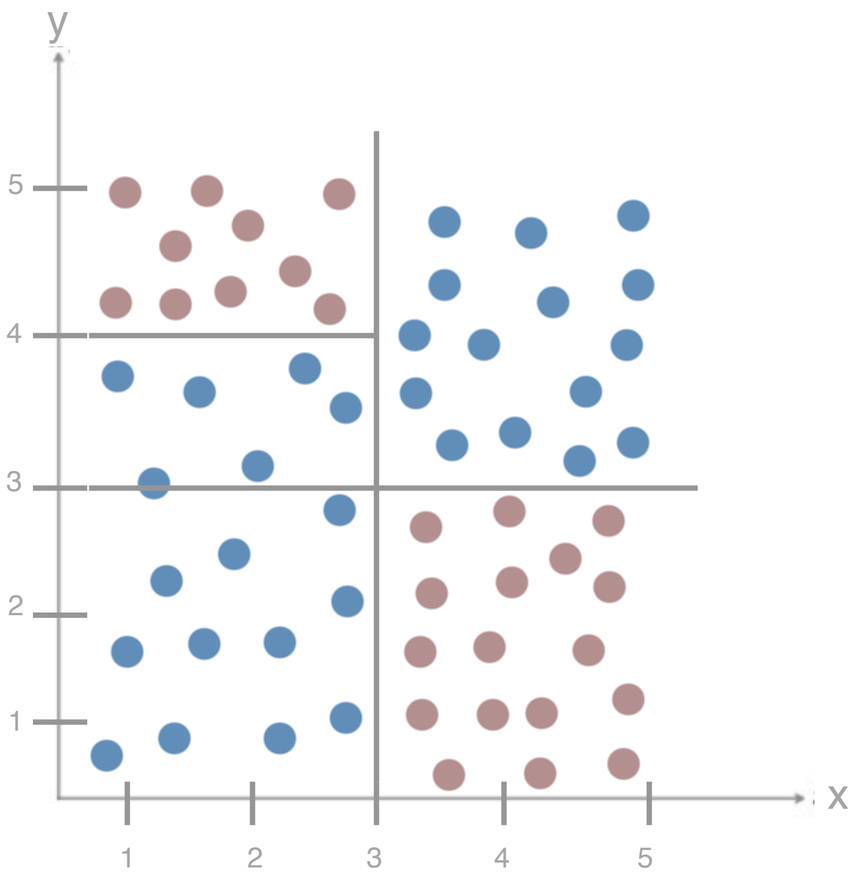
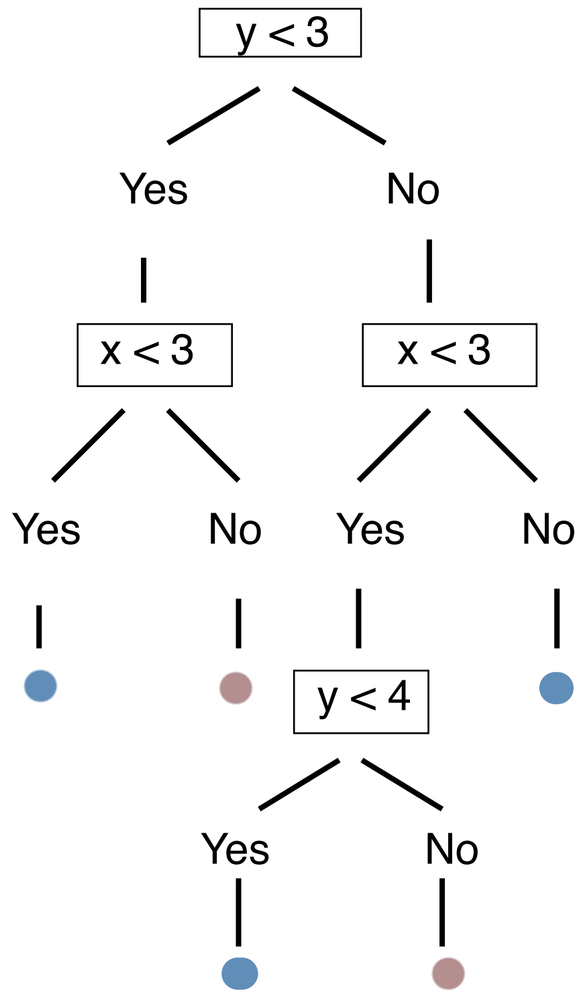




Splitting Strategy

Can't check all possible partitionings

Instead we'll take a greedy approach

Decide which feature to best split on

Perform split

Repeat on each child node

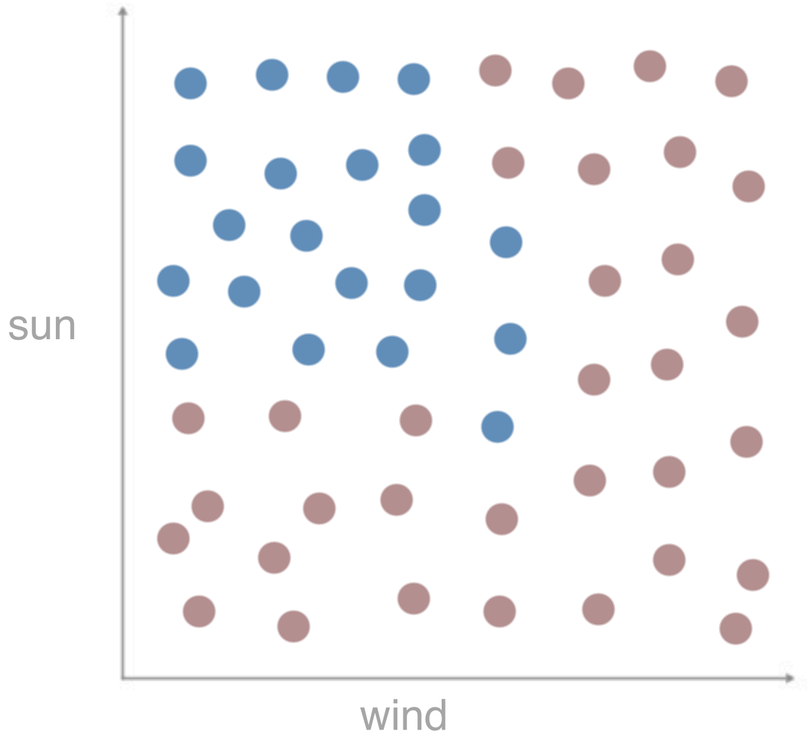
Terminate each branch when all training examples are same class

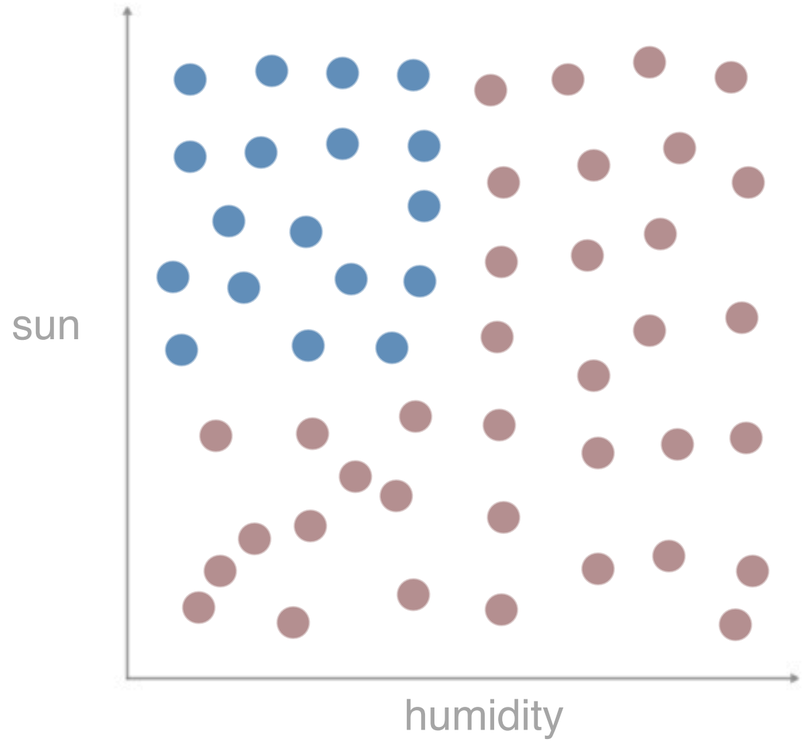
Splitting based on minimizing **Entropy**

Entropy: Measure of impurity of set of examples

Splitting Strategy

Entropy: Measure of impurity of set of examples





Entropy and Best Splitting

Entropy: Measure of impurity of set of examples (are there others??)

Mathematical Representation:

$$\text{entropy} = \sum_{c} -p_c \log_2(p_c)$$

where p_c is the fraction of examples in class c.

Note that for binary classification, let p be fraction in pos class, then

$$\text{entropy} = -p \log_2(p) - (1-p) \log_2(1-p)$$

Question: When is entropy the largest / smallest it can be?

Entropy and Best Splitting

$$\text{entropy} = -p\log_2(p) - (1-p)\log_2(1-p)$$

Question: When is entropy the largest / smallest it can be?

Answer:

- When all examples are same class, $\text{entropy} = 0$
- When samples equally balanced, $\text{entropy} = 1$

Entropy and Best Splitting

Example, consider the tennis problem now with binary features

sun	wind	humidity	tennis
sunny	windy	not humid	tennis
sunny	not windy	not humid	tennis
not sunny	not windy	humid	no tennis
sunny	windy	humid	no tennis

Entropy and Best Splitting

Example, consider the tennis problem now with binary features

sun	wind	humidity	tennis
S	W	$\neg\, H$	T
S	$\neg\, W$	$\neg\, H$	T
$\neg\, S$	$\neg\, W$	H	$\neg\, T$
S	W	H	$\neg\, T$

Question: What is the entropy of the root node?

Easy: The root node is balanced in T and $\neg\, T$ so the entropy is 1

Entropy and Best Splitting

Example, consider the tennis problem now with binary features

sun	wind	humidity	tennis
S	W	$\neg H$	T
S	$\neg W$	$\neg H$	T
$\neg S$	$\neg W$	H	$\neg T$
S	W	H	$\neg T$

Let's check the math anyway. Denoting the fraction of T in the training set by p, we have $p = \frac{1}{2}$

$$\text{entropy} = -\frac{1}{2}\log_2\left(\frac{1}{2}\right) - \frac{1}{2}\log_2\left(\frac{1}{2}\right)$$

Entropy and Best Splitting

Example, consider the tennis problem now with binary features

sun	wind	humidity	tennis
S	W	$\neg H$	T
S	$\neg W$	$\neg H$	T
$\neg S$	$\neg W$	H	$\neg T$
S	W	H	$\neg T$

Let's check the math anyway. Denoting the fraction of T in the training set by p, we have $p = \frac{1}{2}$

$$\text{entropy} = -\frac{1}{2}\log_2 2^{-1} - \frac{1}{2}\log_2 2^{-1}$$

Entropy and Best Splitting

Example, consider the tennis problem now with binary features

sun	wind	humidity	tennis
S	W	$\neg H$	T
S	$\neg W$	$\neg H$	T
$\neg S$	$\neg W$	H	$\neg T$
S	W	H	$\neg T$

Let's check the math anyway. Denoting the fraction of T in the training set by p, we have $p = \frac{1}{2}$

$$\text{entropy} = +\frac{1}{2}\log_2 2 + \frac{1}{2}\log_2 2 = 1$$

Information Gain and Best Splitting

Goal: Pick a feature and split that decreases impurity the most

Information Gain: Consider a parent node and it's children after a split on feature $\mathbf{x}_i$. Define the following

- D_{par}: training subset of the parent node
- D_{left}: training subset of the left child node
- D_{right}: training subset of the right child node
- I: An impurity function (for now, entropy)

Idea: Information gain is the difference between impurity at the parent and (weighted average) of impurity at the children

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- I: An impurity function (for now, entropy)

$$IG(D_{par}, \mathbf{x}_i) = I(D_{par}) - \frac{|D_{left}|}{|D_{par}|} I(D_{left}) - \frac{|D_{right}|}{|D_{par}|} I(D_{right})$$

Information Gain and Best Splitting

$$IG(D_{par}, \mathbf{x}_i) = I(D_{par}) - \frac{|D_{left}|}{|D_{par}|} I(D_{left}) - \frac{|D_{right}|}{|D_{par}|} I(D_{right})$$

For each feature $\mathbf{x}_i$ compute it's information gain

Split on feature with largest information gain

Information Gain and Best Splitting

Determine the best first splitting for the Tennis data

sun	wind	humidity	tennis
S	W	$\neg\, H$	T
S	$\neg\, W$	$\neg\, H$	T
$\neg\, S$	$\neg\, W$	H	$\neg\, T$
S	W	H	$\neg\, T$

We need to compute $IG(D_{par}, \mathbf{x}_i)$ for each feature, where D_{par} is the full training set

Information Gain and Best Splitting

$IG(D_{par}, \text{sun})$:

- $D_{par} = \{(S, T),\ (S, T),\ (\neg S, \neg T), (S, \neg T)\}$
- $D_{left} = \{(S, T),\ (S, T), (S, \neg T)\}$
- $D_{right} = \{(\neg S, \neg T)\}$

Q: What is $I(D_{par})$?

Information Gain and Best Splitting

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Q: What is $I(D_{par})$?

A: Already computed this, $I(D_{par}) = 1$

Information Gain and Best Splitting

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- $D_{par} = \{(S, T),\ (S, T),\ (\neg S, \neg T), (S, \neg T)\}$
- $D_{left} = \{(S, T),\ (S, T), (S, \neg T)\}$
- $D_{right} = \{(\neg S, \neg T)\}$

$$I(D_{par}) = 1,$$

Q: What are the weights in the average: $\frac{|D_{left}|}{|D_{par}|}$ and $\frac{|D_{right}|}{|D_{par}|}$?

Information Gain and Best Splitting

$IG(D_{par}, \text{sun})$:

- $D_{par} = \{(S, T),\ (S, T),\ (\neg S, \neg T), (S, \neg T)\}$
- $D_{left} = \{(S, T),\ (S, T), (S, \neg T)\}$
- $D_{right} = \{(\neg S, \neg T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{3}{4}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{4}$$

Q: What is the entropy $I(D_{left})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{sun})$:

- $D_{par} = \{(S, T),\ (S, T),\ (\neg S, \neg T), (S, \neg T)\}$
- $D_{left} = \{(S, T),\ (S, T), (S, \neg T)\}$
- $D_{right} = \{(\neg S, \neg T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{3}{4}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{4}$$

$$p = \frac{2}{3} \quad \Rightarrow \quad I(D_{left}) = -\frac{2}{3}\log_2 \frac{2}{3} - \frac{1}{3}\log_2 \frac{1}{3} = 0.918$$

Information Gain and Best Splitting

$IG(D_{par}, \text{sun})$:

- $D_{par} = \{(S, T),\ (S, T),\ (\neg S, \neg T), (S, \neg T)\}$
- $D_{left} = \{(S, T),\ (S, T), (S, \neg T)\}$
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$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{3}{4}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{4}, \quad I(D_{left}) = 0.918$$

Q: What is $I(D_{right})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{sun})$:

- $D_{par} = \{(S, T),\ (S, T),\ (\neg S, \neg T), (S, \neg T)\}$
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$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{3}{4}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{4}, \quad I(D_{left}) = 0.918$$

$$p = 0 \quad \Rightarrow \quad I(D_{right}) = 0$$

Information Gain and Best Splitting

$IG(D_{par}, \text{sun})$:

- $D_{par} = \{(S, T),\ (S, T),\ (\neg S, \neg T), (S, \neg T)\}$
- $D_{left} = \{(S, T),\ (S, T), (S, \neg T)\}$
- $D_{right} = \{(\neg S, \neg T)\}$

Q: What is $IG(D_{par}, \text{sun})$?

$$
\begin{aligned}
IG(D_{par}, \text{sun}) &= I(D_{par}) - \frac{|D_{left}|}{|D_{par}|} I(D_{left}) - \frac{|D_{right}|}{|D_{par}|} I(D_{right}) \\
&= 1 - \tfrac{3}{4} \cdot 0.918 - \tfrac{1}{4} \cdot 0 \\
&= 0.3112
\end{aligned}
$$

Information Gain and Best Splitting

Determine the best first splitting for the Tennis data

sun	wind	humidity	tennis
S	W	$\neg\, H$	T
S	$\neg\, W$	$\neg\, H$	T
$\neg\, S$	$\neg\, W$	H	$\neg\, T$
S	W	H	$\neg\, T$

We need to compute $IG(D_{par}, \mathbf{x}_i)$ for each feature, where D_{par} is the full training set

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg\, W, T),\ (\neg\, W, \neg\, T), (W, \neg\, T)\}$
- $D_{left} = \{(W, T),\ (W, \neg\, T)\}$
- $D_{right} = \{(\neg\, W, \neg\, T),\ (\neg\, W, T)\}$

Q: What is $I(D_{par})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg\, W, T),\ (\neg\, W, \neg\, T), (W, \neg\, T)\}$
- $D_{left} = \{(W, T),\ (W, \neg\, T)\}$
- $D_{right} = \{(\neg\, W, \neg\, T),\ (\neg\, W, T)\}$

Q: What is $I(D_{par})$?

A: Already computed this, $I(D_{par}) = 1$

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg W, T),\ (\neg W, \neg T), (W, \neg T)\}$
- $D_{left} = \{(W, T),\ (W, \neg T)\}$
- $D_{right} = \{(\neg W, \neg T),\ (\neg W, T)\}$

$$I(D_{par}) = 1,$$

Q: What are the weights in the average: $\frac{|D_{left}|}{|D_{par}|}$ and $\frac{|D_{right}|}{|D_{par}|}$?

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg\, W, T),\ (\neg\, W, \neg\, T), (W, \neg\, T)\}$
- $D_{left} = \{(W, T),\ (W, \neg\, T)\}$
- $D_{right} = \{(\neg\, W, \neg\, T),\ (\neg\, W, T)\}$

$$I(D_{par}) = 1, \quad \frac{|\,D_{left}\,|}{|\,D_{par}\,|} = \frac{1}{2}, \quad \frac{|\,D_{right}\,|}{|\,D_{par}\,|} = \frac{1}{2}$$

Q: What is the entropy $I(D_{left})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg W, T),\ (\neg W, \neg T), (W, \neg T)\}$
- $D_{left} = \{(W, T),\ (W, \neg T)\}$
- $D_{right} = \{(\neg W, \neg T),\ (\neg W, T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{1}{2}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{2}$$

$$p = \frac{1}{2} \quad \Rightarrow \quad I(D_{left}) = -\frac{1}{2}\log_2 \frac{1}{2} - \frac{1}{2}\log_2 \frac{1}{2} = 1$$

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg W, T),\ (\neg W, \neg T), (W, \neg T)\}$
- $D_{left} = \{(W, T),\ (W, \neg T)\}$
- $D_{right} = \{(\neg W, \neg T),\ (\neg W, T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{1}{2}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{2}, \quad I(D_{left}) = 1$$

Q: What is $I(D_{right})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg W, T),\ (\neg W, \neg T), (W, \neg T)\}$
- $D_{left} = \{(W, T),\ (W, \neg T)\}$
- $D_{right} = \{(\neg W, \neg T),\ (\neg W, T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{1}{2}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{2}, \quad I(D_{left}) = 1$$

$$p = \frac{1}{2} \quad \Rightarrow \quad I(D_{right}) = -\frac{1}{2}\log_2 \frac{1}{2} - \frac{1}{2}\log_2 \frac{1}{2} = 1$$

Information Gain and Best Splitting

$IG(D_{par}, \text{wind})$:

- $D_{par} = \{(W, T),\ (\neg W, T),\ (\neg W, \neg T), (W, \neg T)\}$
- $D_{left} = \{(W, T),\ (W, \neg T)\}$
- $D_{right} = \{(\neg W, \neg T),\ (\neg W, T)\}$

Q: What is $IG(D_{par}, \text{wind})$?

$$
\begin{aligned}
IG(D_{par}, \text{wind}) &= I(D_{par}) - \frac{|D_{left}|}{|D_{par}|} I(D_{left}) - \frac{|D_{right}|}{|D_{par}|} I(D_{right}) \\
&= 1 - \frac{1}{2} \cdot 1 - \frac{1}{2} \cdot 1 \\
&= 0
\end{aligned}
$$

Information Gain and Best Splitting

Determine the best first splitting for the Tennis data

sun	wind	humidity	tennis
S	W	$\neg\, H$	T
S	$\neg\, W$	$\neg\, H$	T
$\neg\, S$	$\neg\, W$	H	$\neg\, T$
S	W	H	$\neg\, T$

We need to compute $IG(D_{par}, \mathbf{x}_i)$ for each feature, where D_{par} is the full training set

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

Q: What is $I(D_{par})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

Q: What is $I(D_{par})$?

A: Already computed this, $I(D_{par}) = 1$

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

$$I(D_{par}) = 1,$$

Q: What are the weights in the average: $\frac{|D_{left}|}{|D_{par}|}$ and $\frac{|D_{right}|}{|D_{par}|}$?

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{1}{2}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{2}$$

Q: What is the entropy $I(D_{left})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{1}{2}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{2}$$

$$p = 1 \quad \Rightarrow \quad I(D_{left}) = 1 \log_2 1 - 0 \log_2 0 = 0$$

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{1}{2}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{2}, \quad I(D_{left}) = 1$$

Q: What is $I(D_{right})$?

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

$$I(D_{par}) = 1, \quad \frac{|D_{left}|}{|D_{par}|} = \frac{1}{2}, \quad \frac{|D_{right}|}{|D_{par}|} = \frac{1}{2}, \quad I(D_{left}) = 1$$

$$p = 0 \quad \Rightarrow \quad I(D_{right}) = 0 \log_2 0 - 1 \log_2 1 = 0$$

Information Gain and Best Splitting

$IG(D_{par}, \text{humid})$:

- $D_{par} = \{(\neg H, T),\ (\neg H, T),\ (H, \neg T), (H, \neg T)\}$
- $D_{left} = \{(H, \neg T), (H, \neg T)\}$
- $D_{par} = \{(\neg H, T),\ (\neg H, T)\}$

Q: What is $IG(D_{par}, \text{humid})$?

$$
\begin{aligned}
IG(D_{par}, \text{humid}) &= I(D_{par}) - \frac{|D_{left}|}{|D_{par}|} I(D_{left}) - \frac{|D_{right}|}{|D_{par}|} I(D_{right} \\
&= 1 - \frac{1}{2} \cdot 0 - \frac{1}{2} \cdot 0 \\
&= 1
\end{aligned}
$$

Information Gain and Best Splitting

So we have ...

$$IG(D_{par}, \text{sun}) = 0.3112$$

$$IG(D_{par}, \text{wind}) = 0$$

$$IG(D_{par}, \text{humid}) = 1$$

Q: Which feature should we split on?

Information Gain and Best Splitting

So we have ...

$$IG(D_{par}, \text{sun}) = 0.3112$$

$$IG(D_{par}, \text{wind}) = 0$$

$$IG(D_{par}, \text{humid}) = 1$$

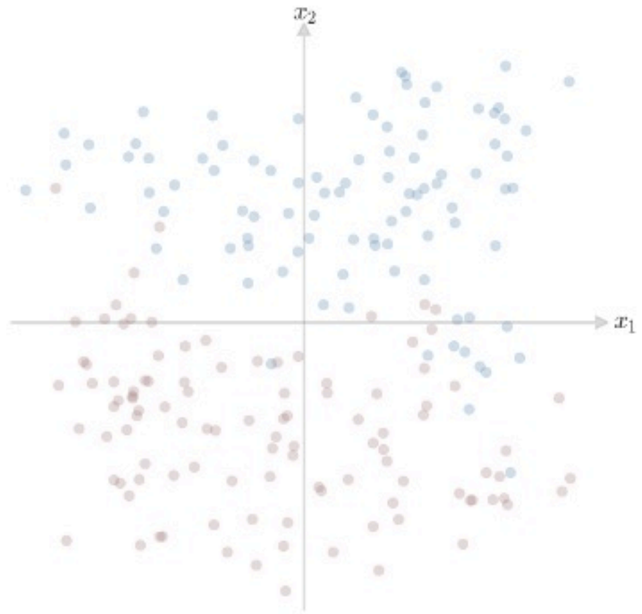
Q: Which feature should we split on?

A: We split on **humid** because it gives the largest information gain!

So Many Questions ...

- How well do these things work anyway?

In general, Decision Trees are very high variance methods and prone to overfitting



So Many Questions ...

- How well do these things work anyway?

In general, Decision Trees are very high variance methods and prone to overfitting. How do we combat this?