CSCI567 Machine Learning (Fall 2024)

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Outline

Decision tree

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- linear models, neural nets and other nonlinear models induced by kernels

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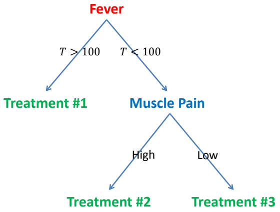
- used to be very popular; ensemble of trees (i.e. "forest") can still be very effective
- not to be confused with the "tree reduction" in Lec 4

Example

Many decisions are made based on some tree structure

Medical treatment



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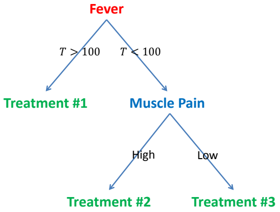
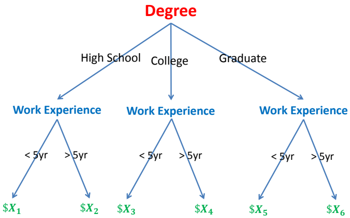
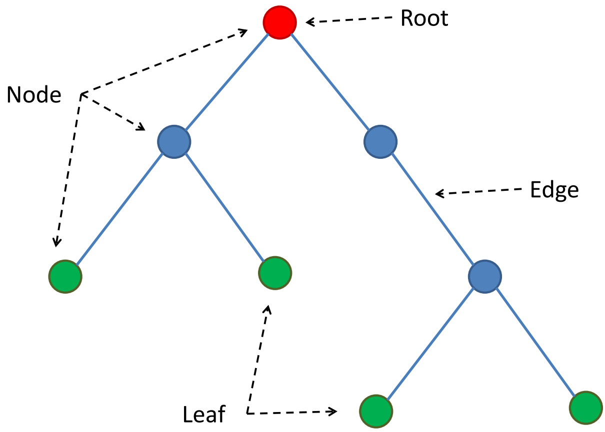


Salary in a company

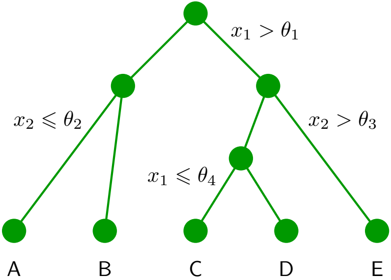


Tree terminology



A more abstract example of decision trees

Input: $\boldsymbol{x} = (x_1, x_2)$



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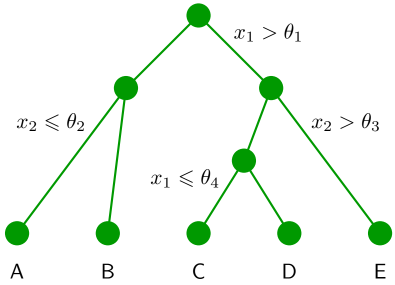

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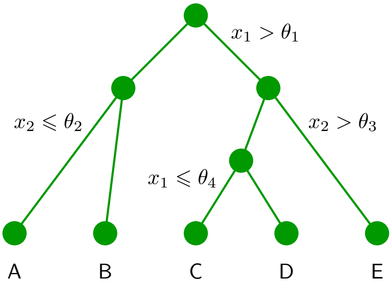

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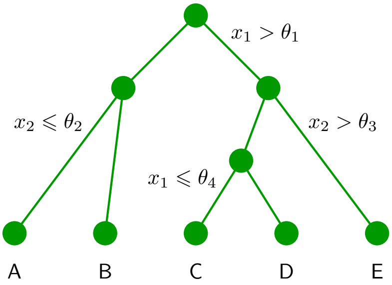

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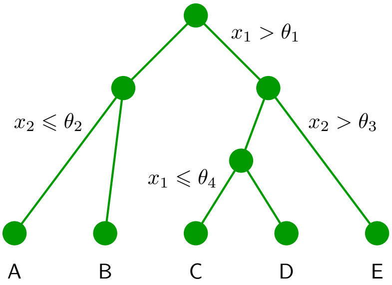

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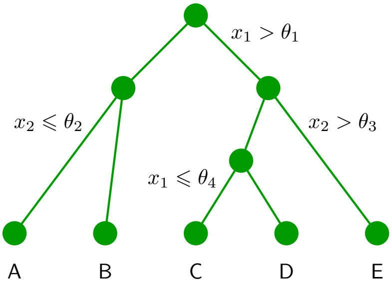

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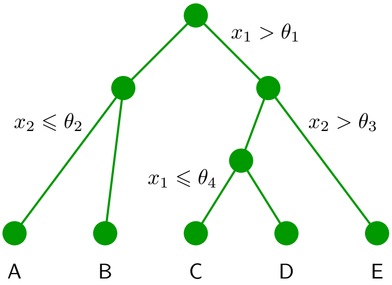

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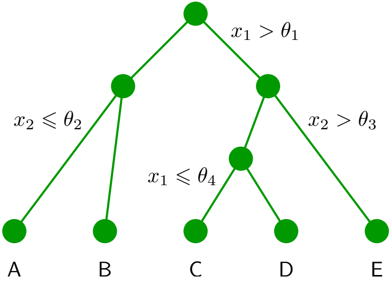
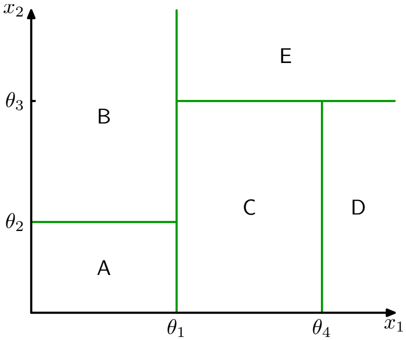
Complex to formally write down, but easy to represent pictorially or as codes.

The decision boundary

Corresponds to a classifier with boundaries:





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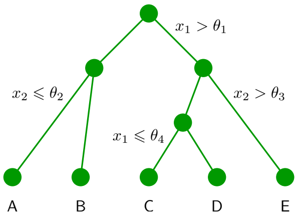

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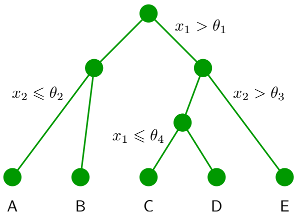

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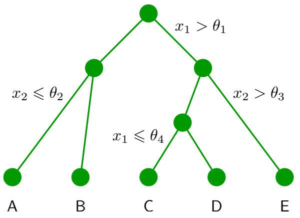

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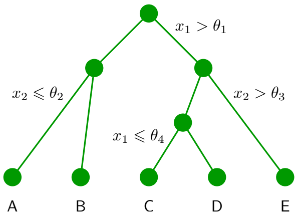

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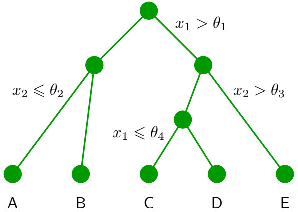

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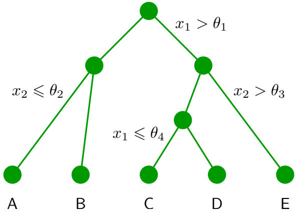

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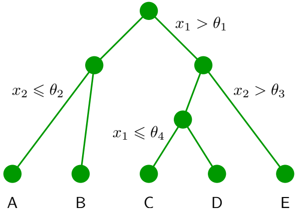

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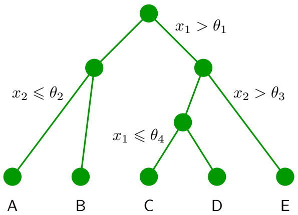

- the value/prediction of the leaves (A, B, ...)

Learning the parameters

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Instead, we turn to some **greedy top-down approach**.

A running example

[Russell & Norvig, AIMA]

- predict whether a customer will wait for a table at a restaurant
- 12 training examples
- 10 features (all discrete)

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

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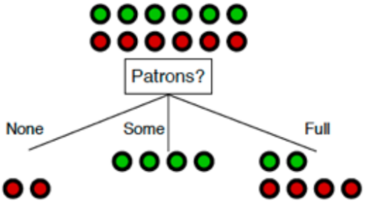
I.e., which feature should we test at the root? Examples:



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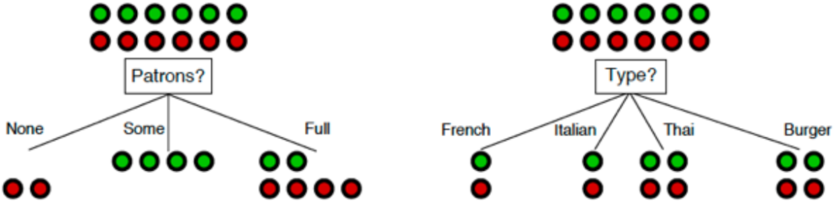

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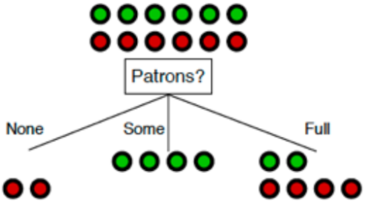

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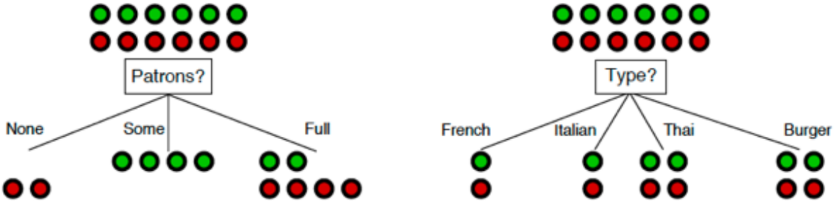

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- intuitively "patrons" is a better feature since it leads to "more pure" or "more certain" children
- how to quantify this intuition?

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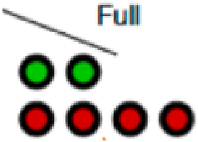

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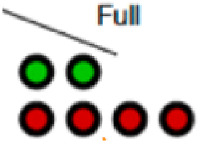

One classic uncertainty measure of a distribution is its *(Shannon) entropy*:

$$H(P) = -\sum_{k=1}^{\mathsf{C}} P(Y=k)\log P(Y=k)$$

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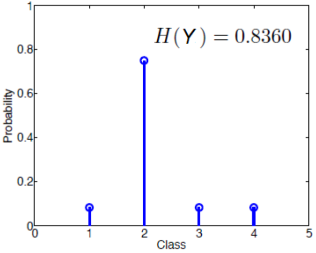
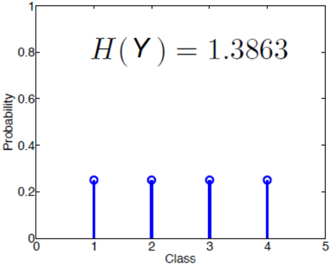
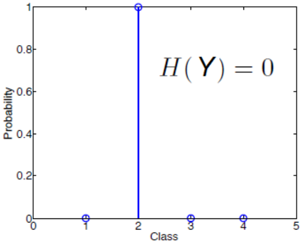
  - $0 \log 0$ is defined naturally as $\lim_{z \to 0+} z \log z = 0$

Examples of computing entropy

With base e and 4 classes:







Another example

Entropy in each child if root tests on "patrons"

For "None" branch

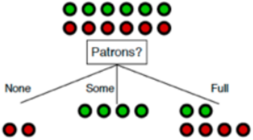
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

For "Some" branch

$$-\left(\frac{4}{4+0}\log\frac{4}{4+0}+\frac{0}{4+0}\log\frac{0}{4+0}\right)=0$$

For "Full" branch

$$-\left(\frac{2}{2+4}\log\frac{2}{2+4}+\frac{4}{2+4}\log\frac{4}{2+4}\right)\approx 0.9$$



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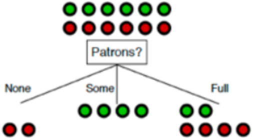

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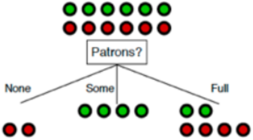

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Very naturally, we take the weighted average of entropy:

$$\frac{2}{12}\times 0+\frac{4}{12}\times 0+\frac{6}{12}\times 0.9=0.45$$

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&= \sum_a P(A = a) \left(- \sum_{k=1}^{\mathsf{C}} P(Y \mid A = a) \log P(Y \mid A = a) \right)
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&= \sum_a P(A=a) \left(-\sum_{k=1}^{\mathsf{C}} P(Y \mid A=a) \log P(Y \mid A=a) \right) \\
&= \sum_a \text{“fraction of example at node } A=a\text{”} \times \text{“entropy at node } A=a\text{”}
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&= \sum_a P(A=a) \left(-\sum_{k=1}^{\mathsf{C}} P(Y \mid A=a) \log P(Y \mid A=a) \right) \\
&= \sum_a \text{“fraction of example at node } A=a\text{”} \times \text{“entropy at node } A=a\text{”}
\end{aligned}
$$

Pick the feature that leads to the smallest conditional entropy.

Deciding the root

For "French" branch

$$-\left(\frac{1}{1+1}\log\frac{1}{1+1}+\frac{1}{1+1}\log\frac{1}{1+1}\right)=1$$

For "Italian" branch

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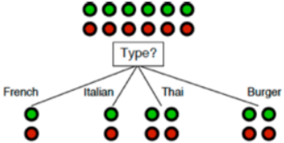

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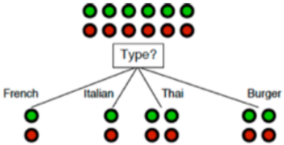

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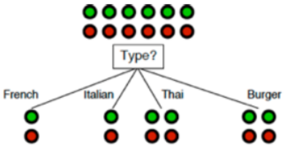

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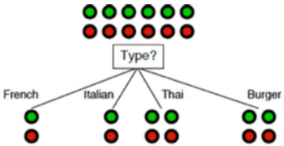

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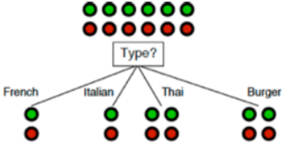

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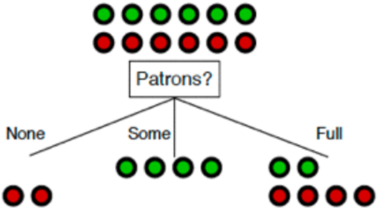
We are now done with building the root (this is also called a **stump**).

Repeat recursively

Split each child in the same way.



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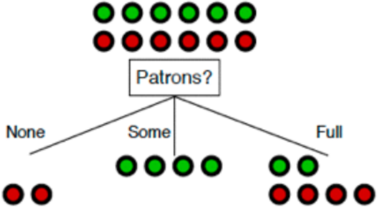

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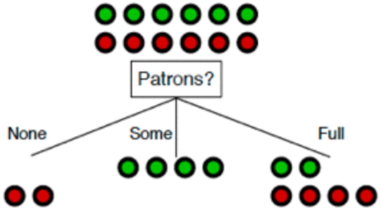
- but no need to split children "none" and "some": they are pure already and become leaves
- for "full", repeat, focusing on those 6 examples:



	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
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X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
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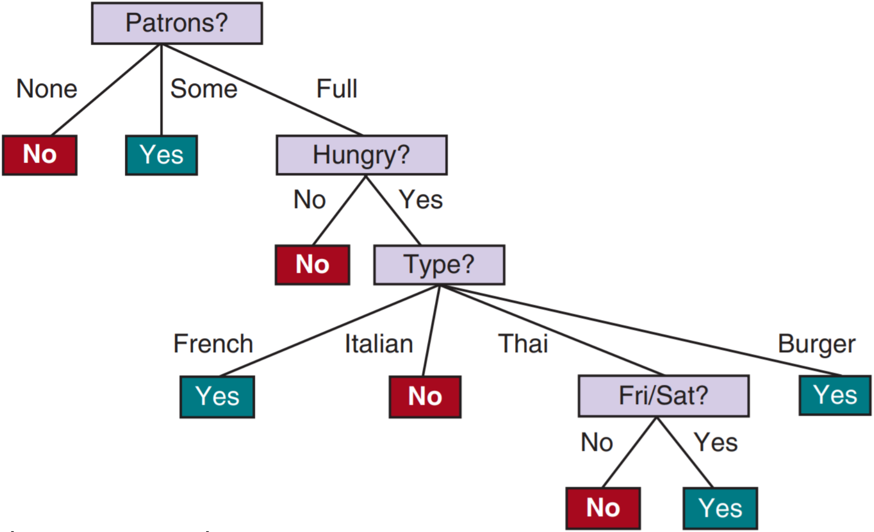
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T



Again, very easy to interpret.

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- else if Examples is empty, <u>return a leaf with majority class of parent</u>
- else

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- if a feature is continuous, we need to find a threshold that leads to minimum conditional entropy or Gini impurity. *Think about how to do it efficiently.*

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Outline

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We again focus on binary classification.

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- repeat ...
- final classifier is the (weighted) majority vote of all weak classifiers

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- even if it's not obvious how to deal with weight directly, we can always resample according to D to create a new unweighted dataset

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AdaBoost is one of the most successful boosting algorithms.

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$$\beta_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right) \qquad (\beta_t > 0 \Leftrightarrow \epsilon_t < 0.5)$$

where $\epsilon_t = \sum_{n: h_t(\boldsymbol{x}_n) \neq y_n} D_t(n)$ is the weighted error of h_t.

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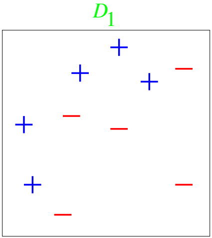
Output the final classifier $H(\boldsymbol{x}) = \text{sgn}\left(\sum_{t=1}^{T} \beta_t h_t(\boldsymbol{x})\right)$

Example

10 data points in $\mathbb{R}^2$

The size of $+$ or - indicates the weight, which starts from uniform D_1



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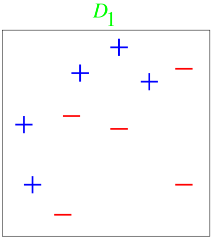

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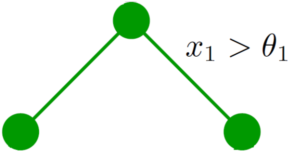

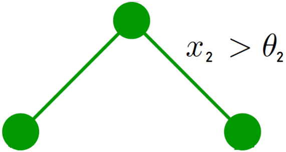

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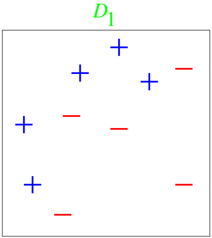

Base algorithm is decision stump:

Observe that *no stump can predict very accurately for this dataset*

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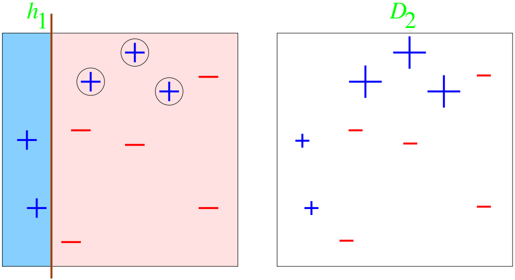

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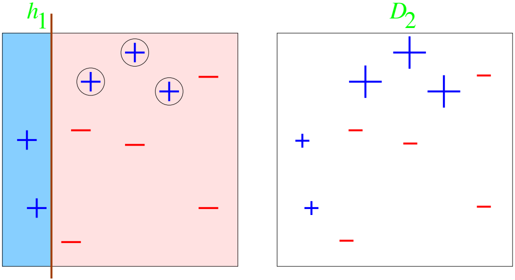

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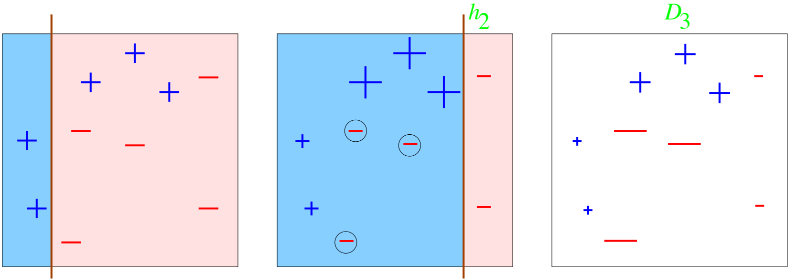
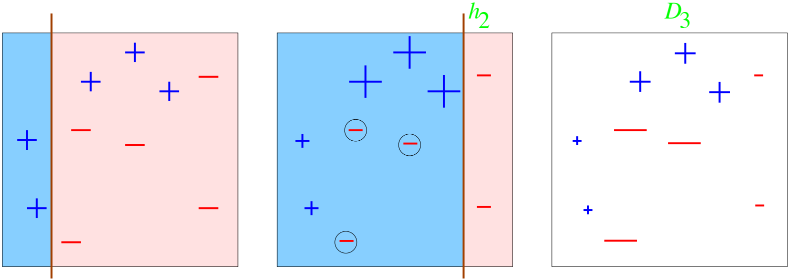
- D_2 puts more weights on those examples

Round 2: $t = 2$



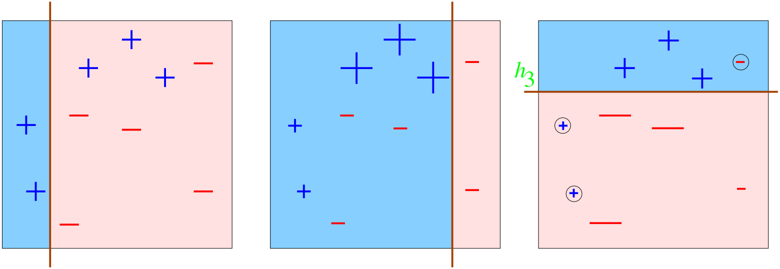
- 3 misclassified (circled): $\epsilon_2 = 0.21 \rightarrow \beta_2 = 0.65$.

Round 2: $t = 2$



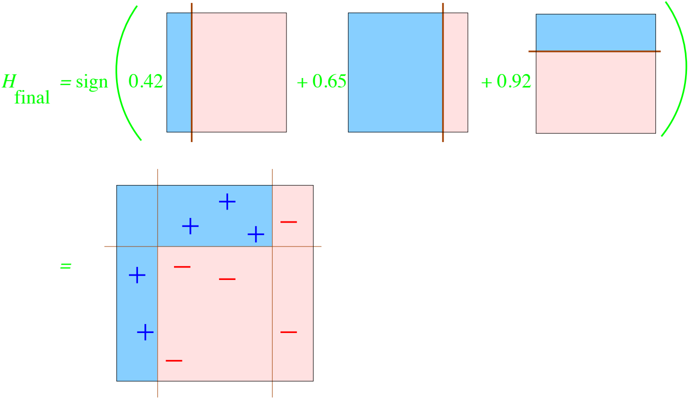
- 3 misclassified (circled): $\epsilon_2 = 0.21 \rightarrow \beta_2 = 0.65$.
- D_3 puts more weights on those examples

Round 3: $t = 3$



- again 3 misclassified (circled): $\epsilon_3 = 0.14 \rightarrow \beta_3 = 0.92$.

Final classifier: combining 3 classifiers



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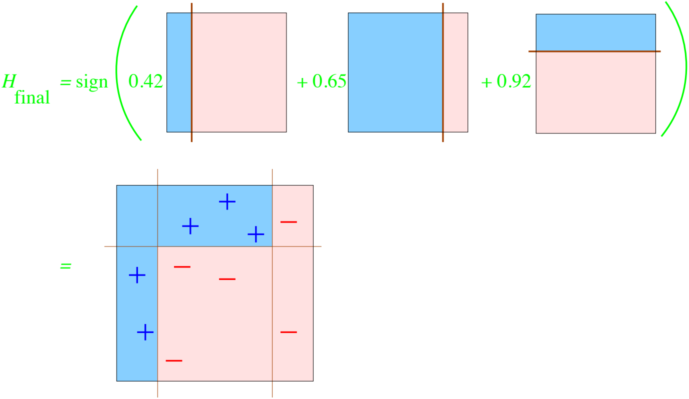

All data points are now classified correctly, even though each weak classifier makes 3 mistakes.

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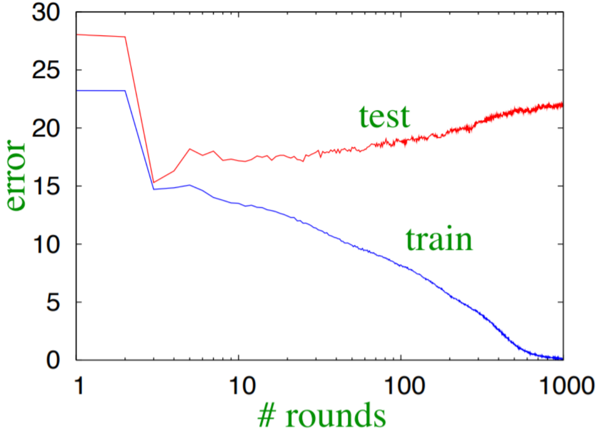

(boosting "stumps" on heart-disease dataset)

Resistance to overfitting

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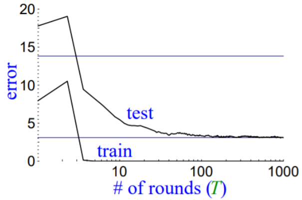

(boosting C4.5 on "letter" dataset)

- test error does not increase, even after 1000 rounds
  - (total size > 2,000,000 nodes)
- test error continues to drop even after training error is zero!

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train error	0.0	0.0	0.0
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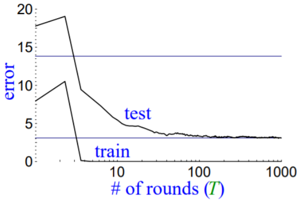

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Used to be a mystery, but by now rigorous theory has been developed to explain this phenomenon.

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In fact, *AdaBoost also follows the general framework of minimizing some surrogate loss*.

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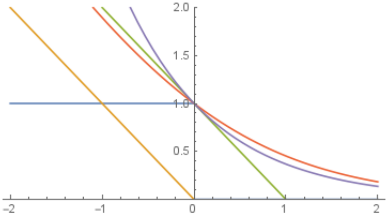

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where the last step is by the definition of weights

$$D_t(n) \propto D_{t-1}(n) \exp\left(-y_n \beta_{t-1} h_{t-1}(\boldsymbol{x}_n)\right) \propto \cdots \propto \exp\left(-y_n f_{t-1}(\boldsymbol{x}_n)\right)$$

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(recall $\epsilon_t = \sum_{n: y_n \neq h_t(\boldsymbol{x}_n)} D_t(n)$)

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This greedy step is abstracted out through a base algorithm.

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When h_t (and thus ϵ_t) is fixed, we then find β_t to minimize

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Keep doing this greedy minimization gives the AdaBoost algorithm.

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