CSCI567 Machine Learning (Fall 2018)

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U of Southern California

Oct 10, 2018

Administration

Midterm:

- grading is in process
- depending on the final outcomes, we will decide whether to curve the exam and to discuss some of the problems in class

Homework 2 was due on 10/7

W3 is available, P3 will be available soon

Outline

1. Review of last lecture
2. Decision tree
3. Boosting

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Support Vector Machine

SVM: **max-margin linear classifier**

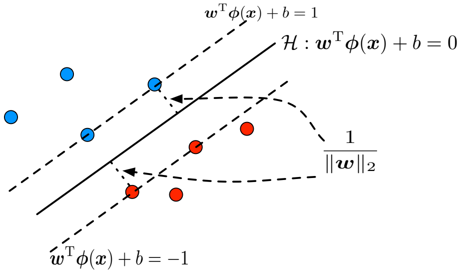
Primal (equivalent to minimizing L2 regularized hinge loss):

$$\begin{aligned} \min_{\boldsymbol{w}, b, \{\xi_n\}} \quad & C \sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t.} \quad & 1 - y_n(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b) \leq \xi_n, \quad \forall\ n \\ & \xi_n \geq 0, \quad \forall\ n \end{aligned}$$

Dual (kernelizable, reveals what training points are support vectors):

$$\begin{aligned} \max_{\{\alpha_n\}} \quad & \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) \\ \text{s.t.} \quad & \sum_n \alpha_n y_n = 0 \quad \text{and} \quad 0 \leq \alpha_n \leq C, \quad \forall\ n \end{aligned}$$

Separable Case



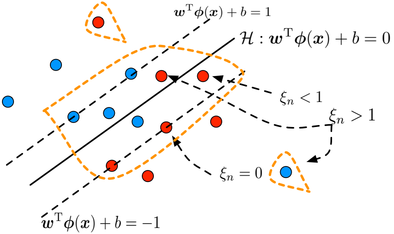
Geometric interpretation of support vectors

A support vector satisfies $\alpha_n^* \neq 0$ and

$$1 - \xi_n^* - y_n(\boldsymbol{w}^{*\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b^*) = 0$$

When

- $\xi_n^* = 0$, $y_n(\boldsymbol{w}^{*\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b^*) = 1$ and thus the point is $1/\|\boldsymbol{w}^*\|_2$ away from the hyperplane.
- $\xi_n^* < 1$, the point is classified correctly but does not satisfy the large margin constraint.
- $\xi_n^* > 1$, the point is misclassified.



Support vectors (circled with the orange line) are *the only points that matter!*

The Karush-Kuhn-Tucker (KKT) conditions

If $\boldsymbol{w}^*$ and $\{\lambda_j^*\}$ are the primal and dual solution respectively, then:

Stationarity:

$$\nabla_{\boldsymbol{w}} L\left(\boldsymbol{w}^*, \{\lambda_j^*\}\right) = \nabla F(\boldsymbol{w}^*) + \sum_{j=1}^{\mathsf{J}} \lambda_j^* \nabla h_j(\boldsymbol{w}^*) = \boldsymbol{0}$$

Complementary slackness:

$$\lambda_j^* h_j(\boldsymbol{w}^*) = 0 \quad \text{for all } j \in [\mathsf{J}]$$

Feasibility:

$$h_j(\boldsymbol{w}^*) \leq 0 \quad \text{and} \quad \lambda_j^* \geq 0 \quad \text{for all } j \in [\mathsf{J}]$$

These are *necessary conditions*. They are also *sufficient* when F is convex and $h_1, \ldots, h_{\mathsf{J}}$ are continuously differentiable convex functions.

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

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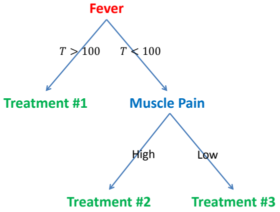
- nonlinear in general
- works for both classification and regression; we focus on classification
- one key advantage is good interpretability
- used to be very popular; ensemble of trees (i.e. "forest") can still be very effective
- not to be confused with the "tree reduction" in Lec 4

Example

Many decisions are made based on some tree structure

Medical treatment



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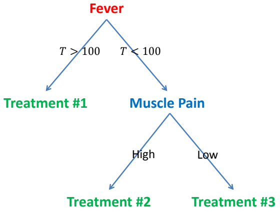
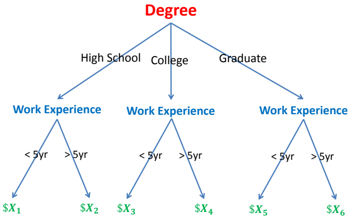
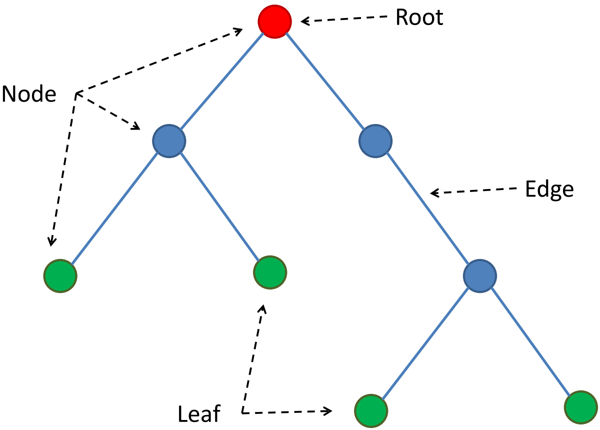


Salary in a company

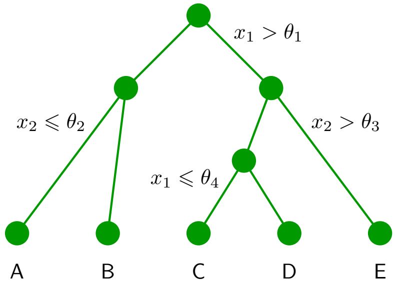


Tree terminology



A more abstract example of decision trees

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



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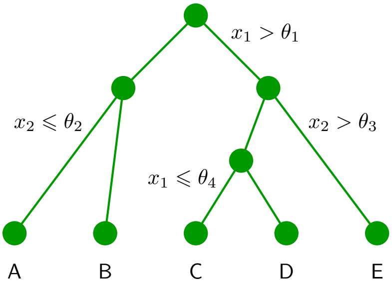

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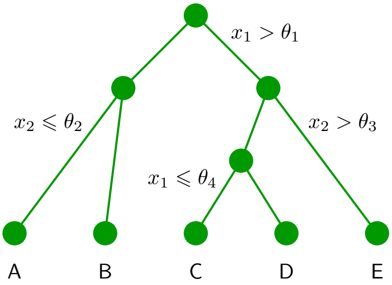

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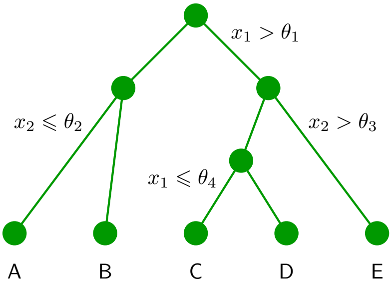

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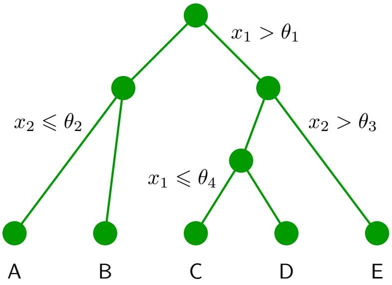

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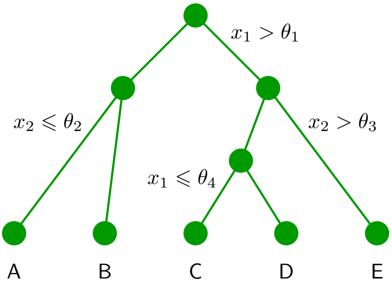

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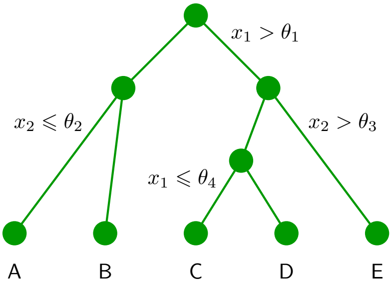

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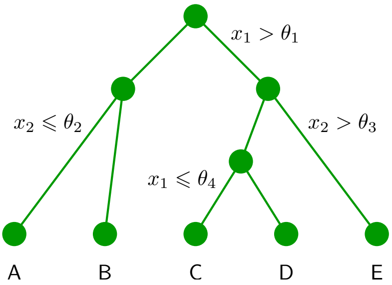
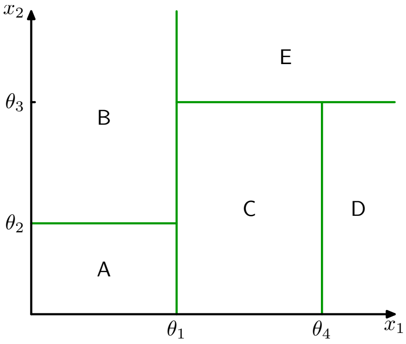
Complex to formally write down, but easy to represent pictorially or as codes.

The decision boundary

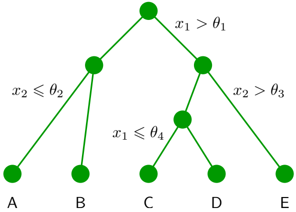
Corresponds to a classifier with boundaries:





Parameters

Parameters to learn for a decision tree:



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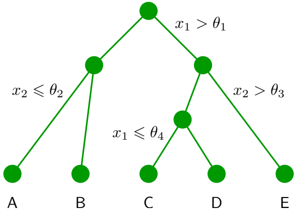

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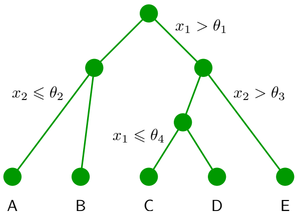

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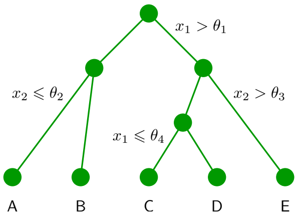

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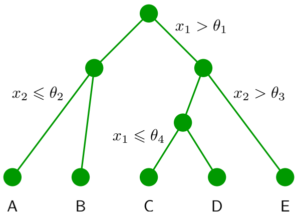

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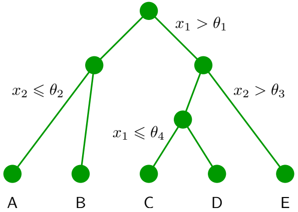

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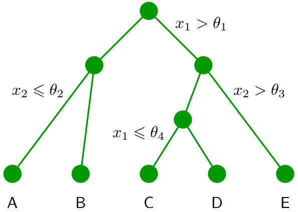

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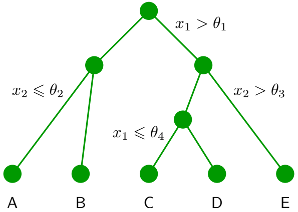

- the value/prediction of the leaves (A, B, ...)

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

A running example

[Russell & Norvig, AIMA]

- 12 examples
- predict whether a customer will wait for a table at a restaurant
- 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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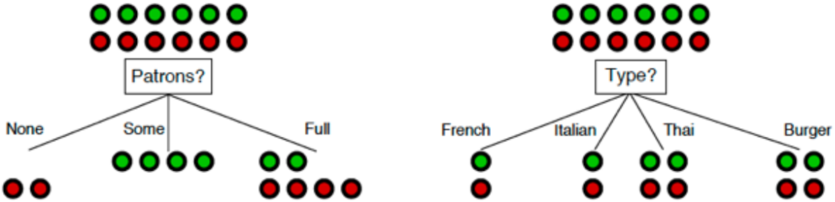
I.e., which feature should we test at the root? Examples:



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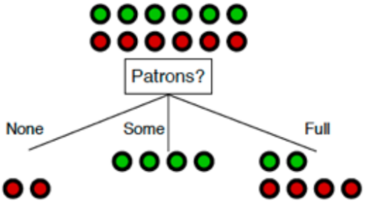

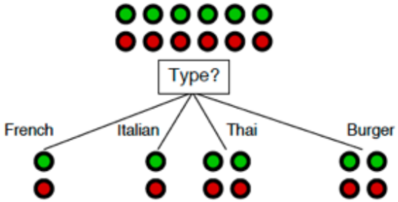

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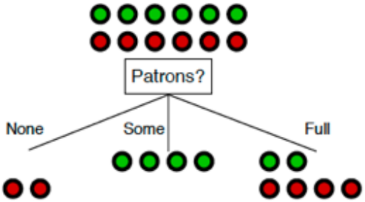

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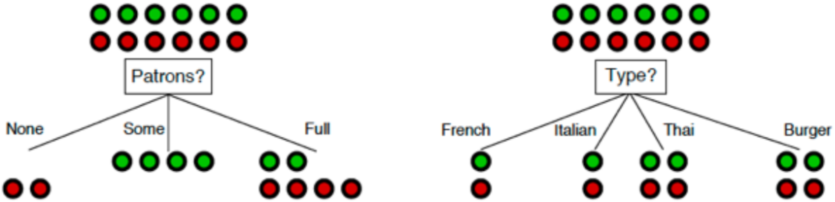

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- how to quantify this intuition?

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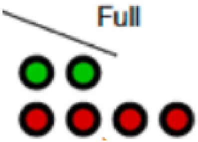

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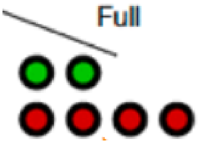

One classic uncertainty measure of a distribution is its *entropy*:

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

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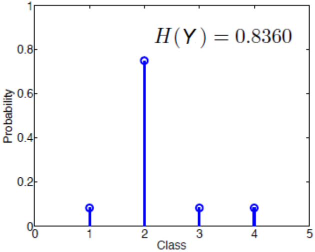
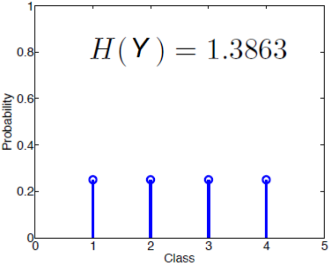
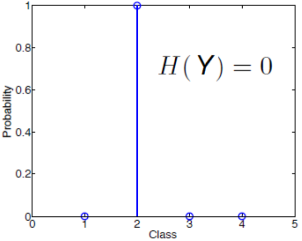
  - $0 \log 0$ is defined naturally as $\lim_{z\to 0+} z \log z = 0$

Examples of computing entropy

With base e and 4 classes:







Another example

Entropy in each child if root tests on "patrons"

For "None" branch

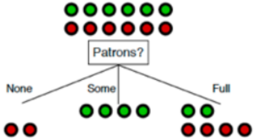
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

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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Entropy in each child if root tests on "patrons"

For "None" branch

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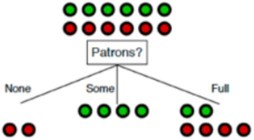

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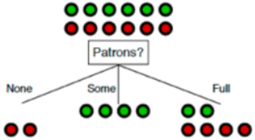

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Very naturally, we take the weighted average of entropy:

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

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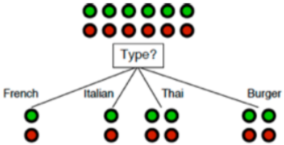
Pick the feature that leads to the smallest conditional entropy.

Deciding the root



For "French" branch

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

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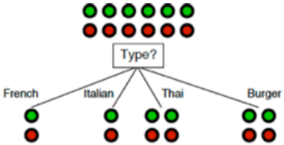

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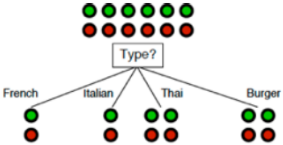

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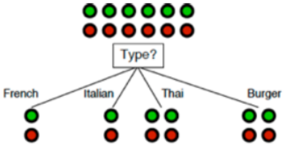

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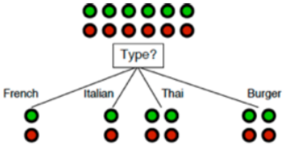

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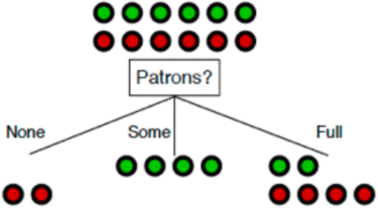
We are now done with building the root (this is also called a **stump**).

Repeat recursively

Split each child in the same way.



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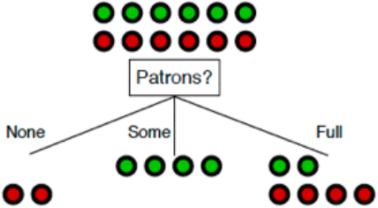

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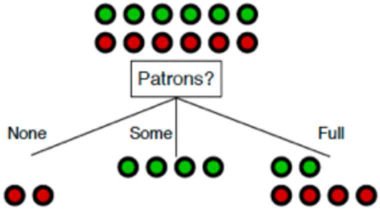
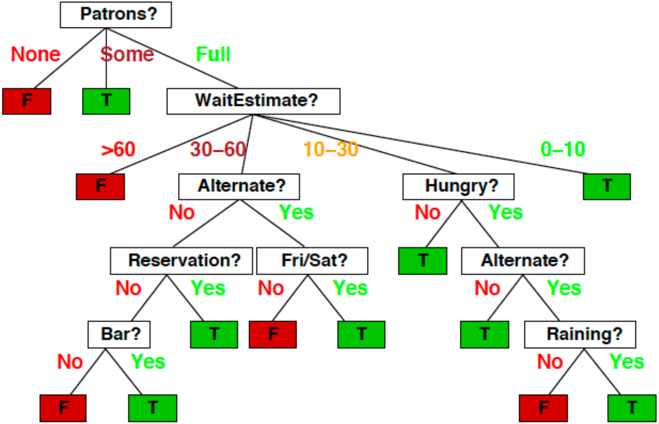
- but no need to split children "none" and "some": they are pure already and become leaves
- for "full", repeat, focusing on those 6 examples:



Example	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

Greedily we build the tree and get this



Again, very easy to interpret.

Putting it together

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

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$$D_{t+1}(n) \propto D_t(n) e^{-\beta_t y_n h_t(\boldsymbol{x}_n)} = \begin{cases} D_t(n) e^{-\beta_t} & \text{if } h_t(x_n) = y_n \\ D_t(n) e^{\beta_t} & \text{else} \end{cases}$$

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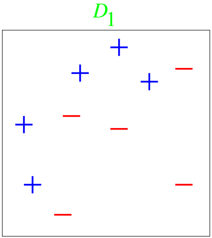
$$D_{t+1}(n) \propto D_t(n) e^{-\beta_t y_n h_t(\boldsymbol{x}_n)} = \begin{cases} D_t(n) e^{-\beta_t} & \text{if } h_t(x_n) = y_n \\ D_t(n) e^{\beta_t} & \text{else} \end{cases}$$

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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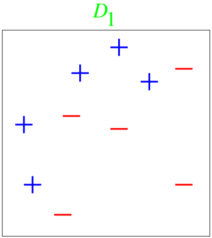

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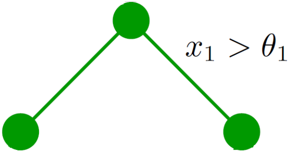

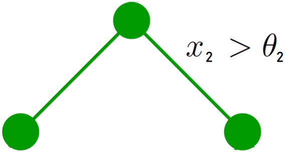

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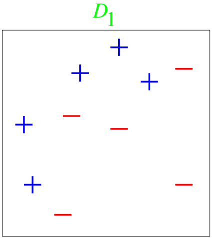
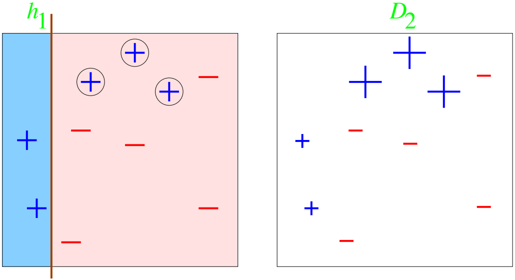


Base algorithm is decision stump:

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

Round 1: $t = 1$



- 3 misclassified (circled): $\epsilon_1 = 0.3 \rightarrow \beta_1 = \frac{1}{2} \ln \left(\frac{1-\epsilon_t}{\epsilon_t} \right) \approx 0.42.$

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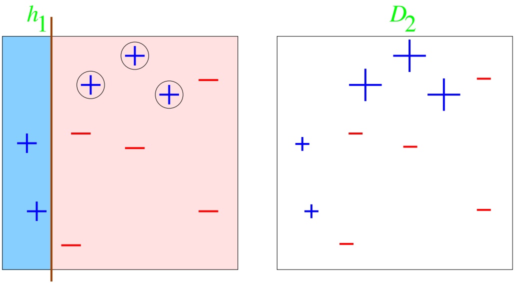

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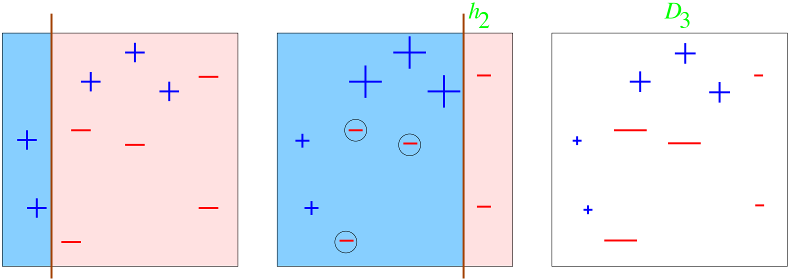

- 3 misclassified (circled): $\epsilon_2 = 0.21 \rightarrow \beta_2 = 0.65$.

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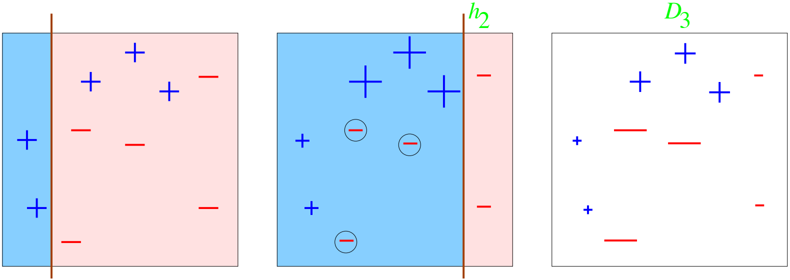

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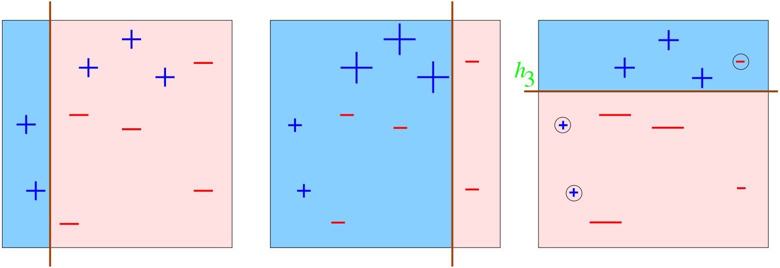
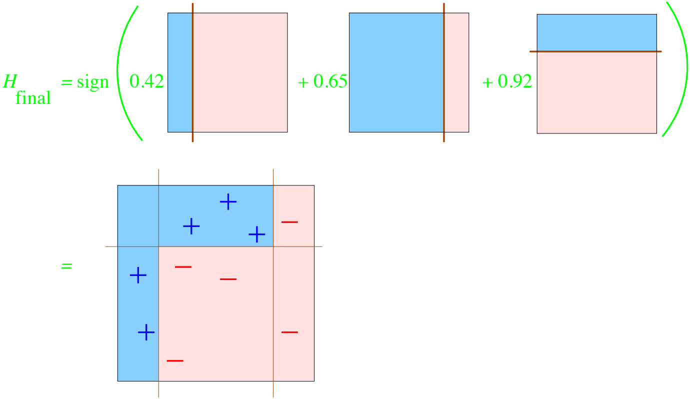
Round 3: $t = 3$



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

Final classifier: combining 3 classifiers



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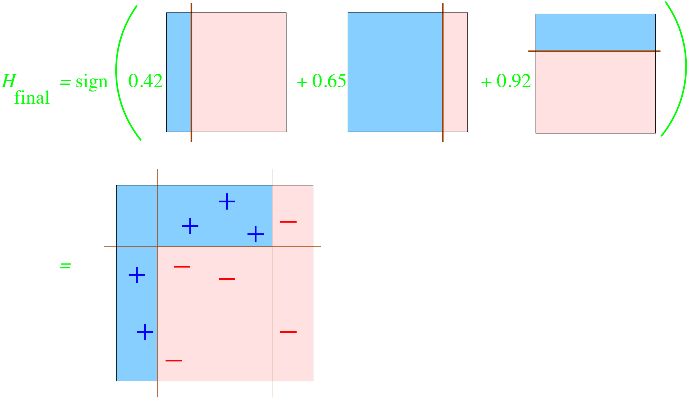

All data points are now classified correctly, even though each weak classifier makes 3 mistakes.

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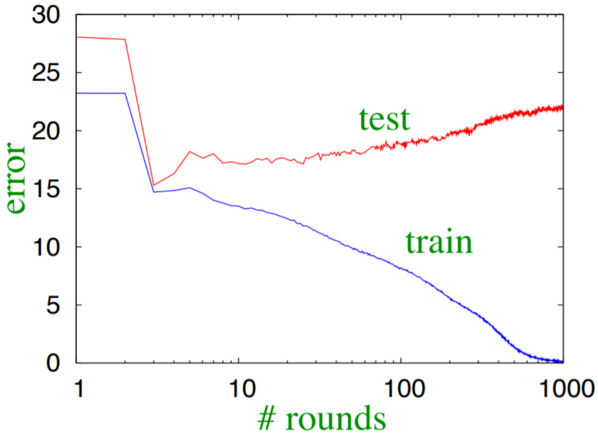

(boosting "stumps" on heart-disease dataset)

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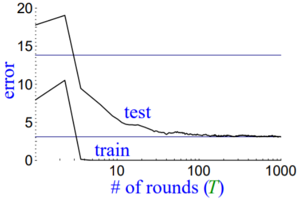

(boosting C4.5 on "letter" dataset)

- 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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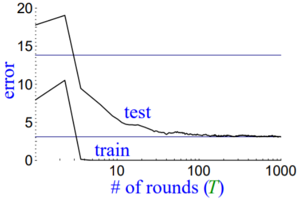

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Used to be a mystery, but by now rigorous theory has been developed to explain this phenomenon.

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

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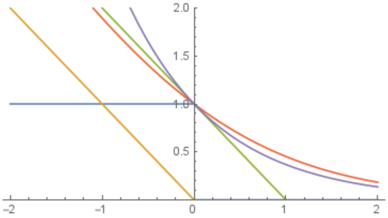

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where the last step is by the definition of weights

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

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This greedy step is abstracted out through a base algorithm.

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Keep doing this greedy minimization gives the AdaBoost algorithm.

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AdaBoost tends to **not overfit**.