CSCI567 Machine Learning (Spring 2025)

Haipeng Luo

University of Southern California

Feb 28, 2025

Quiz 1 Logistics

Date: Friday, March 7th

Time: 1:00-3:20pm

Location: THH 101 (double seating), waiting for an overflow room (will announce on Piazza)

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Individual effort, close-book (no cheat sheet), no calculators or any other electronics, *but need your phone to upload your solutions to Gradescope from 3:20-3:30pm*

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Tips: expect to see variants of questions from discussion/homework

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Most other formulas are not needed (*do not overthink!*)

- Taylor expansion, complete Backprop algorithm in matrix form, KKT conditions, etc.

Outline

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

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Support Vector Machine

SVM: **max-margin linear classifier**

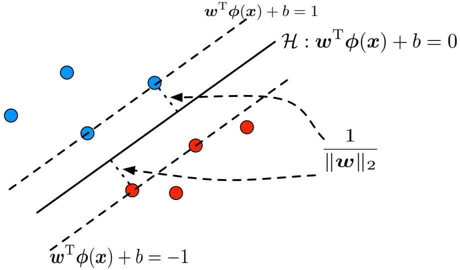
Primal (equivalent to minimizing L2 regularized hinge loss):

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

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



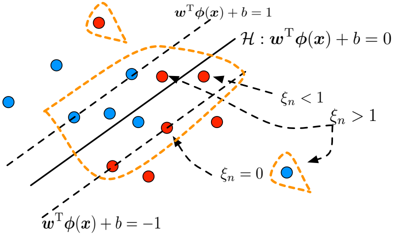
Geometric interpretation of support vectors

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!*

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2 Decision tree
- The model
- Learning a decision tree

3 Boosting

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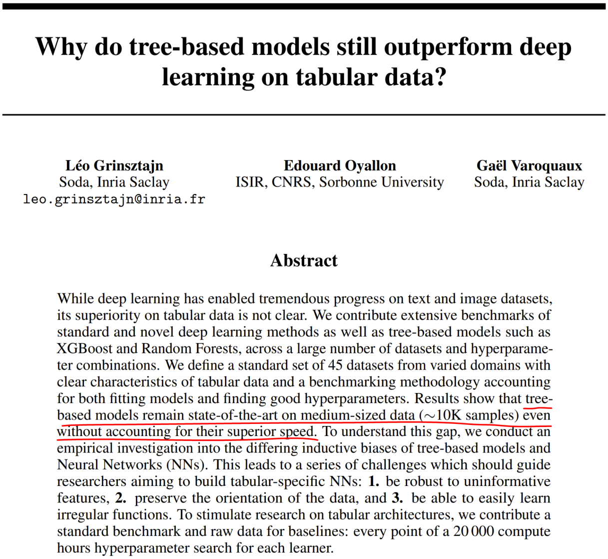
- works for both classification and regression; we focus on classification
- one key advantage is good interpretability
- not to be confused with the "tree reduction" in Lec 4
- still very popular for small tabular data, especially when used in ensemble (i.e. "forest")

Tree-based models outperform neural nets sometimes


Why do tree-based models still outperform deep learning on tabular data?

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Edouard Oyallon
ISIR, CNRS, Sorbonne University

Gaël Varoquaux
Soda, Inria Saclay

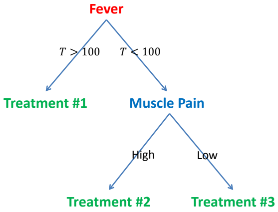
Abstract

While deep learning has enabled tremendous progress on text and image datasets, its superiority on tabular data is not clear. We contribute extensive benchmarks of standard and novel deep learning methods as well as tree-based models such as XGBoost and Random Forests, across a large number of datasets and hyperparameter combinations. We define a standard set of 45 datasets from varied domains with clear characteristics of tabular data and a benchmarking methodology accounting for both fitting models and finding good hyperparameters. Results show that tree-based models remain state-of-the-art on medium-sized data (∼10K samples) even without accounting for their superior speed. To understand this gap, we conduct an empirical investigation into the differing inductive biases of tree-based models and Neural Networks (NNs). This leads to a series of challenges which should guide researchers aiming to build tabular-specific NNs: **1.** be robust to uninformative features, **2.** preserve the orientation of the data, and **3.** be able to easily learn irregular functions. To stimulate research on tabular architectures, we contribute a standard benchmark and raw data for baselines: every point of a 20 000 compute hours hyperparameter search for each learner.

Example

Many decisions are made based on some tree structure

Medical treatment



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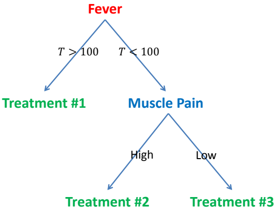
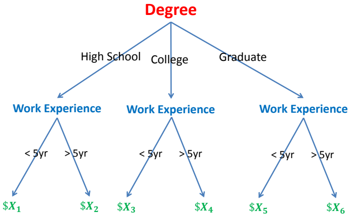
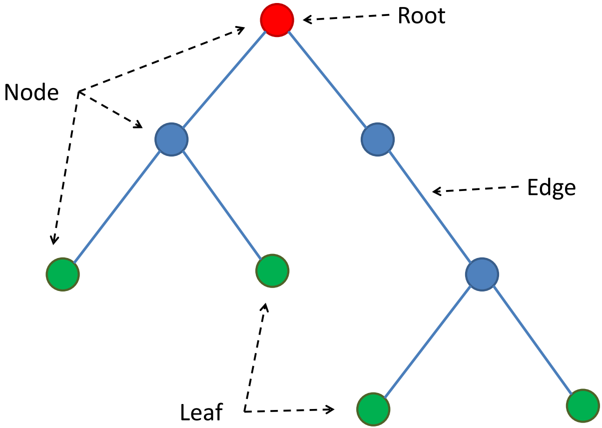


Salary in a company

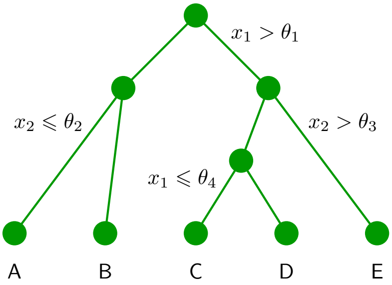


Tree terminology



A more abstract example of decision trees

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



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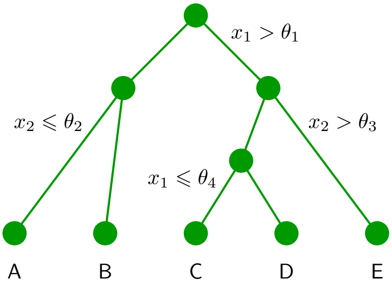

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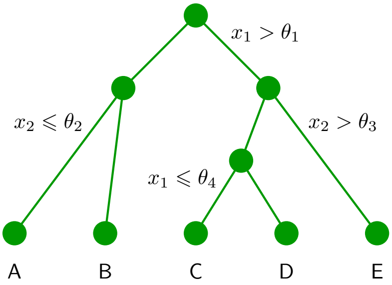

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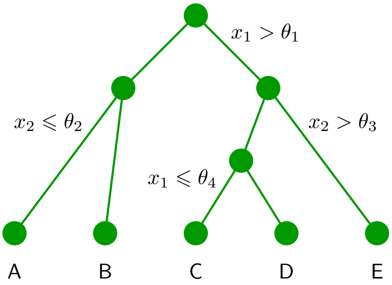

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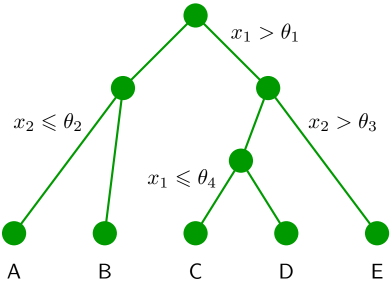

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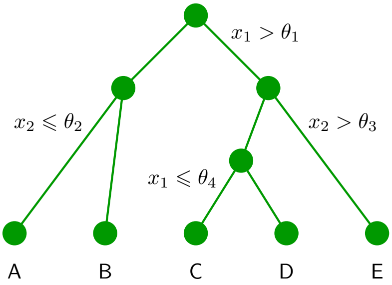

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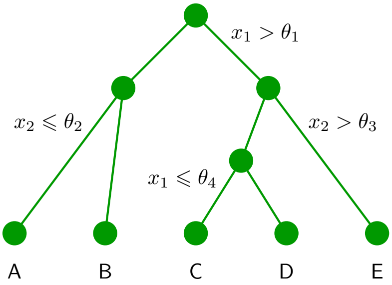

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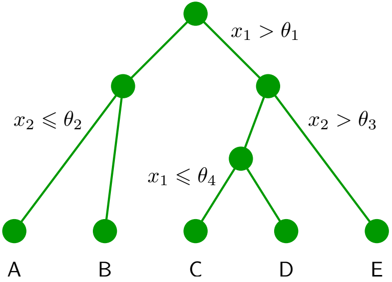
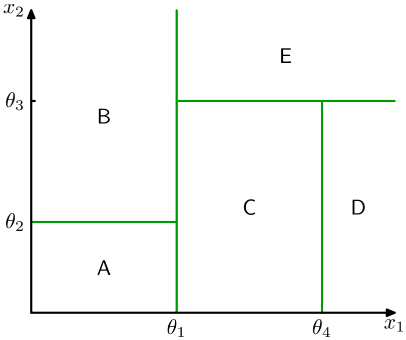
Complex to formally write down, but easy to represent pictorially or as codes.

The decision boundary

Corresponds to a classifier with boundaries:





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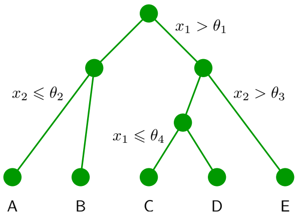

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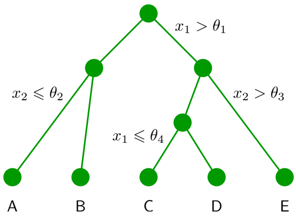

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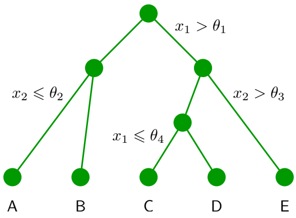

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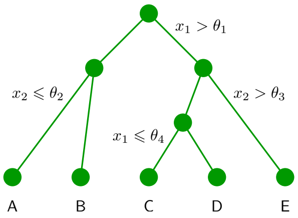

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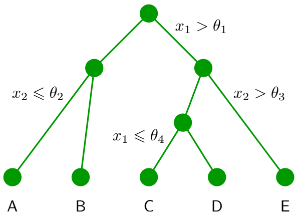

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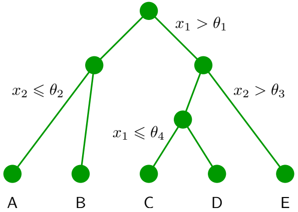

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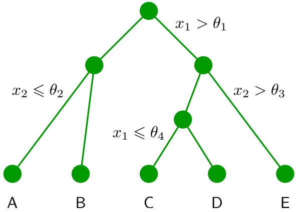

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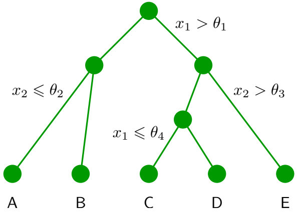

- the value/prediction of the leaves (A, B, ...)

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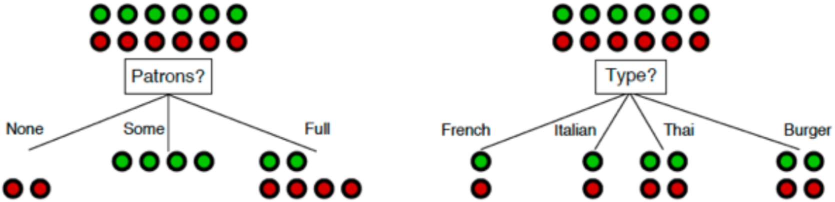
I.e., which feature should we test at the root? Examples:



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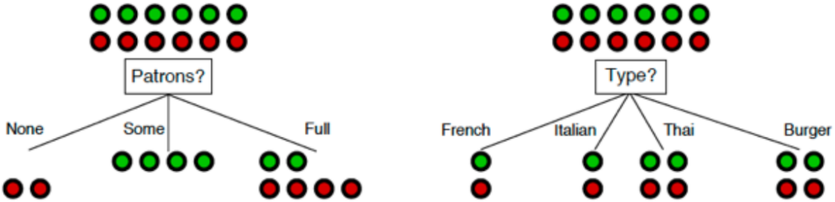

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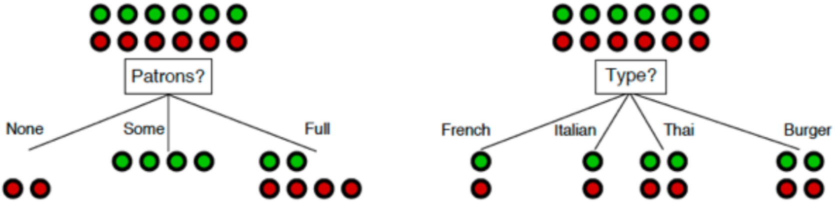

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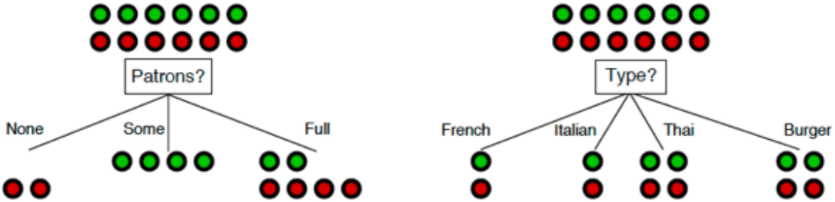

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- intuitively "patrons" is a better feature since it leads to "more pure" or "more certain" children
- how to quantify this intuition?

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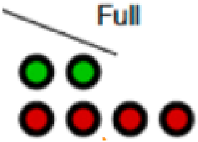

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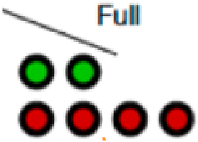
It should be **a function of the distribution of classes**

- e.g. a node with 2 positive and 4 negative examples can be summarized by a distribution P with $P(Y = +1) = 1/3$ and $P(Y = -1) = 2/3$



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

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

Properties of entropy

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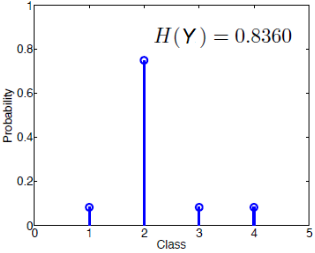
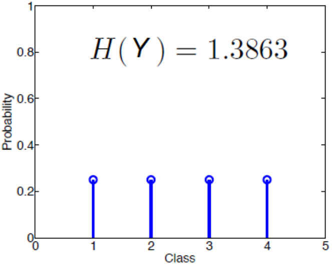
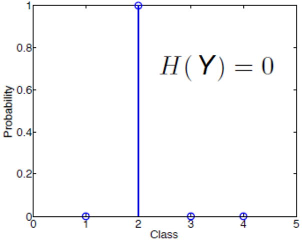
  - $0 \log 0$ is defined naturally as $\lim_{z \to 0+} z \log z = 0$

Examples of computing entropy

With base e and 4 classes:







Another example

Entropy in each child if root tests on "patrons"

For "None" branch

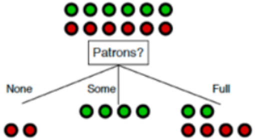
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

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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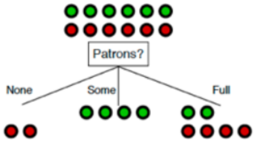

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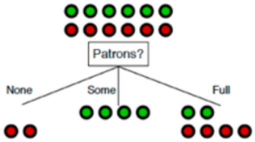

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Very naturally, we take the weighted average of entropy:

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

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Pick the feature that leads to the smallest conditional entropy.

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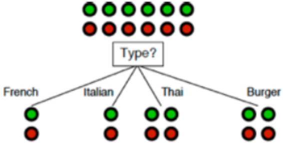

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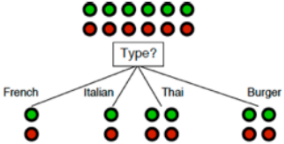

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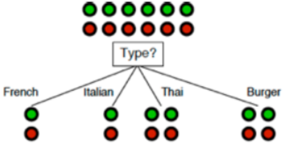

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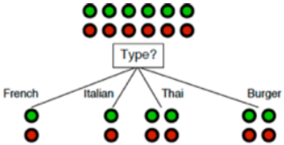

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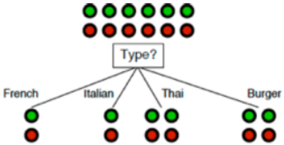

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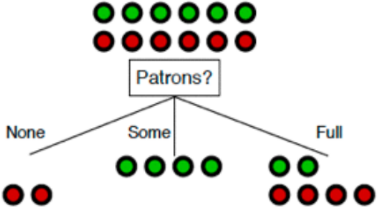
We are now done with building the root (this is also called a **stump**).

Repeat recursively

Split each child in the same way.



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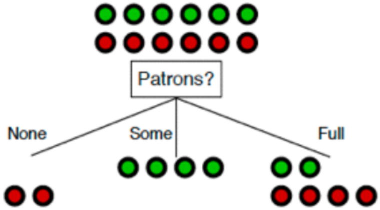
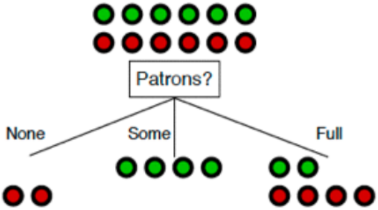


Repeat recursively

Split each child in the same way.

- 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	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
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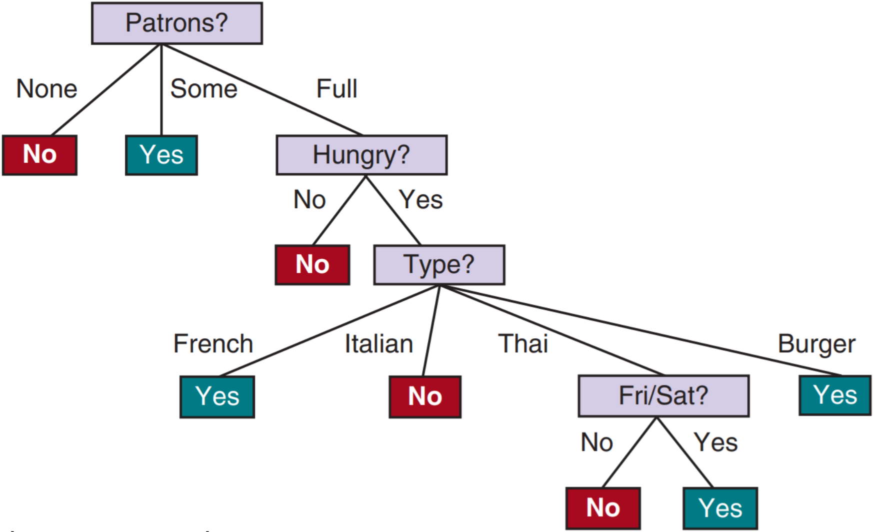
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T



Again, very easy to interpret.

Putting it together

DecisionTreeLearning(Examples, Features)

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- if Examples have the same class, return a leaf with this class
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- else if Examples is empty, return a leaf with majority class of parent
- else

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Variants

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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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- all make use of a validation set

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- much better performance than a single tree, trivially parallelizable!

Outline

1 Review of last lecture

2 Decision tree

3 Boosting
- Examples
- AdaBoost
- Derivation of AdaBoost

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We again focus on binary classification.

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- reweight the examples so that "difficult" ones get more attention
  - e.g. spam that doesn't contain the word "money"
- obtain another classifier by applying the same base algorithm:
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A simple example

Email spam detection:

- given a training set like:
  - ("Want to make money fast? ...", **spam**)
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  - e.g. contains the word "money" ⇒ spam
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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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Focus on AdaBoost, 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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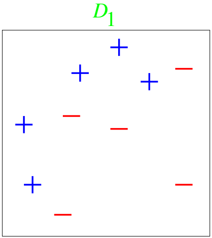
Output the final classifier $H(\boldsymbol{x}) = \text{sgn}\left(\sum_{t=1}^{T} \beta_t h_t(\boldsymbol{x})\right)$

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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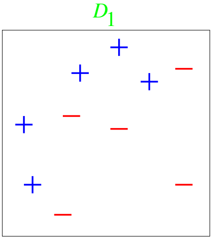

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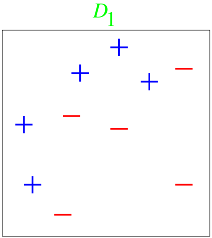

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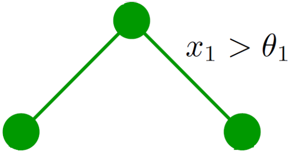
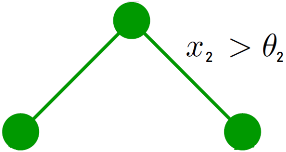
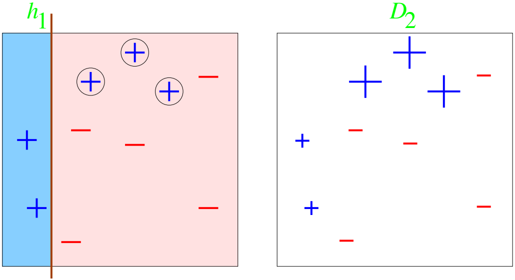




Observe that *no stump can predict very accurately for this dataset*

Round 1: $t = 1$



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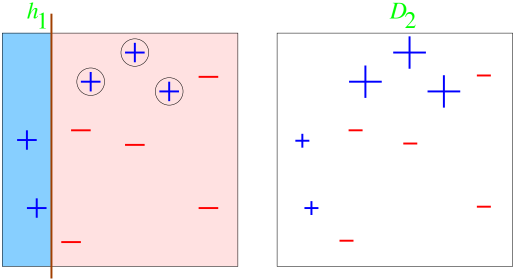

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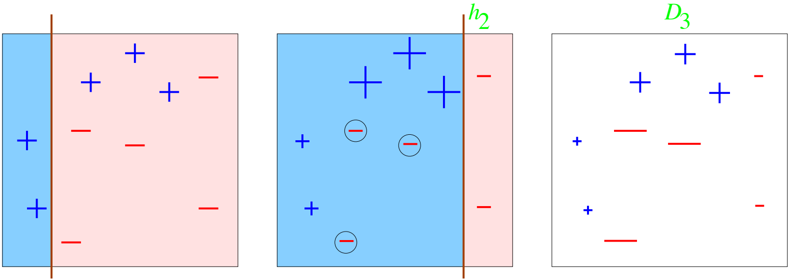

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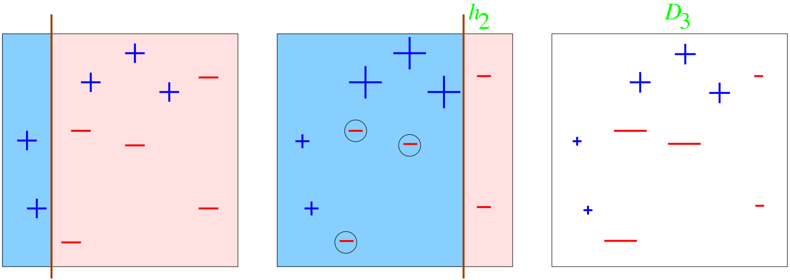

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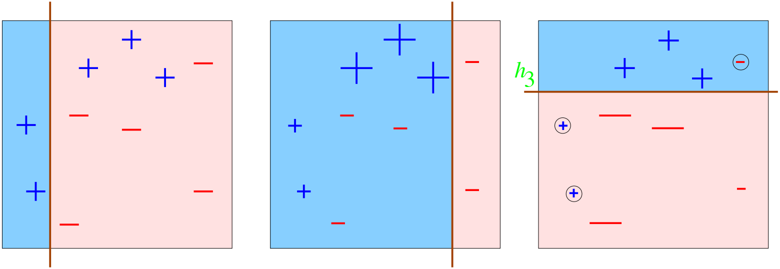
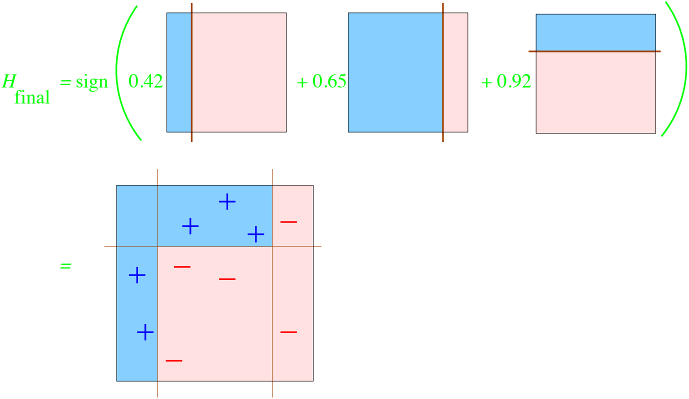
- D_3 puts more weights on those examples

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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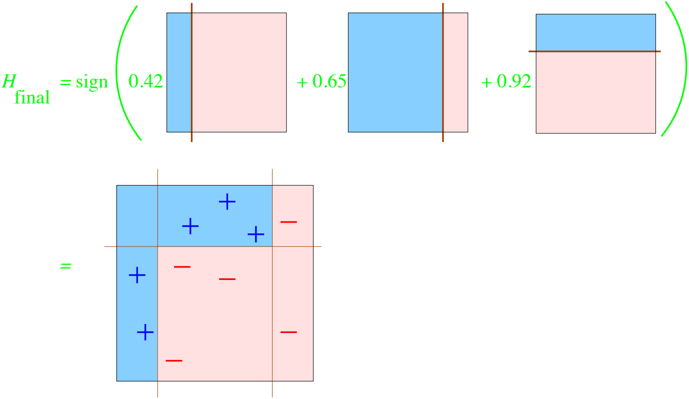

All data points are now classified correctly, even though each weak classifier makes 3 mistakes.

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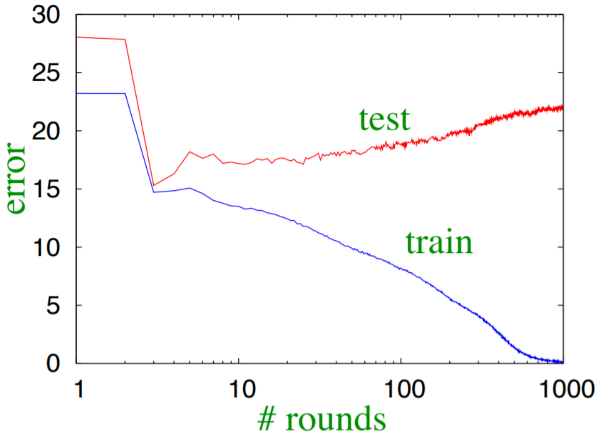

(boosting "stumps" on heart-disease dataset)

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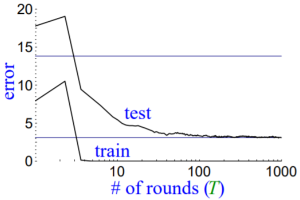

(boosting C4.5 on "letter" dataset)

- test error does not increase, even after 1000 rounds
  - (total size > 2,000,000 nodes)
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train error	0.0	0.0	0.0
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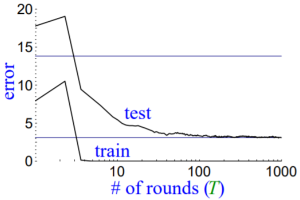

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Used to be a mystery, but by now rigorous theory has been developed to explain this phenomenon.

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

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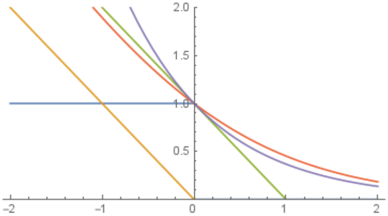

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where the last step is by the definition of weights

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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 is often **resistant to overfitting**.