CSCI567 Machine Learning (Fall 2025)

Haipeng Luo

University of Southern California

Oct 3, 2025

Exam 1 Logistics

Date: Friday, Oct 17th

Time: 2:00-4:00pm

Location: will be announced 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 4:00-4:20pm*

Exam 1 Coverage

Coverage: Lectures 1-6.

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Five problems in total

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  - "which of the following is correct?" *does not imply one correct answer*
- four other homework-like problems, each has a couple sub-problems
  - linear regression, linear classifiers, backpropagation, kernel, SVM

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- make sure to fully understand those problems (solutions to be posted next week)
- no need to remember most formulas from the lectures
- expect to see *variants of these questions*
- sample exam might appear challenging, but hopefully the actual one is less so given the practice from the sample exam

Outline

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Support vector machines (SVM)

- most commonly used classification algorithms before deep learning
- works well with the kernel trick
- strong theoretical guarantees

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We focus on **binary classification** here.

Primal formulation

In one sentence: linear model with L2 regularized hinge loss.

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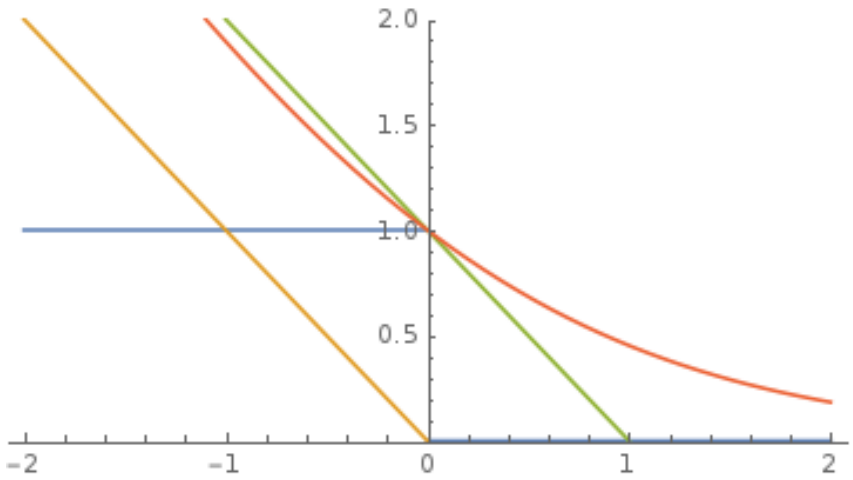

- perceptron loss $\ell_{\text{perceptron}}(z) = \max\{0, -z\} \rightarrow$ Perceptron
- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z)) \rightarrow$ logistic regression
- hinge loss $\ell_{\text{hinge}}(z) = \max\{0, 1 - z\} \rightarrow$ **SVM**

Primal formulation

For a linear model $(\boldsymbol{w}, b)$, this means

$$\min_{\boldsymbol{w},b} \sum_n \max\left\{0, 1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)\right\} + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$$

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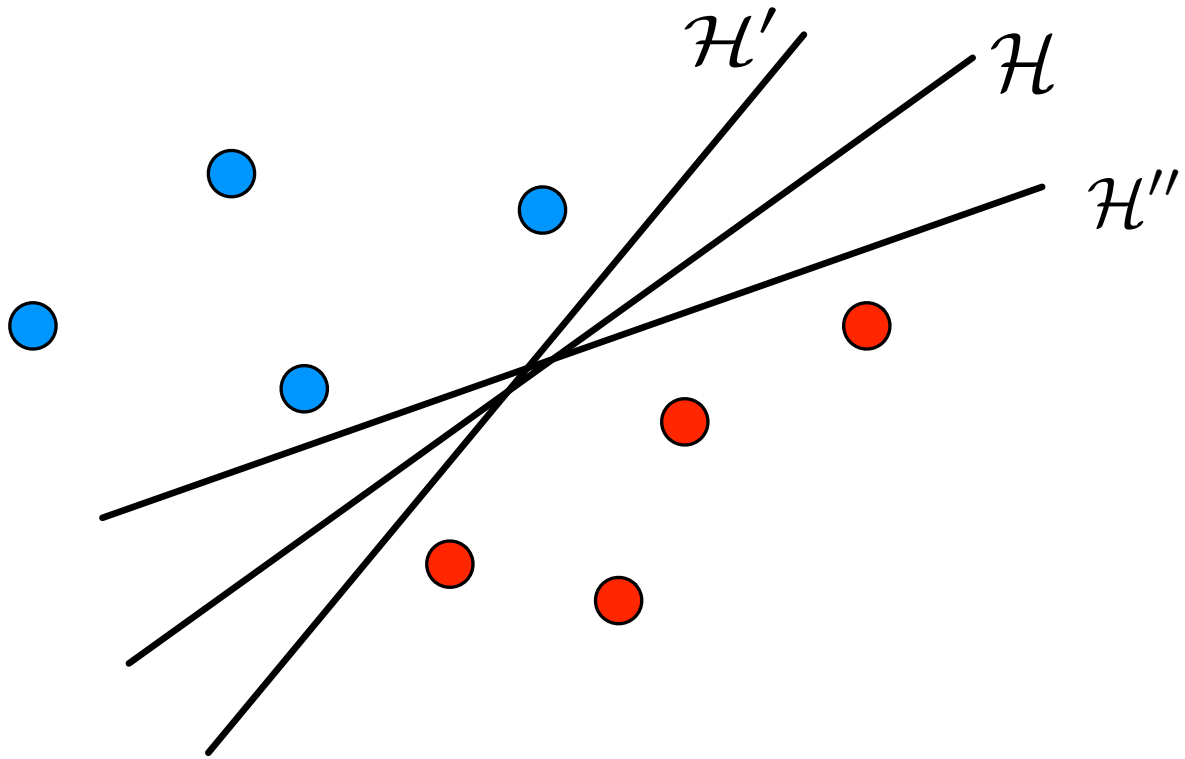
So why L2 regularized hinge loss?

Geometric motivation: separable case

When data is **linearly separable**, there are *infinitely many hyperplanes with zero training error*:



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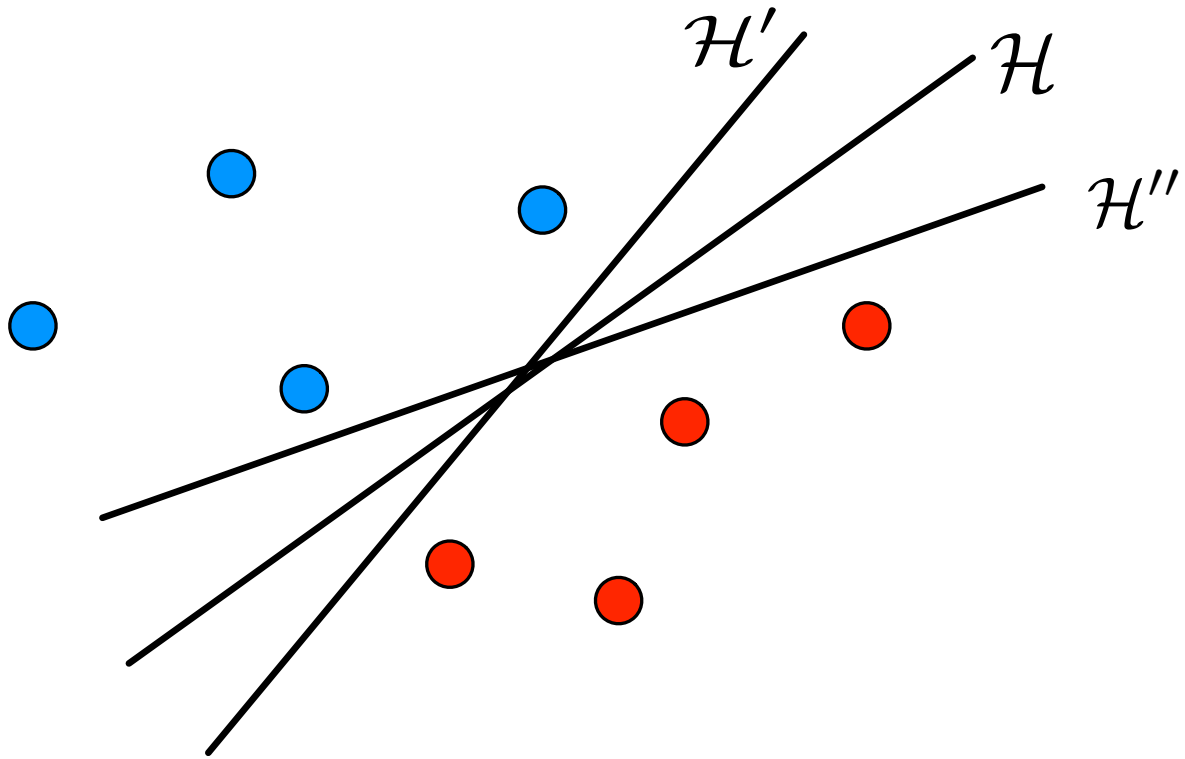
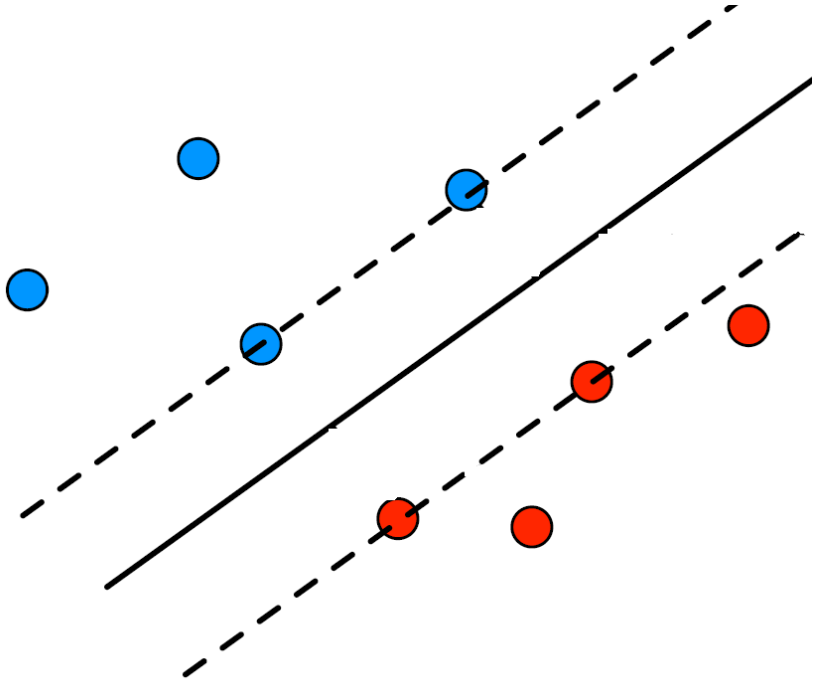


So which one should we choose?

Intuition

The further away from data points the better.



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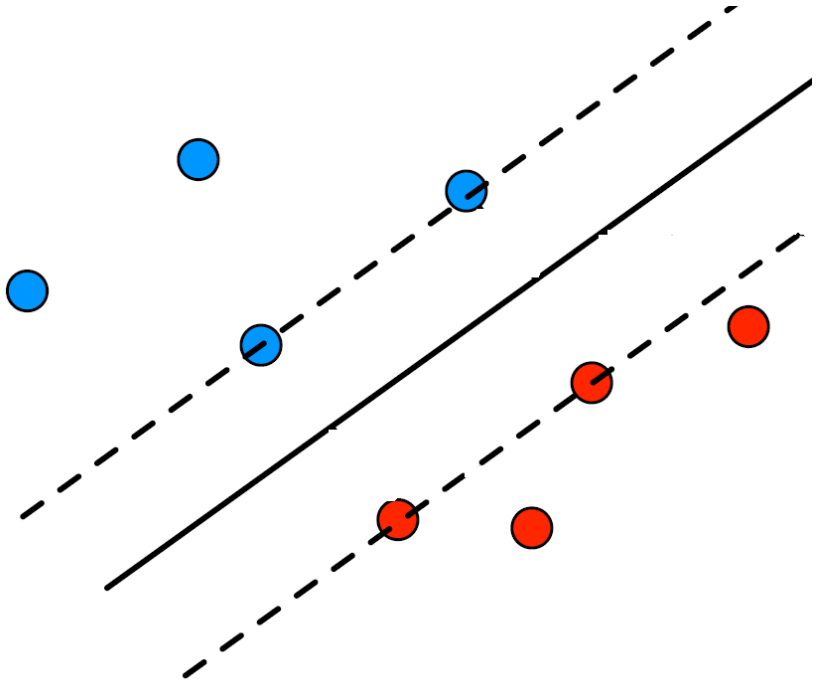

How to formalize this intuition?

Distance to hyperplane

What is the **distance** from a point $\boldsymbol{x}$ to a hyperplane $\{\boldsymbol{x} : \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + b = 0\}$?

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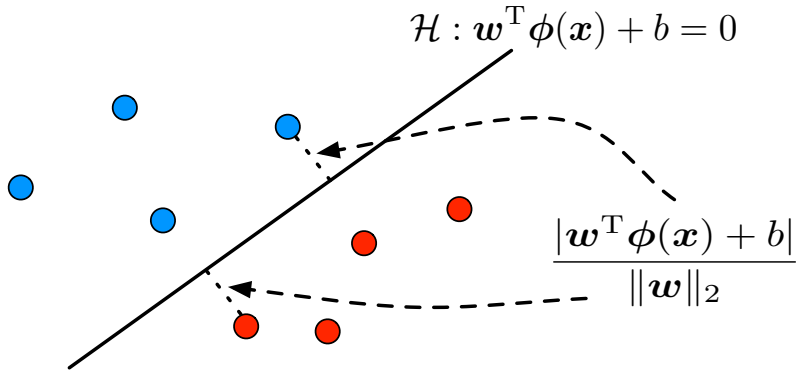
For a hyperplane that correctly classifies $(\boldsymbol{x}, y)$, the distance becomes

$$\frac{y(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + b)}{\|\boldsymbol{w}\|_2}$$

Maximizing margin

Margin: the *smallest* distance from all training points to the hyperplane

$$\text{MARGIN OF } (\boldsymbol{w},\, b) = \min_n \frac{y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)}{\|\boldsymbol{w}\|_2}$$



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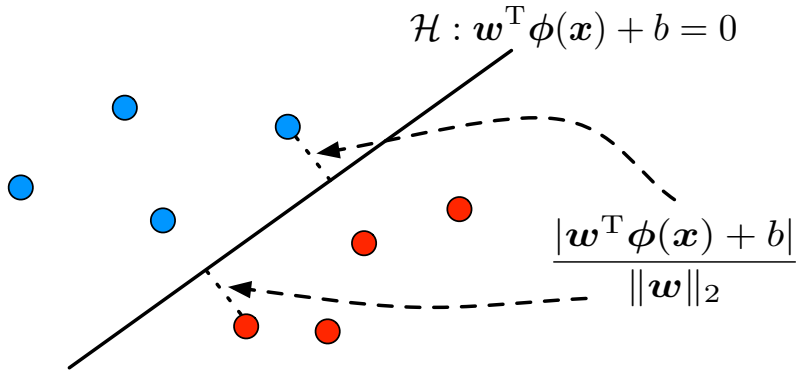

The intuition "**the further away the better**" translates to solving

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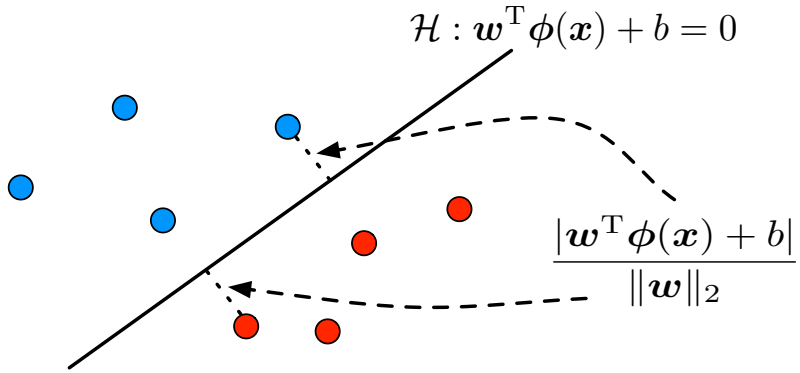

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$$\max_{\boldsymbol{w},b} \min_n \frac{y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)}{\|\boldsymbol{w}\|_2} = \max_{\boldsymbol{w},b} \frac{1}{\|\boldsymbol{w}\|_2} \min_n y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)$$

Rescaling

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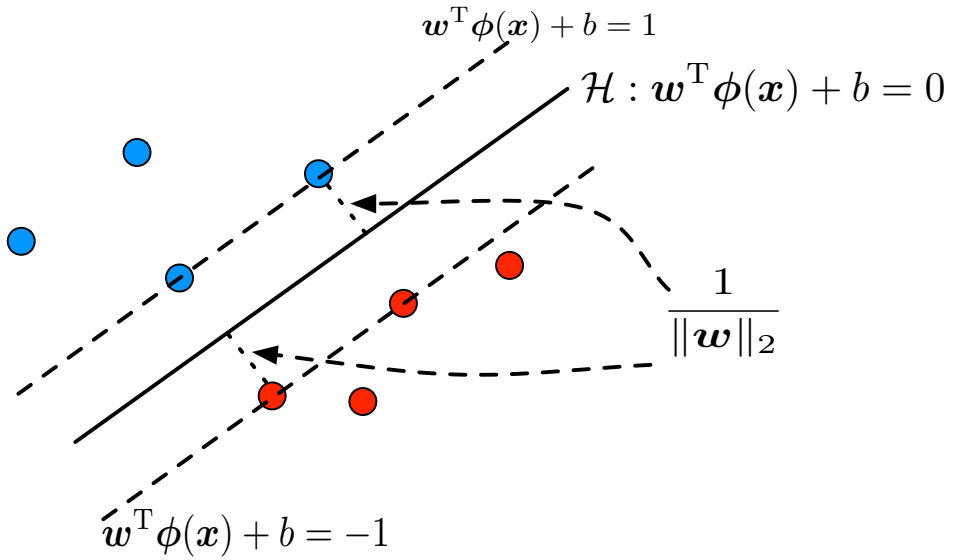

Summary for separable data

For a separable training set, we aim to solve

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SVM is thus also called *max-margin* classifier. The constraints above are called *hard-margin* constraints.

General non-separable case

If data is not linearly separable, the previous constraint

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To deal with this issue, we relax them to **soft-margin** constraints:

$$y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b) \geq 1 - \xi_n, \quad \forall\ n$$

where we introduce **slack variables** $\xi_n \geq 0$.

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We want ξ_n to be as small as possible too. The objective becomes

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

where C is a hyperparameter to balance the two goals.

Equivalent form

Formulation

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

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with $\lambda = 1/C$.

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with $\lambda = 1/C$. *This is exactly minimizing L2 regularized hinge loss!*

Optimization

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- there are **more specialized and efficient** algorithms
- but usually we apply kernel trick, which requires solving the *dual problem*

The dual formulation

Similar to Perceptron, it turns out that the primal solution $\boldsymbol{w}^*$ is also a **linear combination of data**

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- immediately *kernelizable* by replacing $\boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n)$ with $k(\boldsymbol{x}_m, \boldsymbol{x}_n)$

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Hence the name **Support Vector Machine** (SVM).

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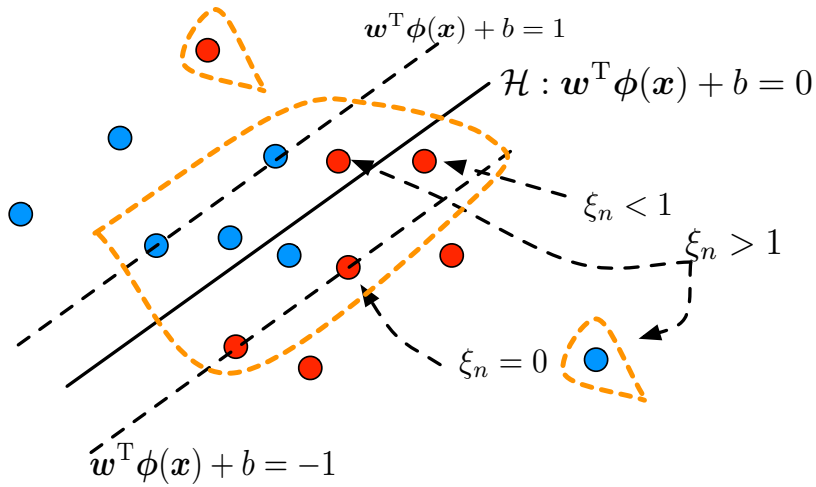

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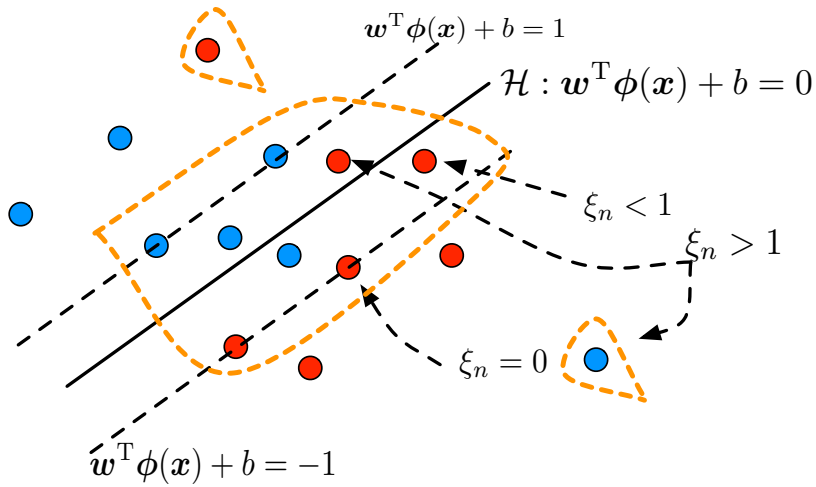

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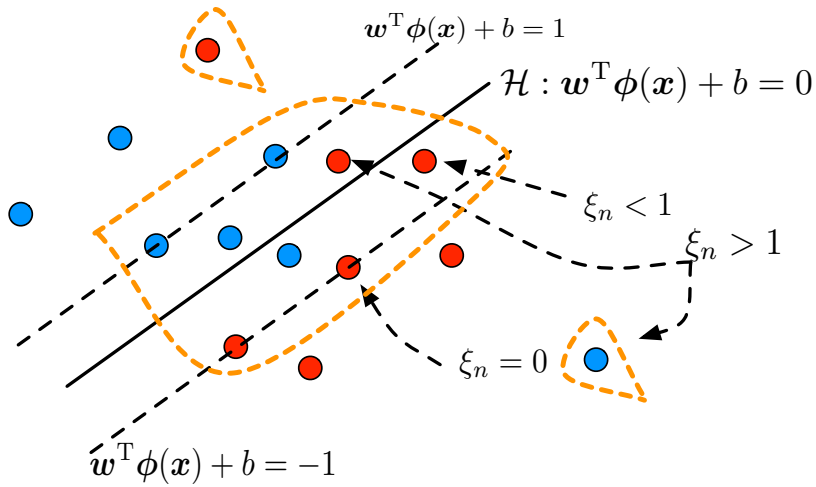

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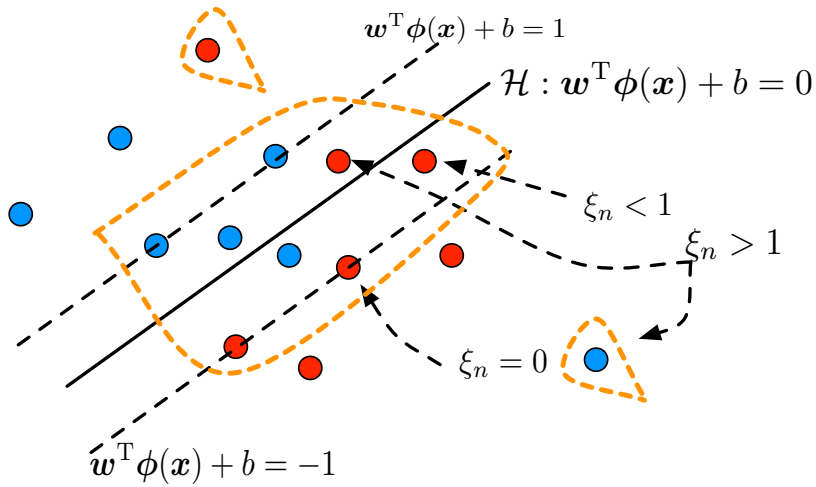

Support vectors (circled with the orange line) are *the only points that matter!*

An example

One drawback of kernel method: **non-parametric**, need to keep all training points potentially

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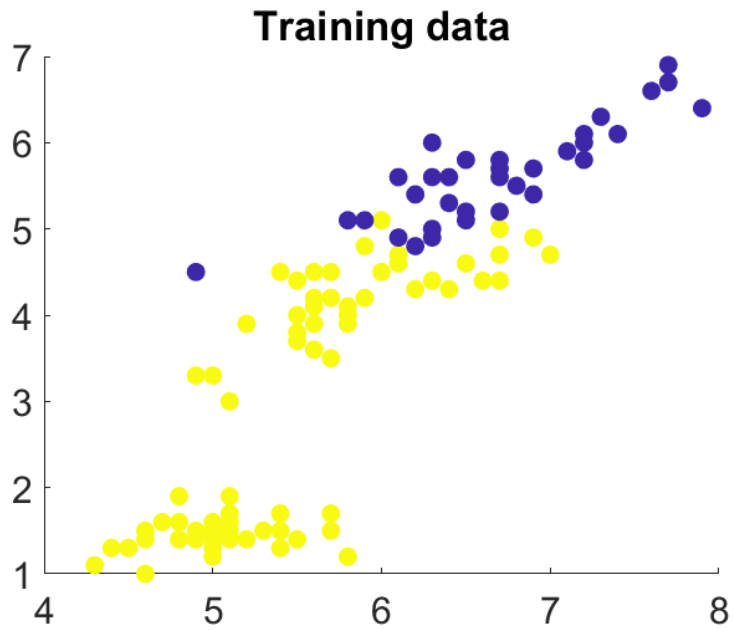

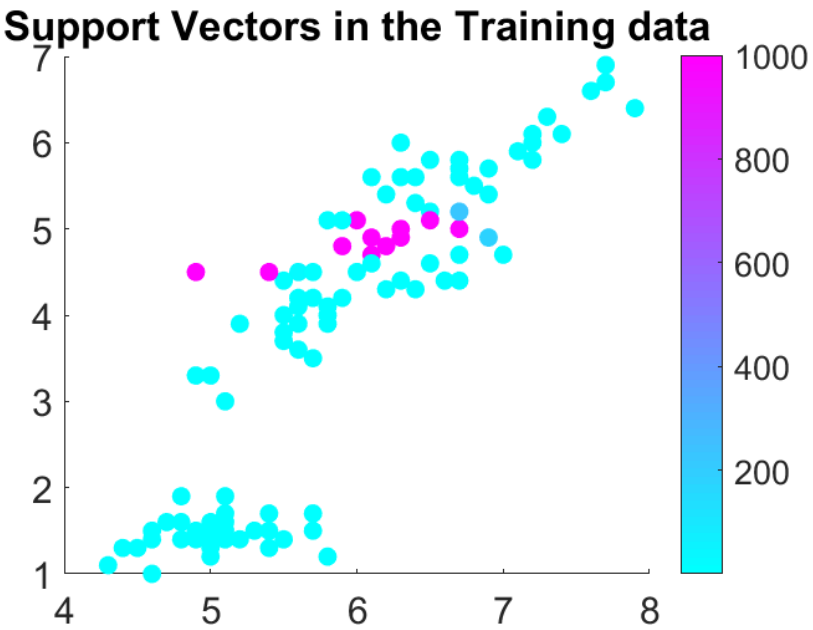

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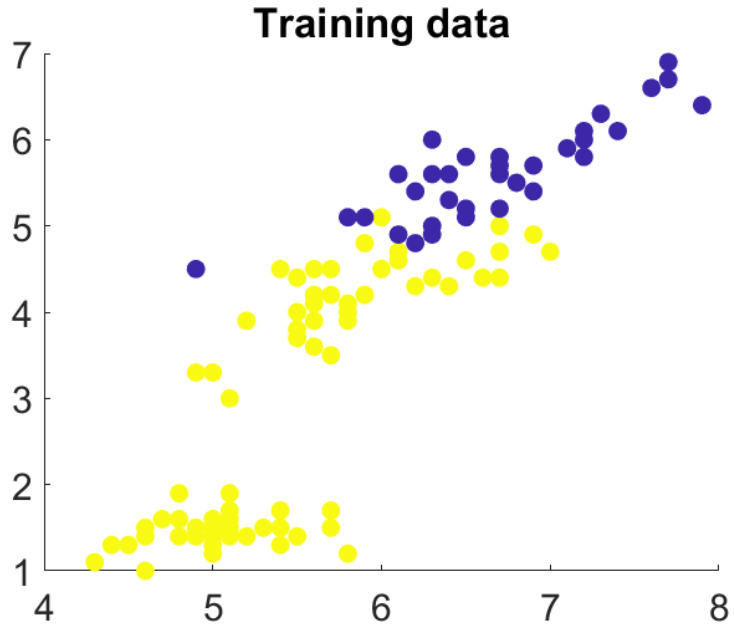

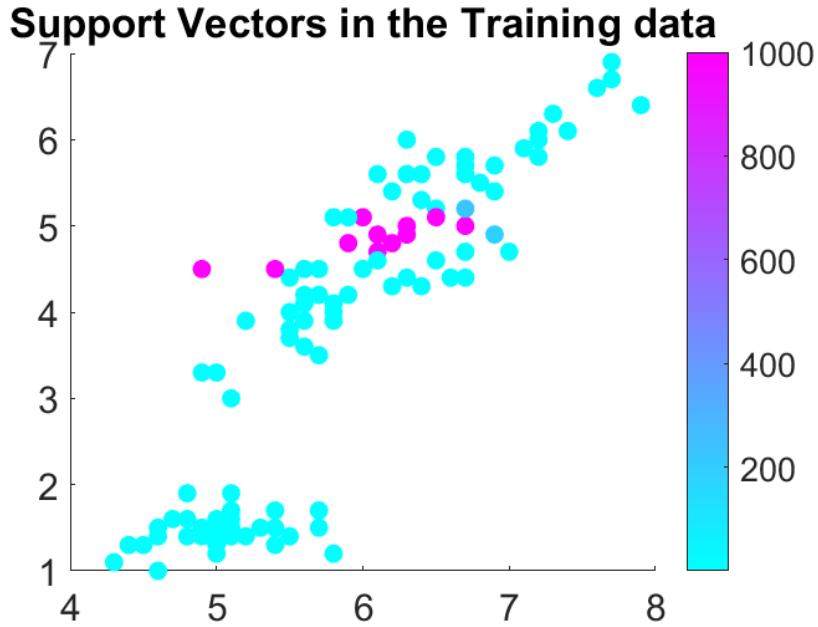

See also Colab demo.

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Primal (equivalent to minimizing L2 regularized hinge loss):

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

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- one key advantage is good interpretability
- 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?

Léo Grinsztajn
Soda, Inria Saclay
leo.grinsztajn@inria.fr

Edouard Oyallon
ISIR, CNRS, Sorbonne University

Gaël Varoquaux
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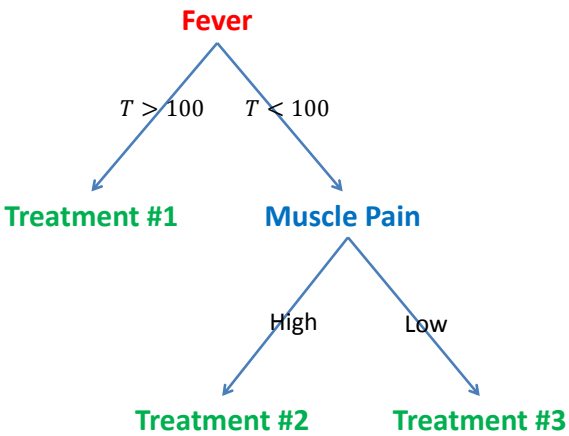
Abstract

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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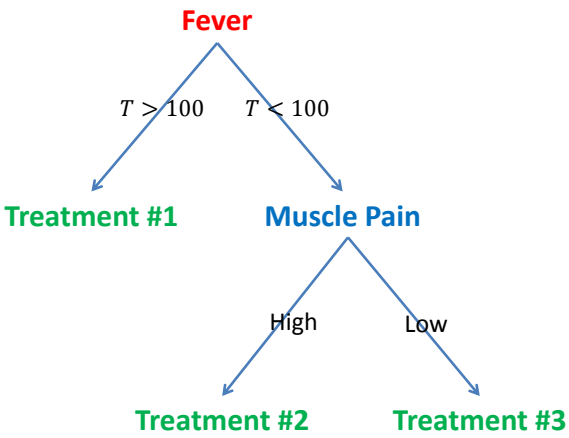
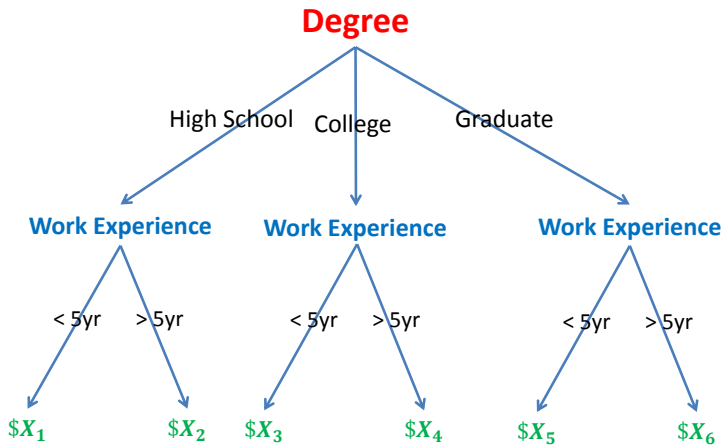
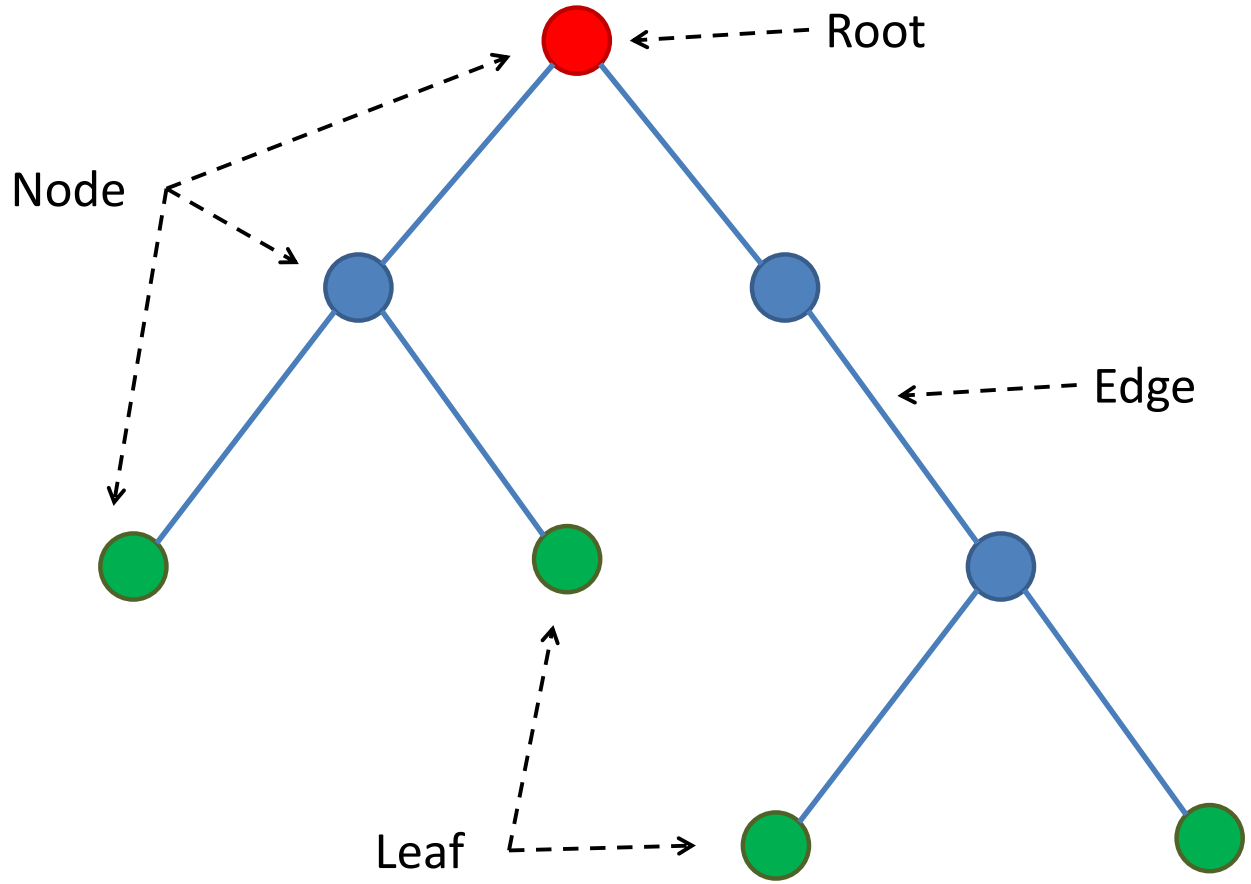


Salary in a company



Tree terminology



A more abstract example of decision trees

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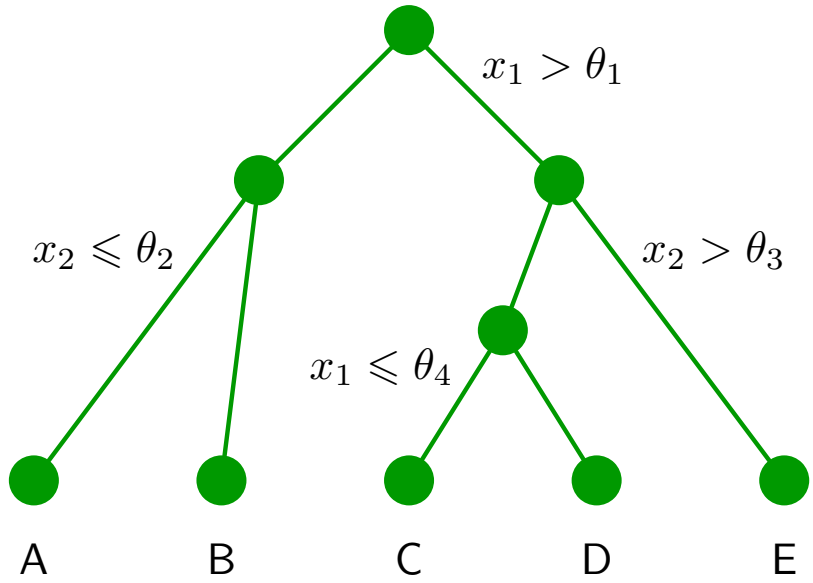

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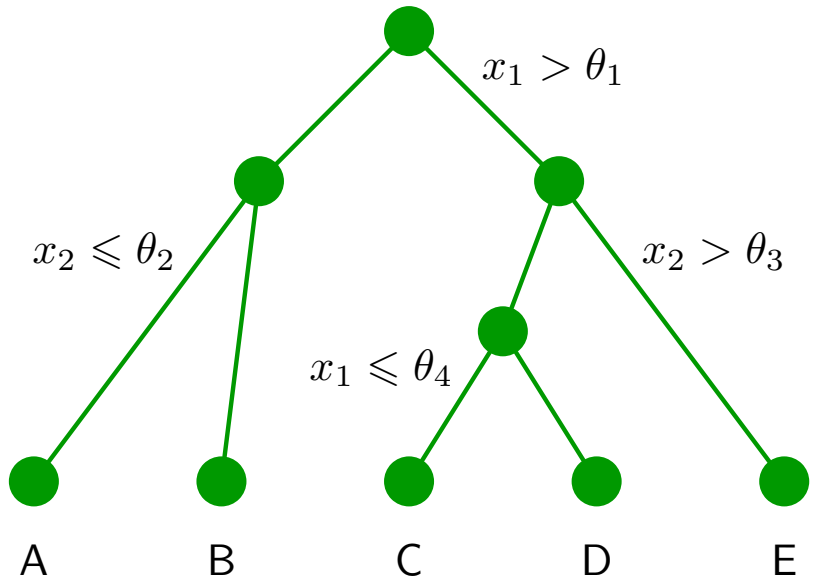

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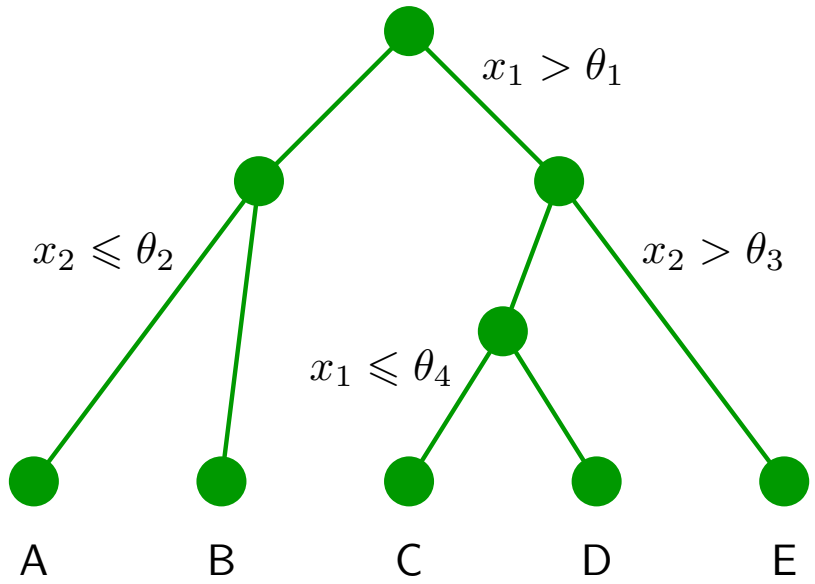

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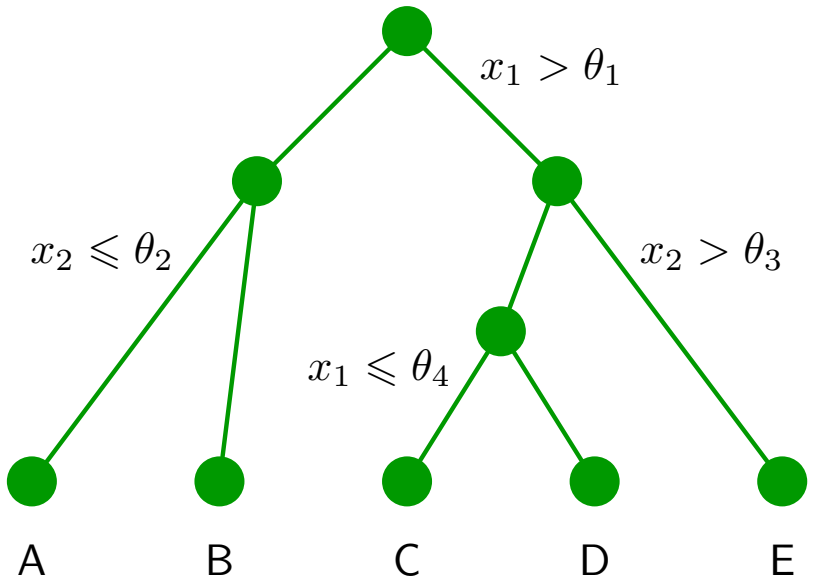

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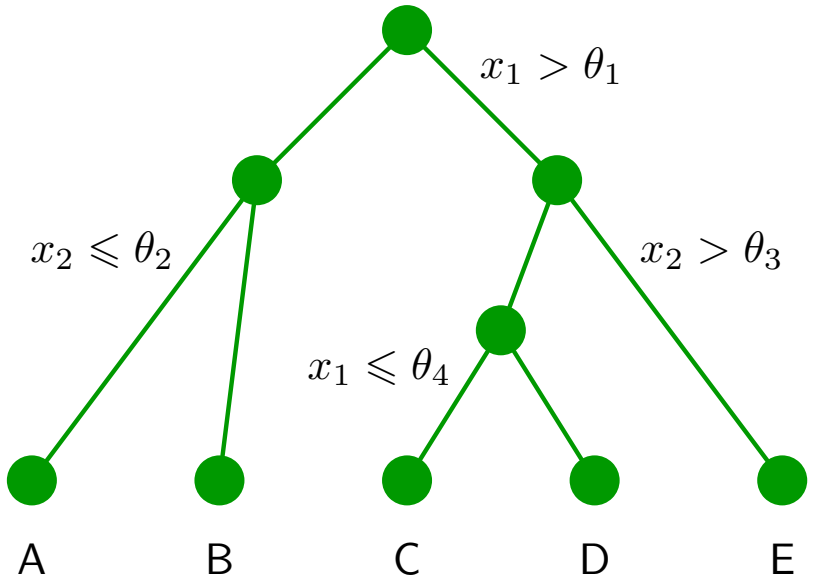

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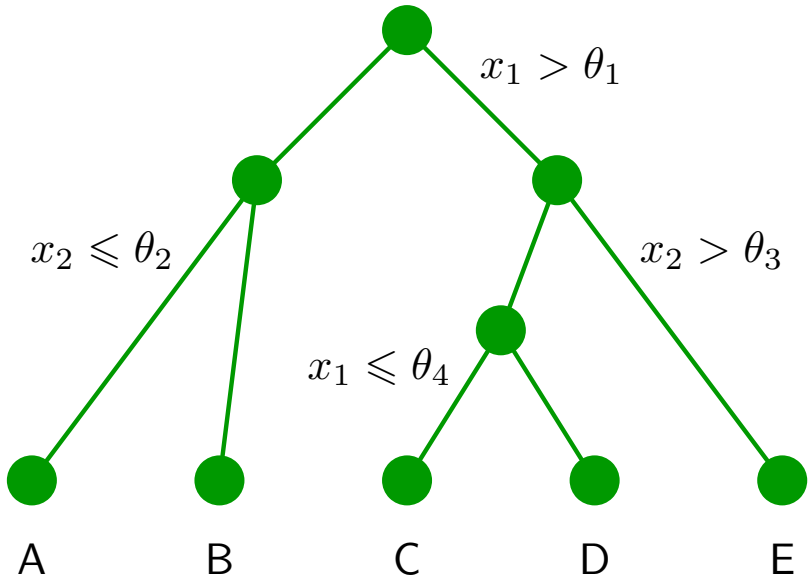

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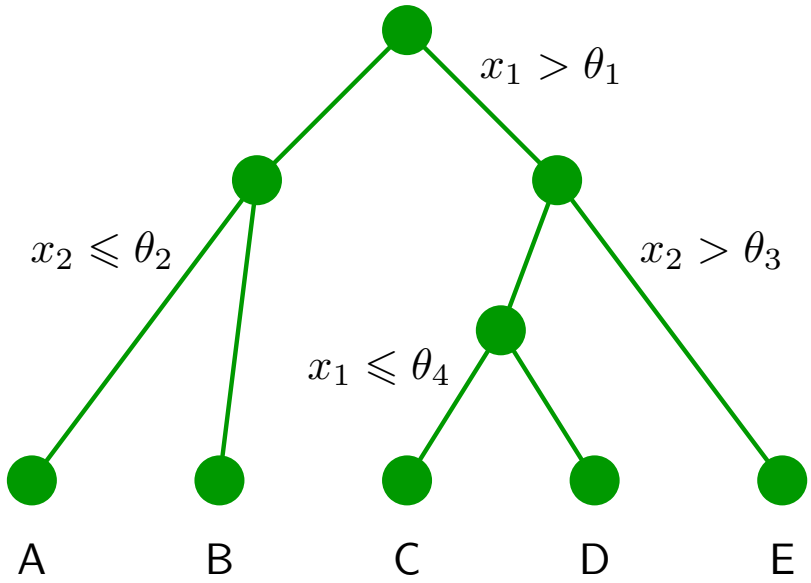

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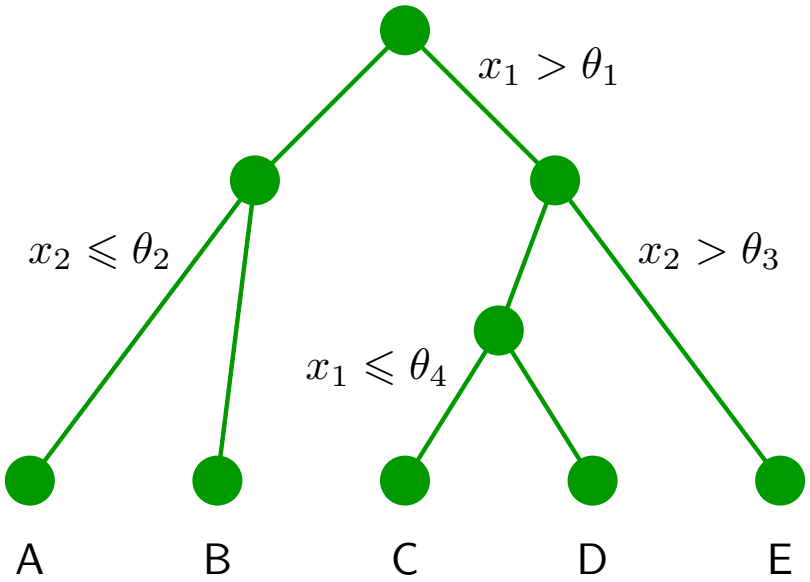
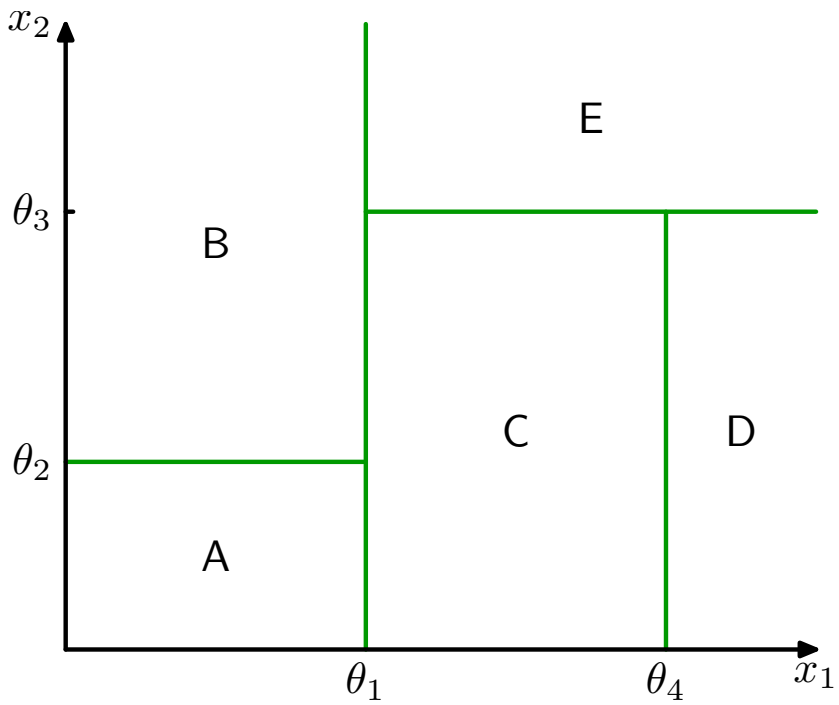
Complex to formally write down, but easy to represent pictorially or as codes.

The decision boundary

Corresponds to a classifier with boundaries:





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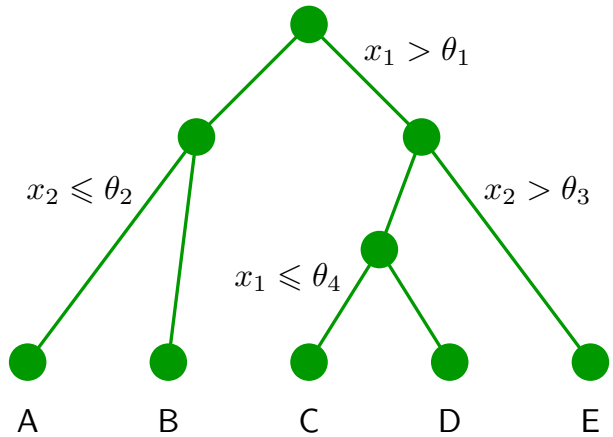

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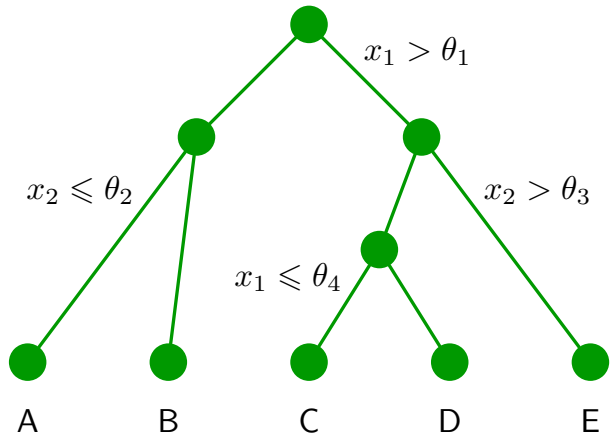

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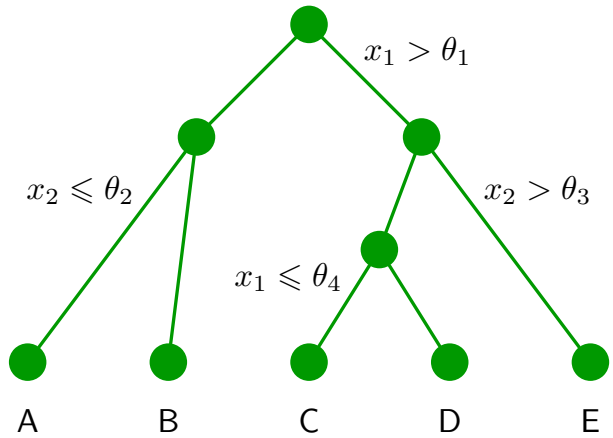

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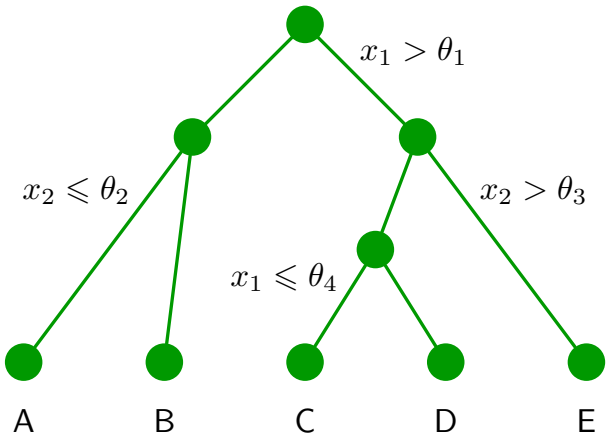

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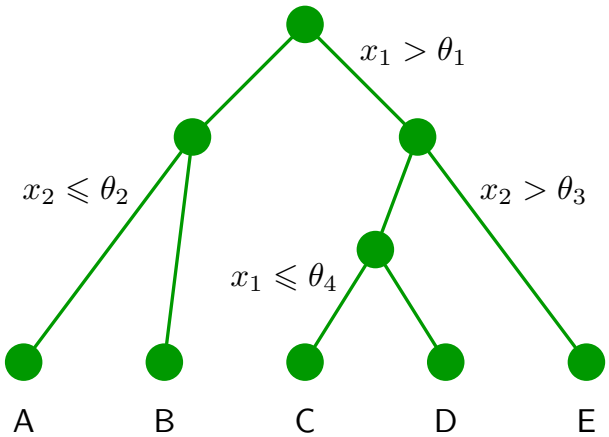

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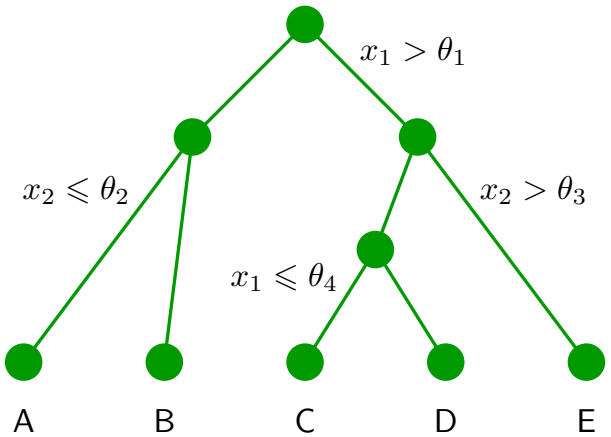
  - which feature(s) to test on?



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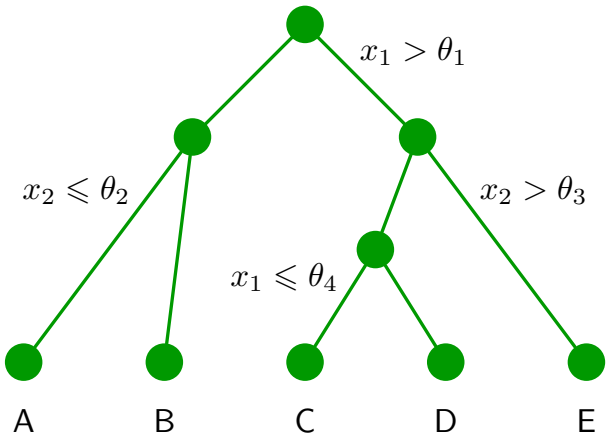
  - unlike typical neural nets, the structure of a tree is *not fixed in advance, but learned from data*
- the test at each internal node
  - which feature(s) to test on?
  - if the feature is continuous, what threshold $(\theta_1, \theta_2, \ldots)$?



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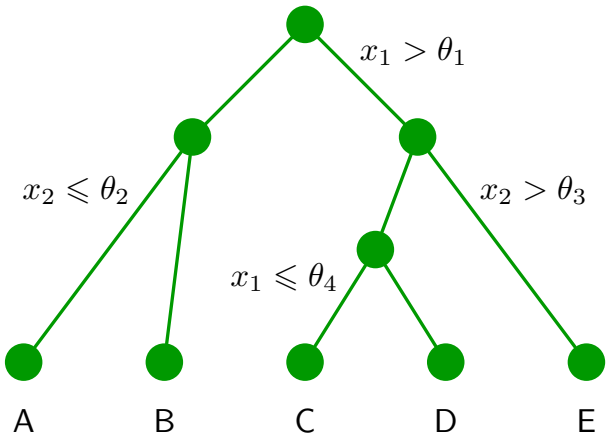

- the value/prediction of the leaves (A, B, ...)

Learning the parameters

So how do we *learn all these 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	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
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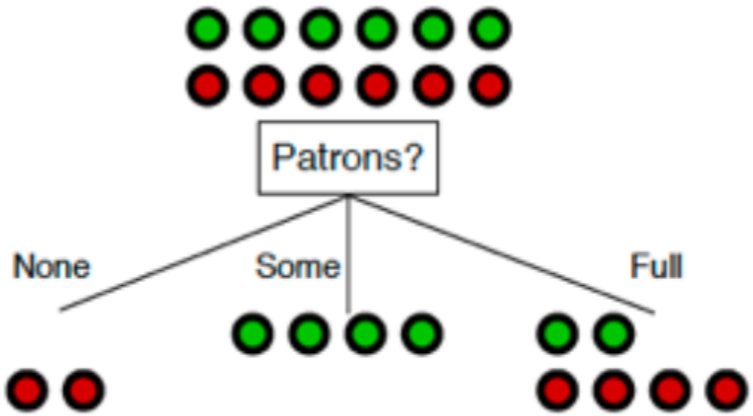
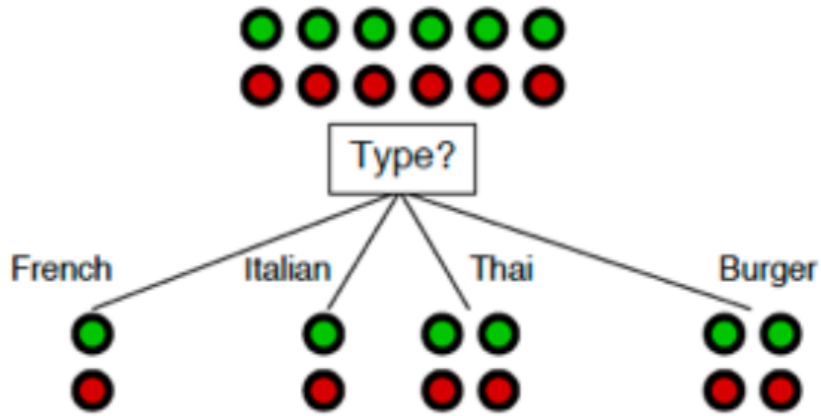
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

First step: how to build the root?

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





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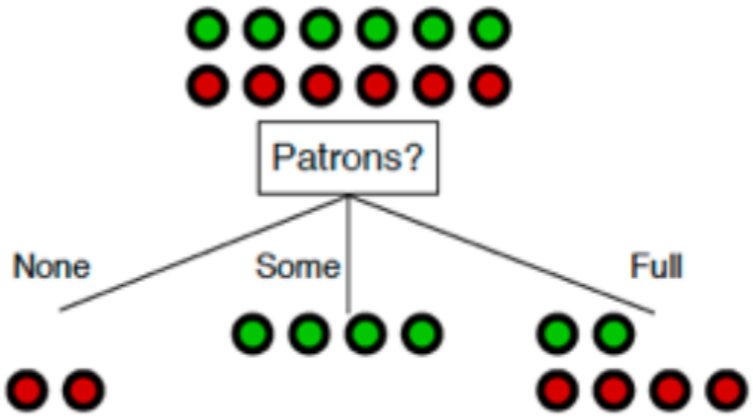

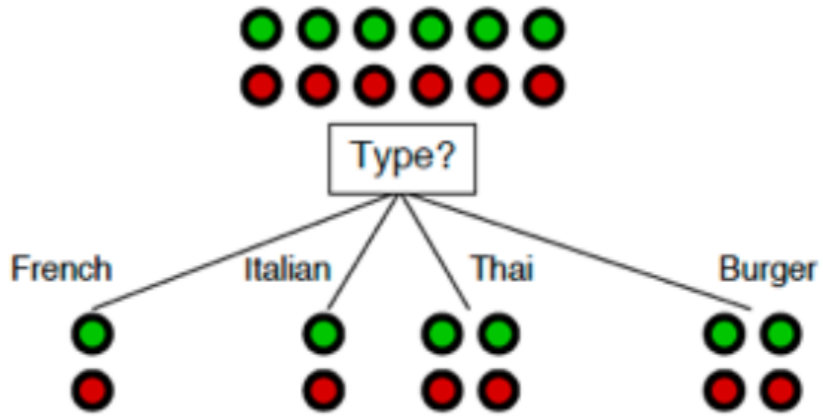

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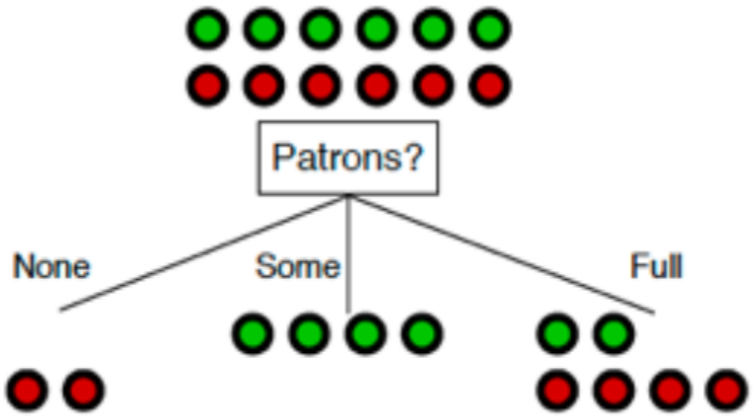

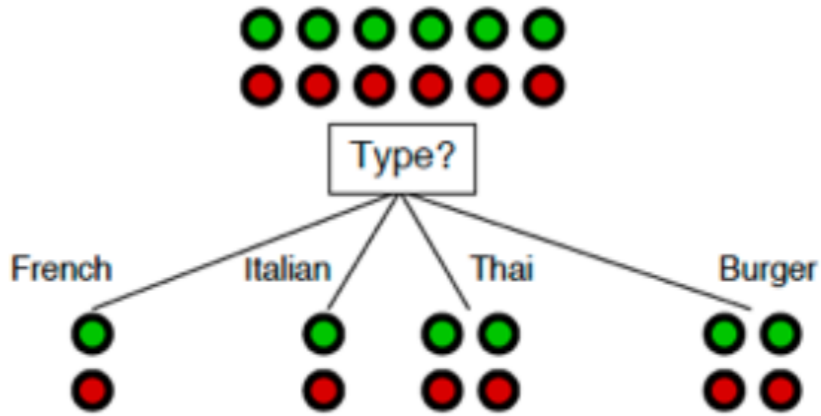

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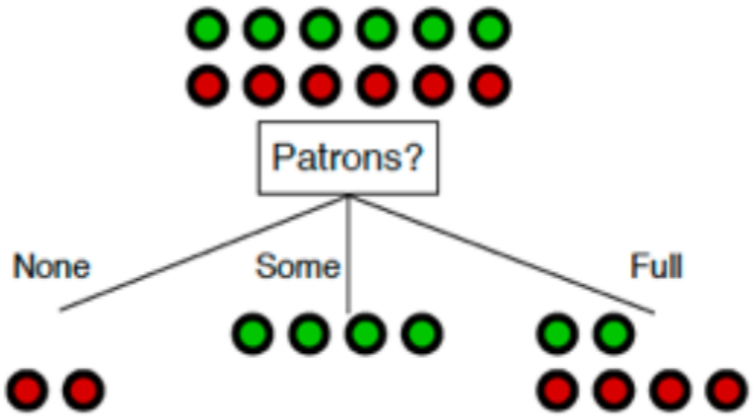

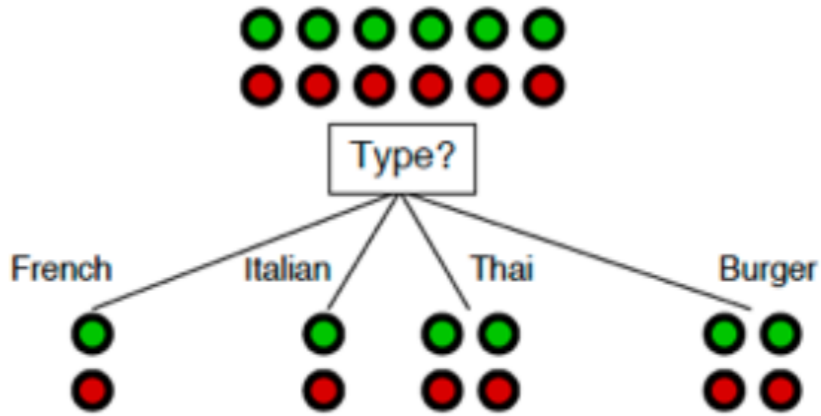

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- intuitively "patrons" is a better feature since it leads to "more pure" or "more certain" children
- how to quantify this intuition?

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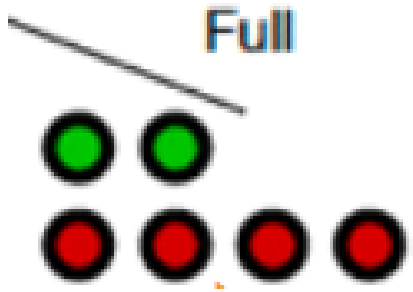

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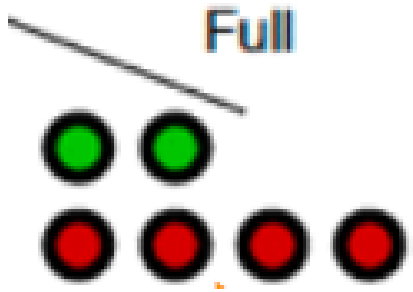

One classic uncertainty measure of a distribution is its *(Shannon) entropy*:

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

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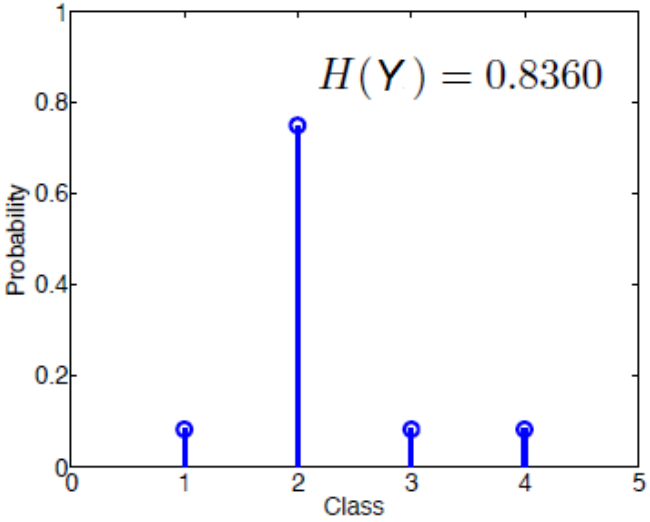
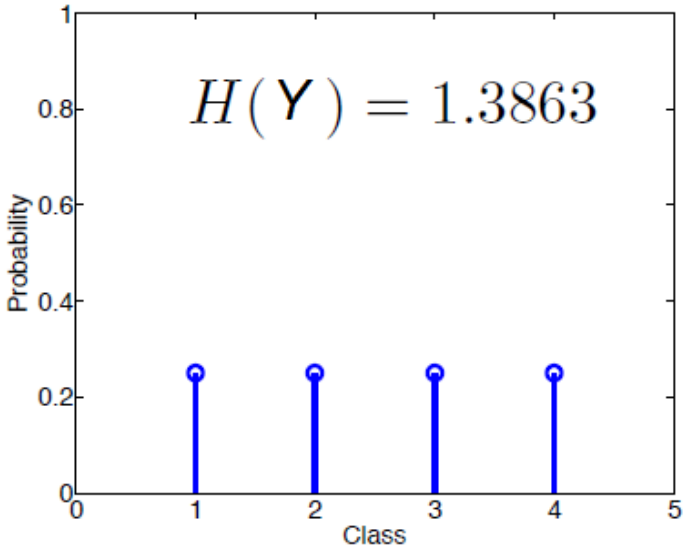
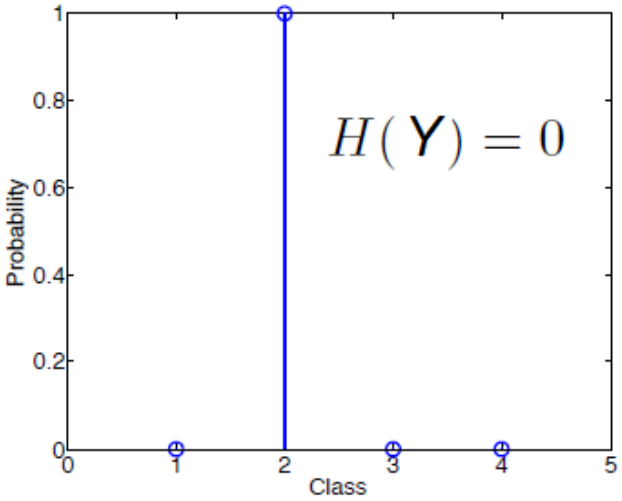
  - $0 \log 0$ is defined naturally as $\lim_{z \to 0+} z \log z = 0$

Examples of computing entropy

With base e and 4 classes:







Another example

Entropy in each child if root tests on "patrons"

For "None" branch

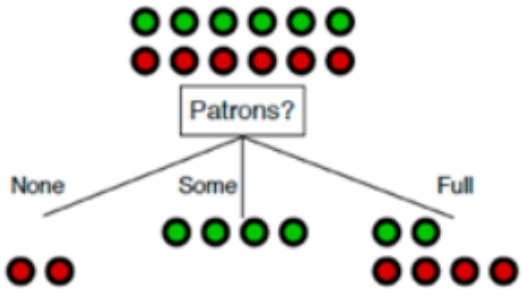
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

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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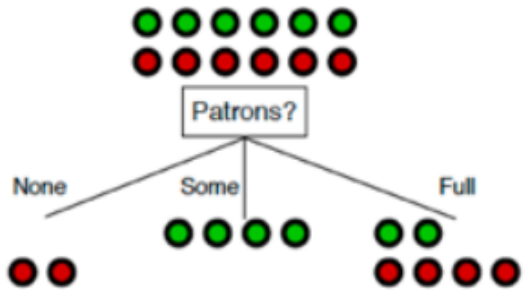

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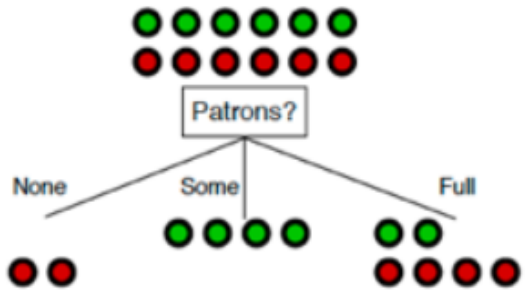

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Very naturally, we take the weighted average of entropy:

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

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Pick the feature that leads to the smallest conditional entropy.

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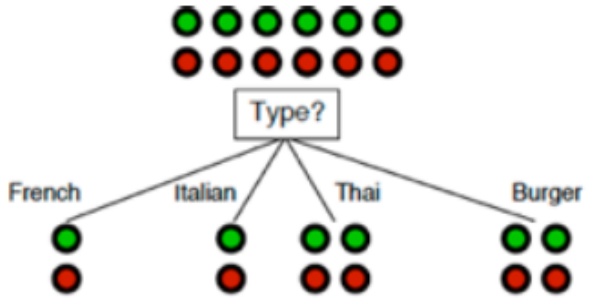

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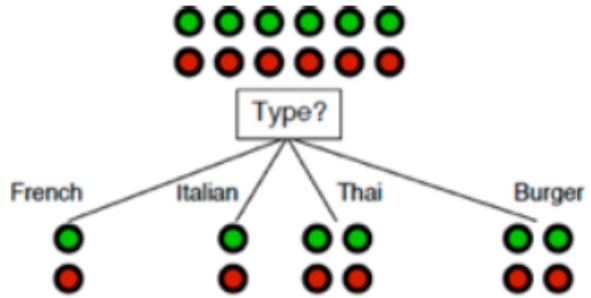

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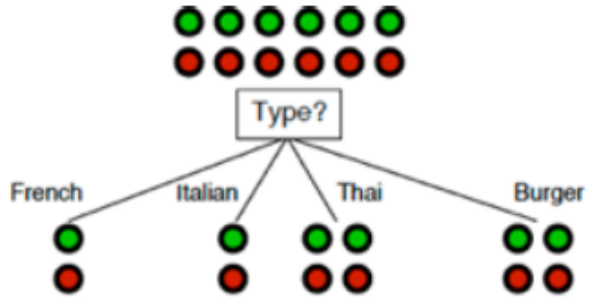

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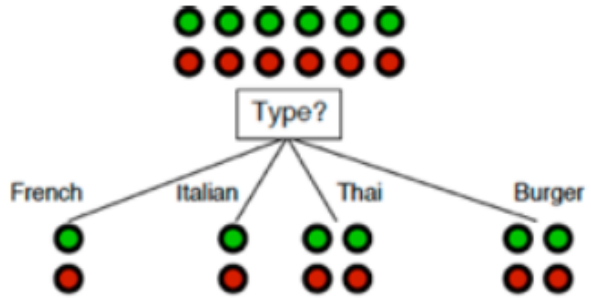

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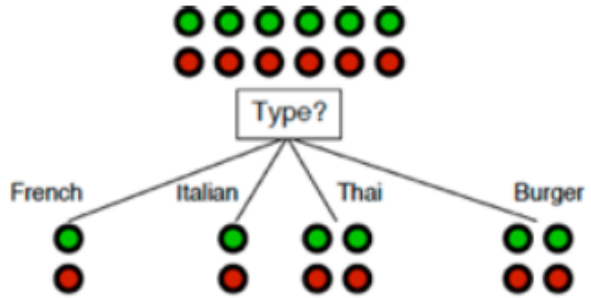

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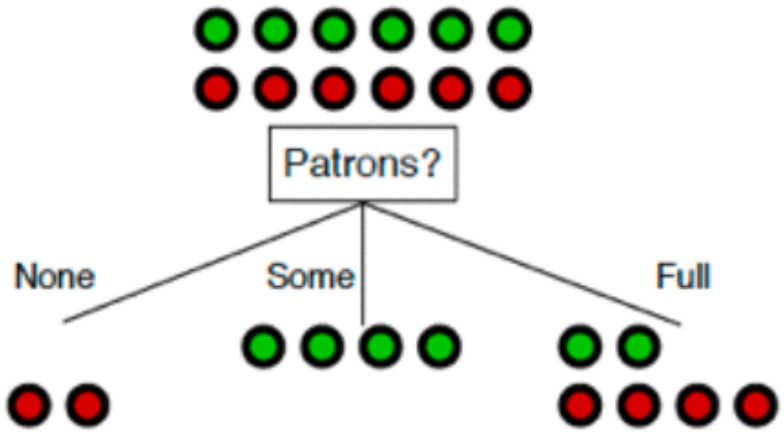
We are now done with building the root (this is also called a **stump**).

Repeat recursively

Split each child in the same way.



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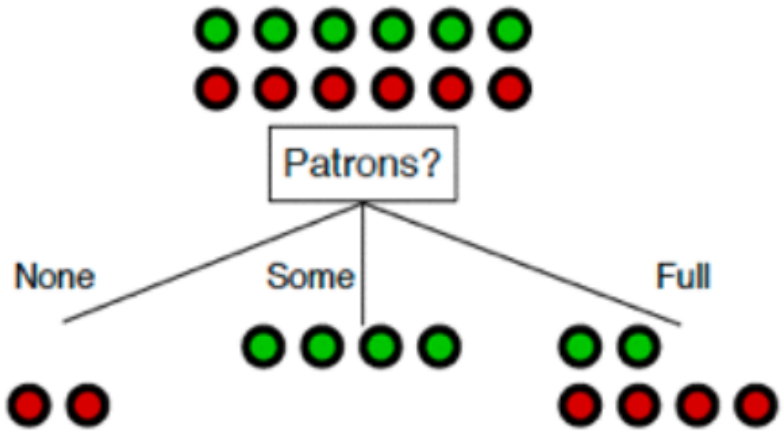

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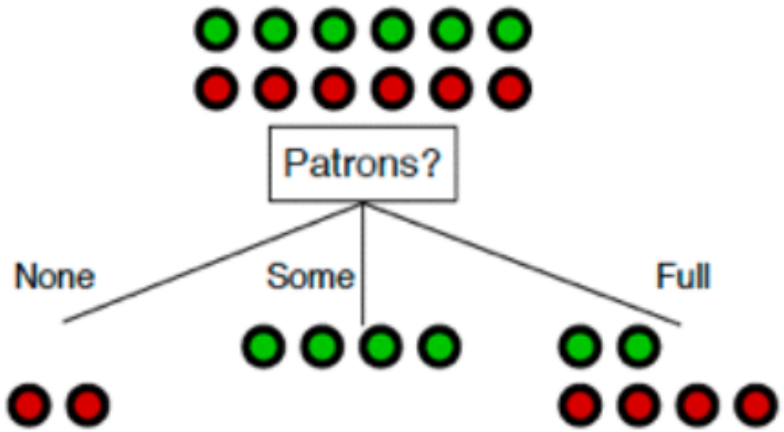
- for "full", repeat, focusing on those 6 examples:



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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	$$	T	T	Thai	0–10	T
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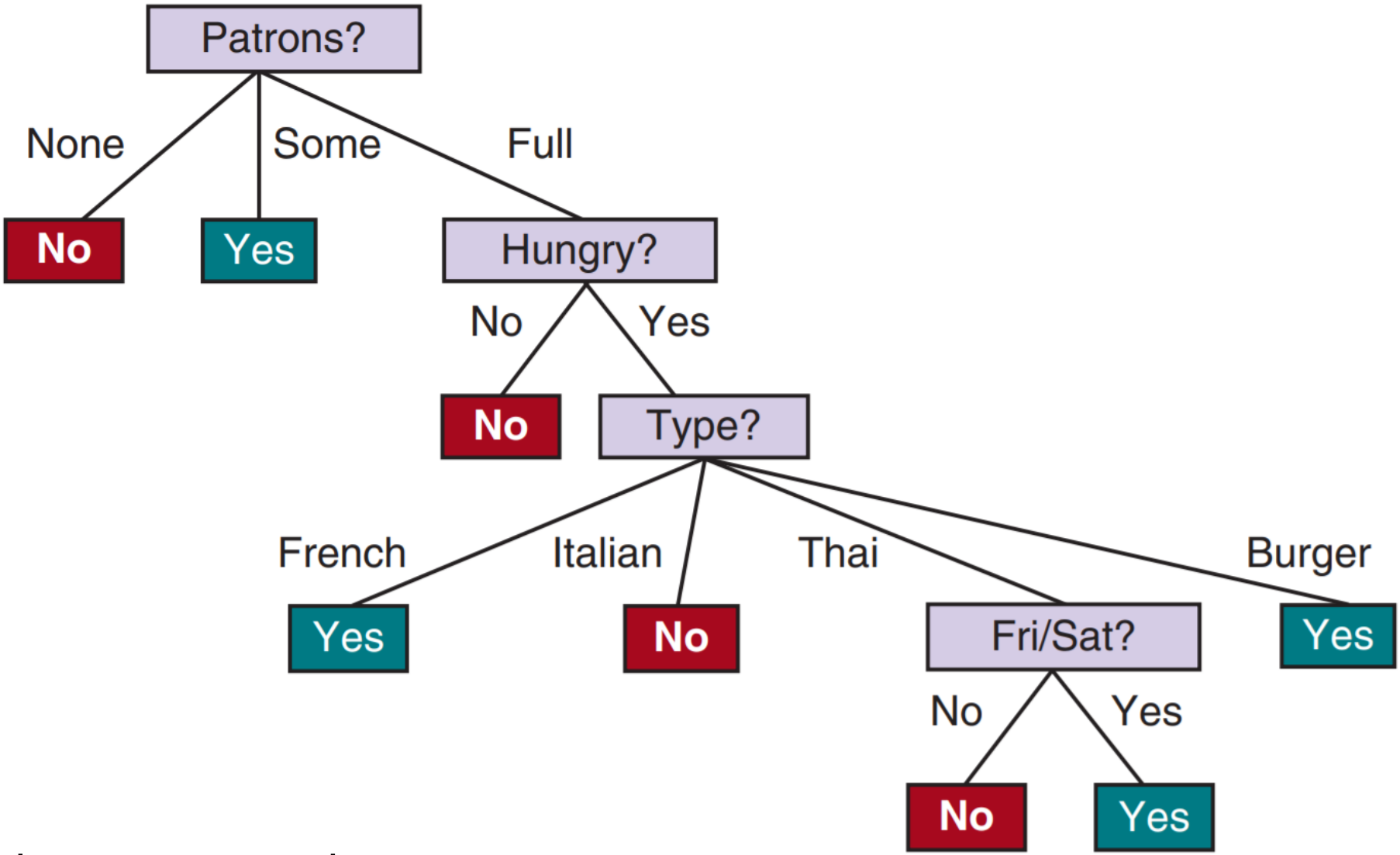
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T



Again, very easy to interpret.

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

Outline

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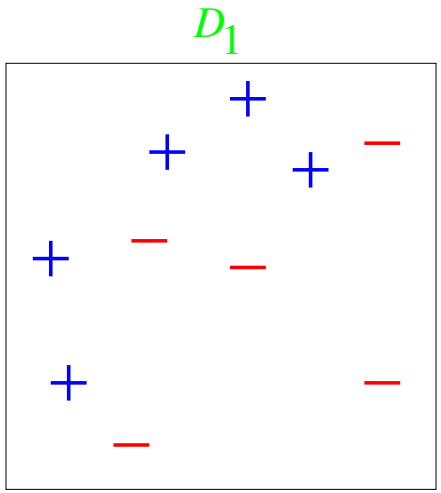
Output the final classifier $H(\boldsymbol{x}) = \text{sgn}\left(\sum_{t=1}^{T} \beta_t h_t(\boldsymbol{x}) \right)$

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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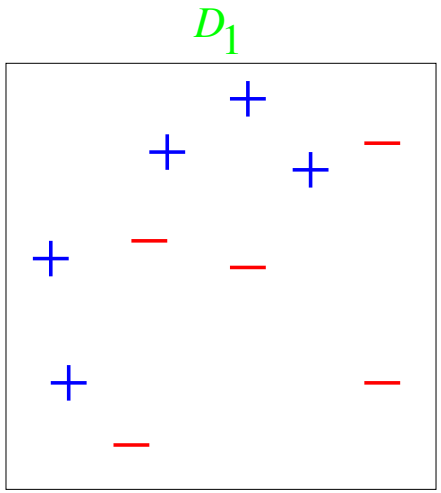
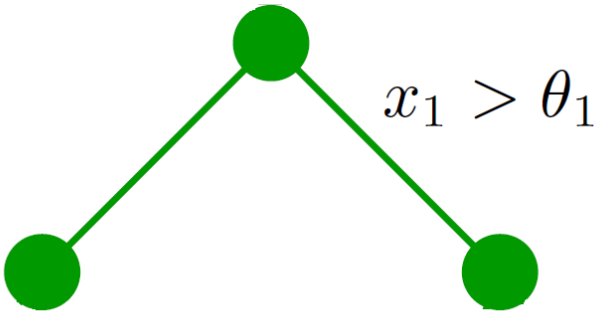
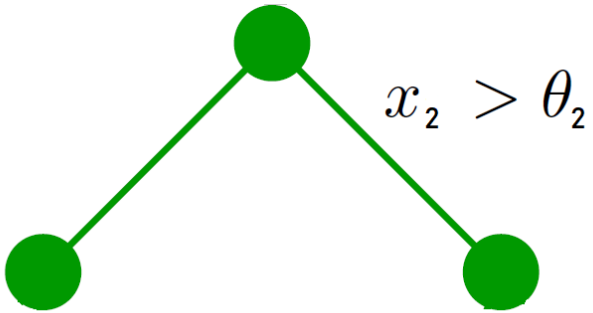


Base algorithm is decision stump:





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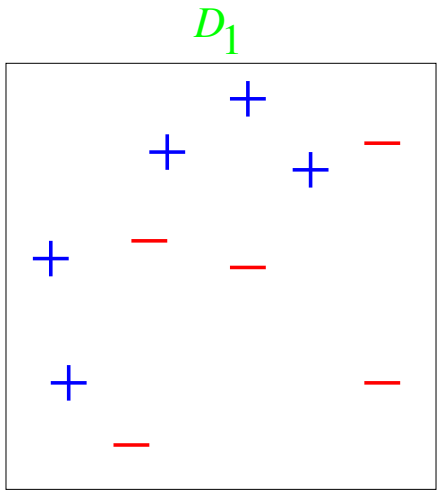

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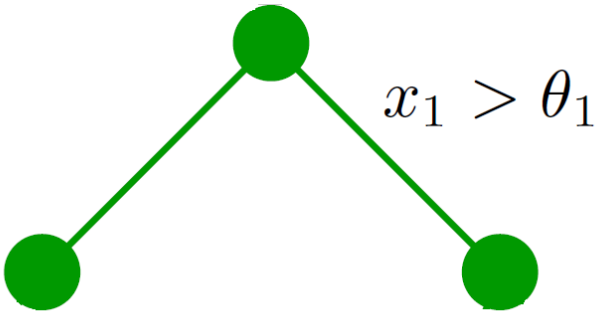
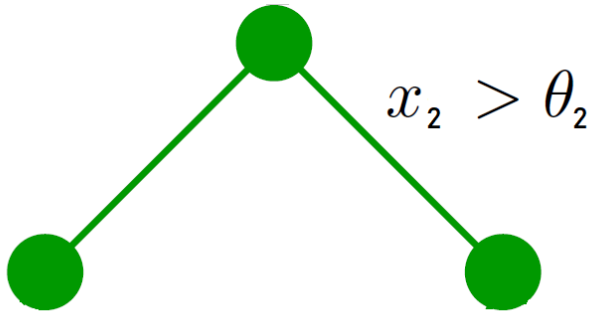
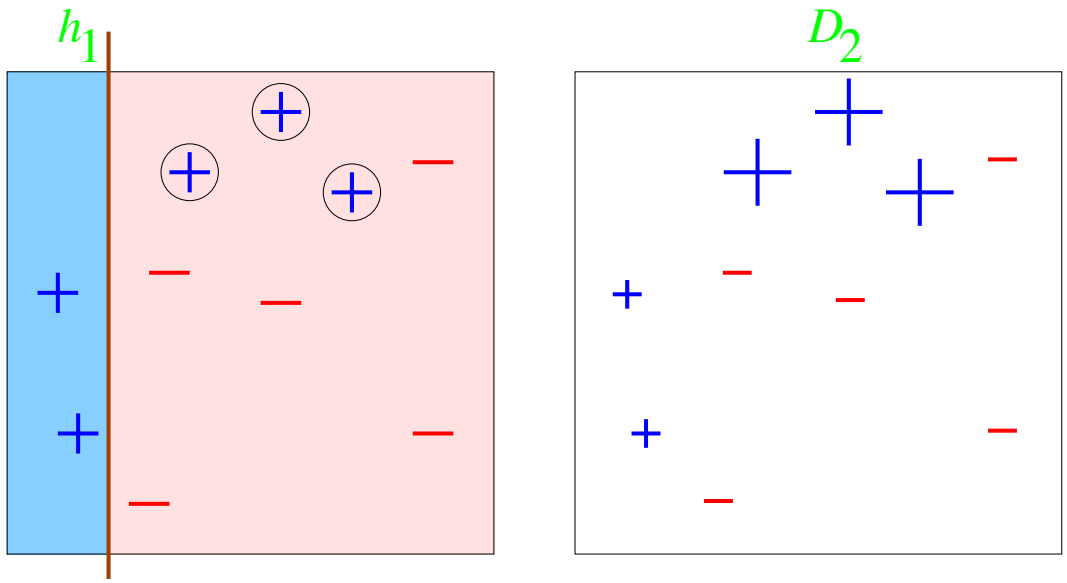




Observe that *no stump can predict very accurately for this dataset*

Round 1: $t = 1$



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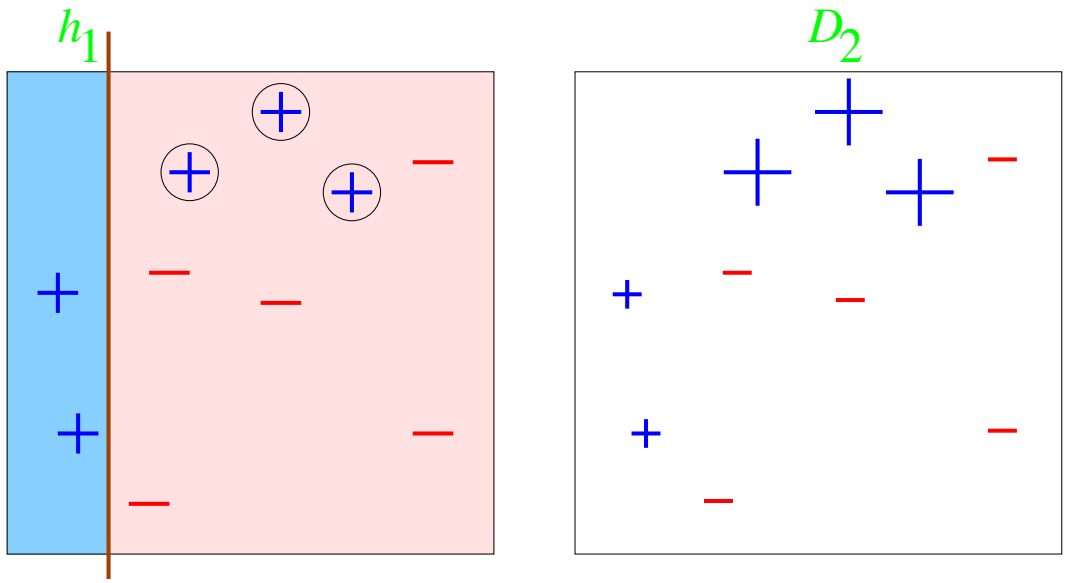

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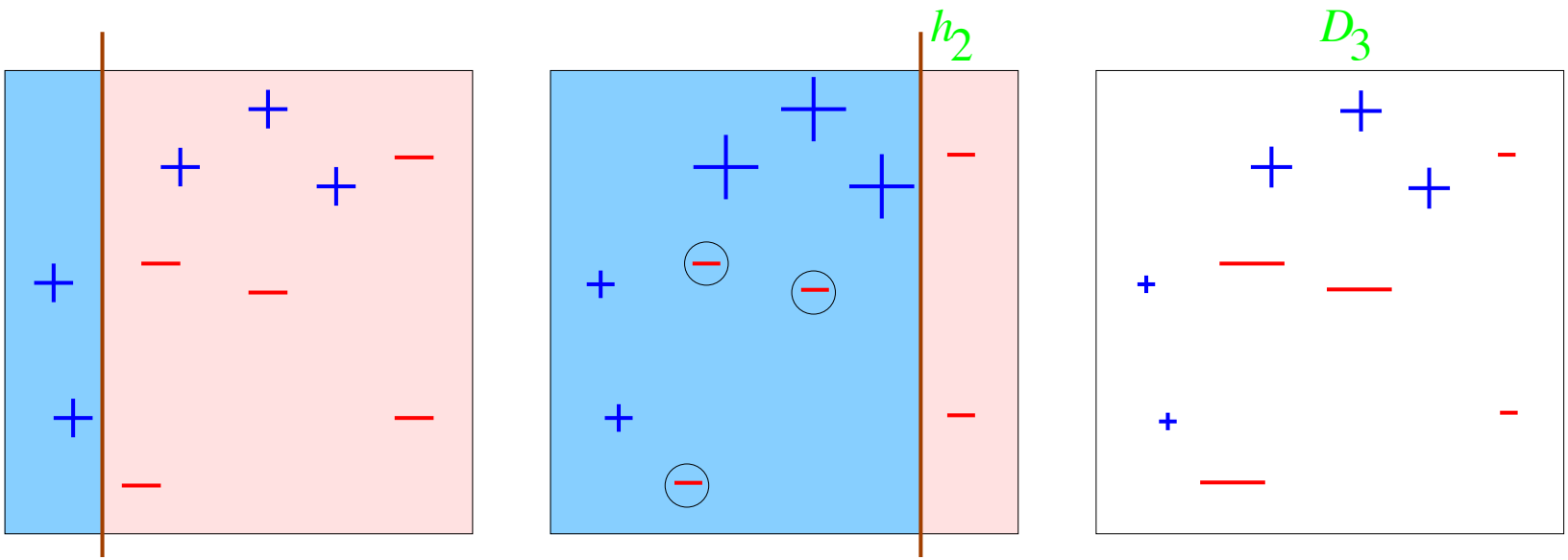

- 3 misclassified (circled): $\epsilon_2 = 0.21 \rightarrow \beta_2 = 0.65$.

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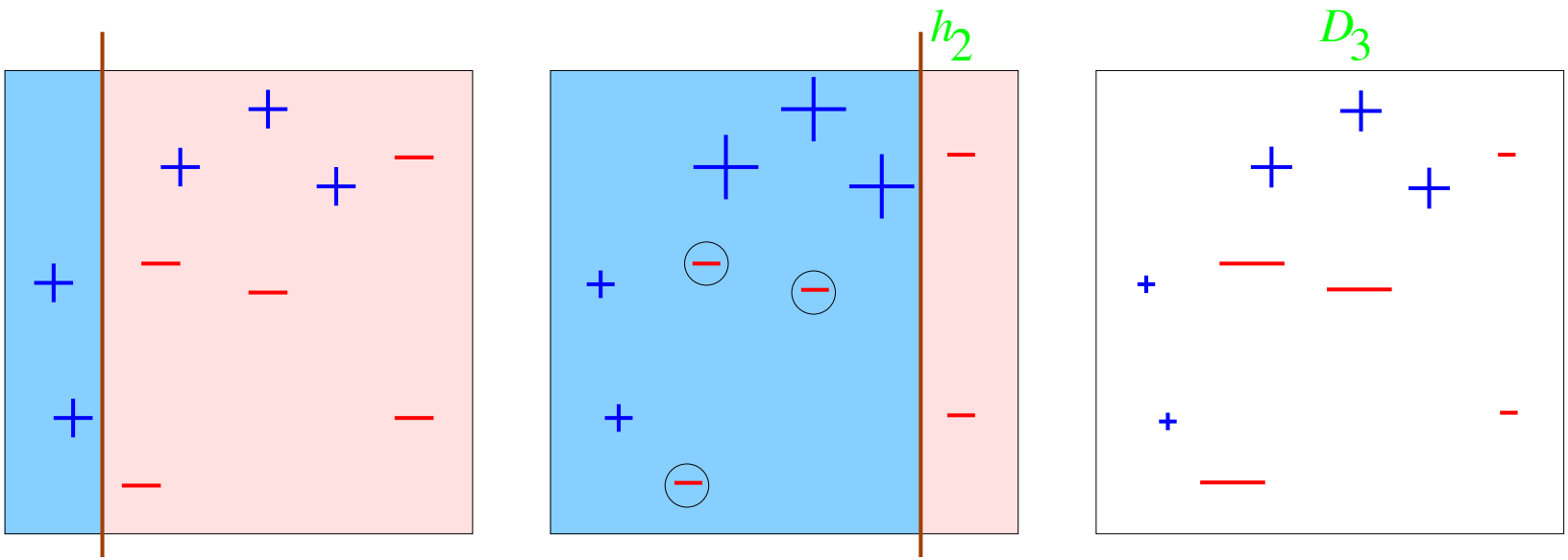

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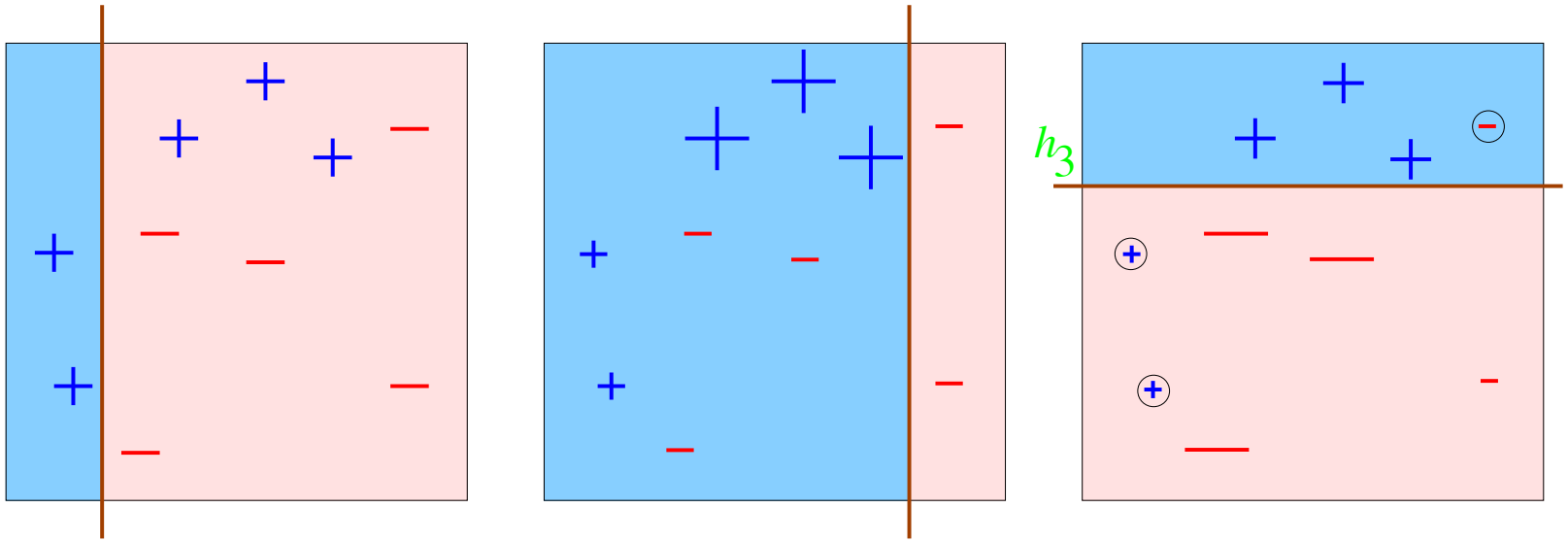
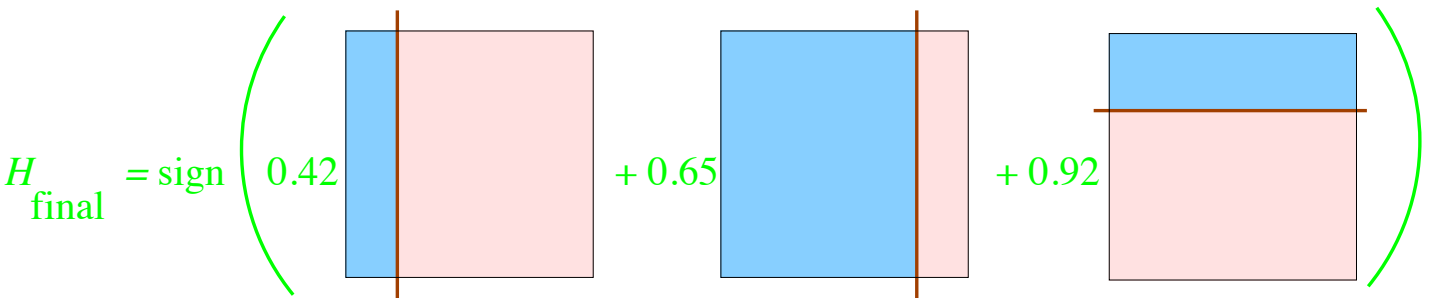
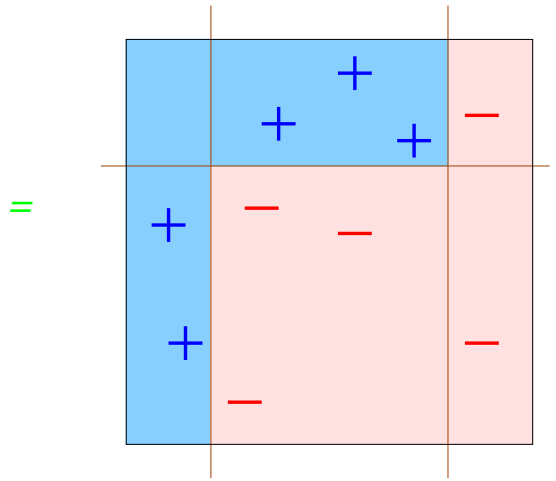


- again 3 misclassified (circled): $\epsilon_3 = 0.14 \rightarrow \beta_3 = 0.92$.

Final classifier: combining 3 classifiers





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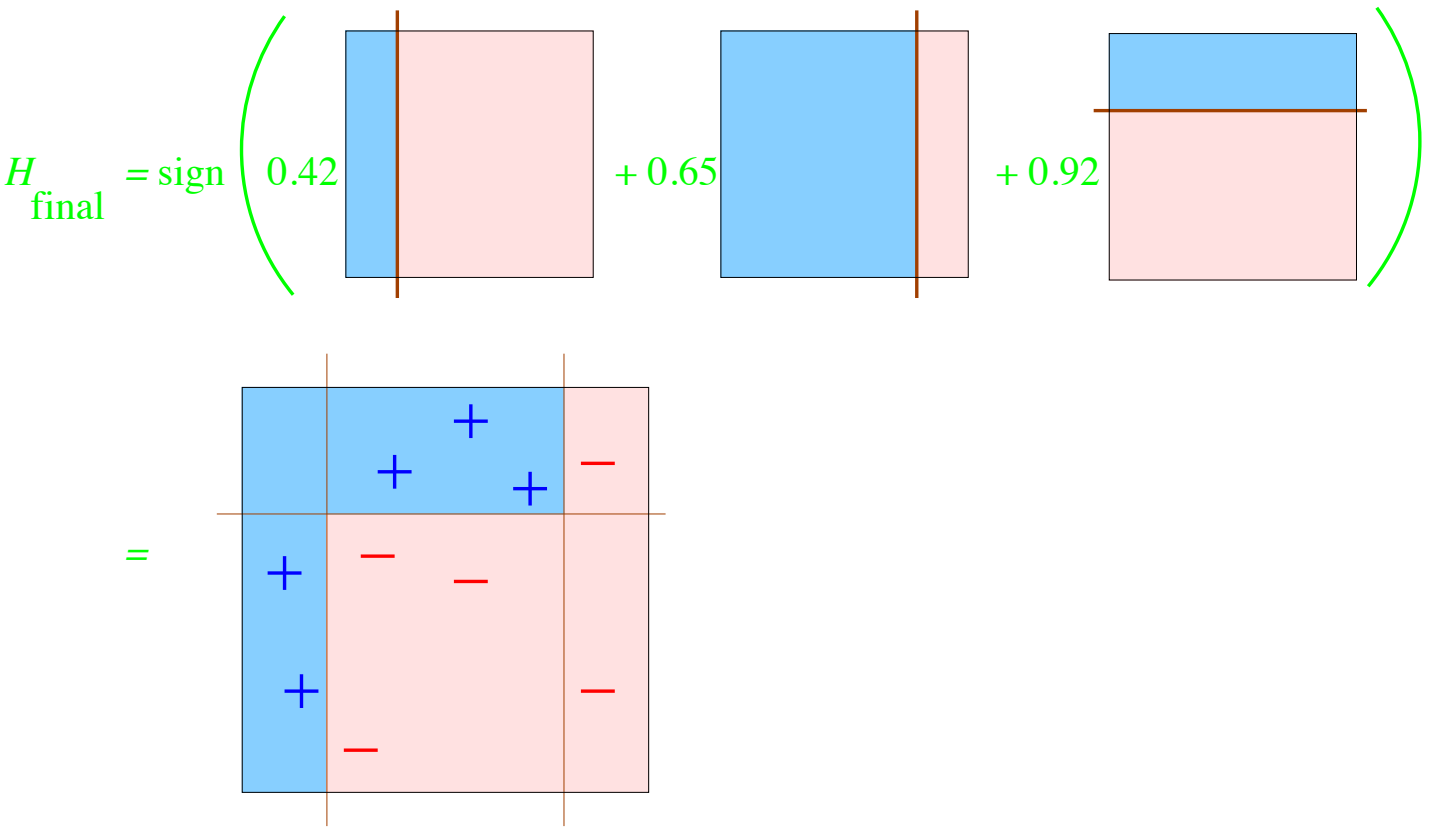

All data points are now classified correctly, even though each weak classifier makes 3 mistakes.

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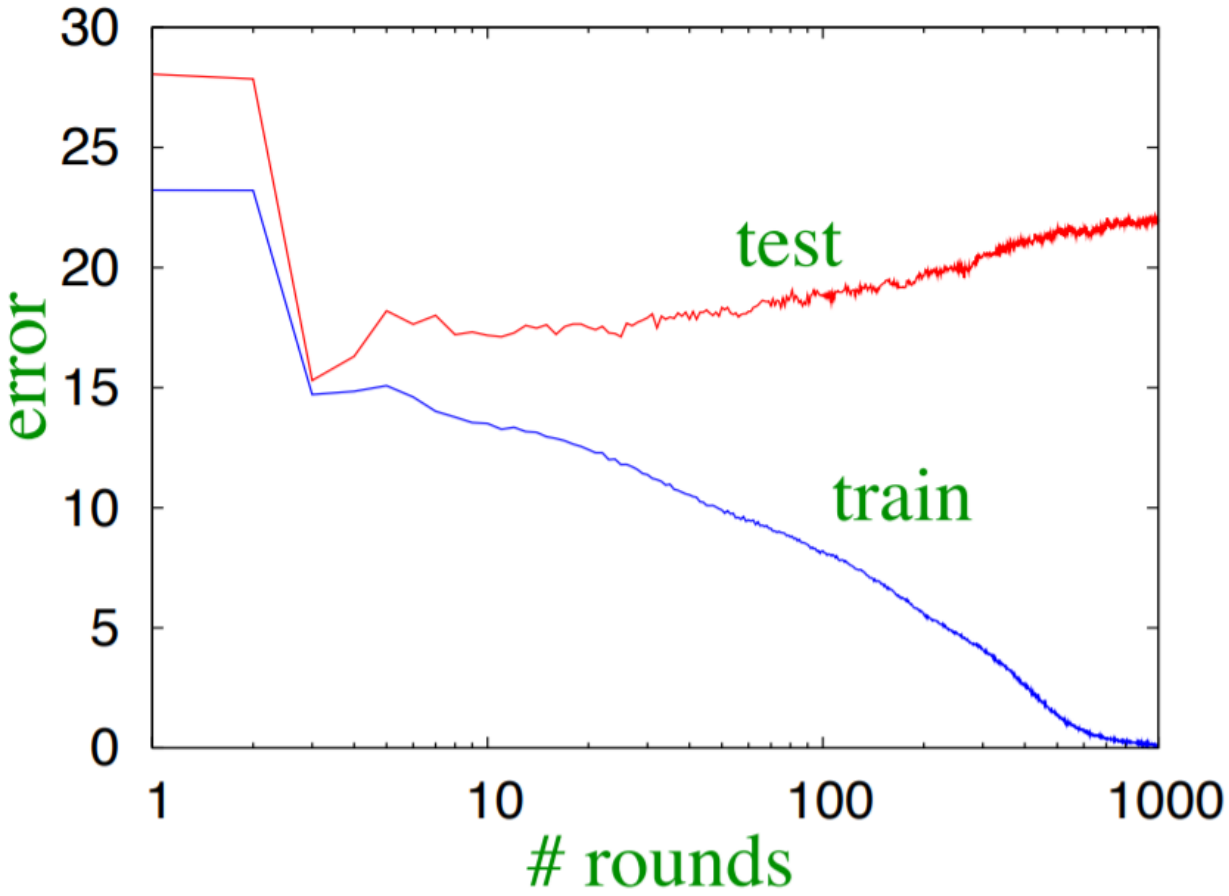

(boosting "stumps" on heart-disease dataset)

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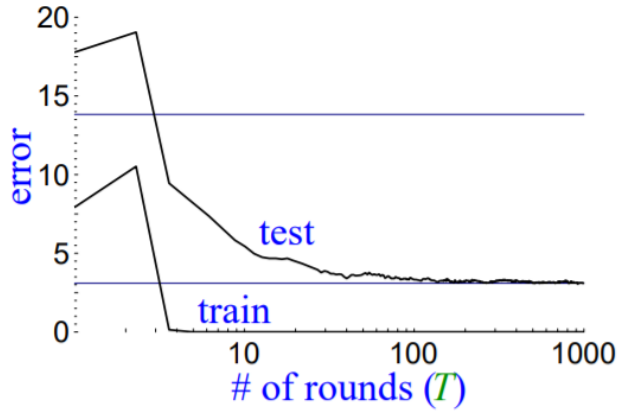

(boosting C4.5 on "letter" dataset)

- 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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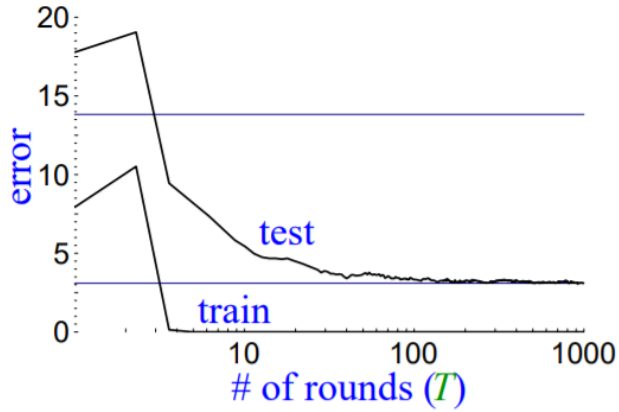

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Used to be a mystery, but by now rigorous theory has been developed to explain this phenomenon.