CSCI567 Machine Learning (Fall 2021)

Prof. Haipeng Luo

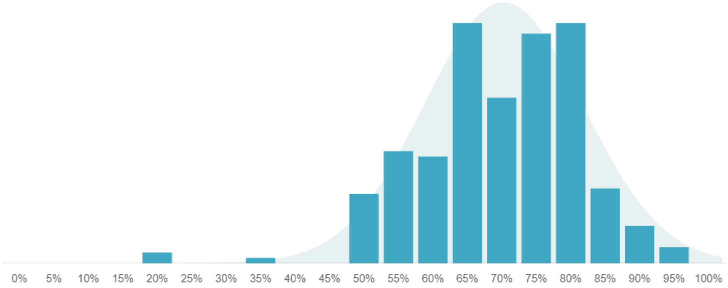
U of Southern California

Oct 21, 2021

Administration

Quiz 1 grading is done:

- mean: 69.7, median: 70.5



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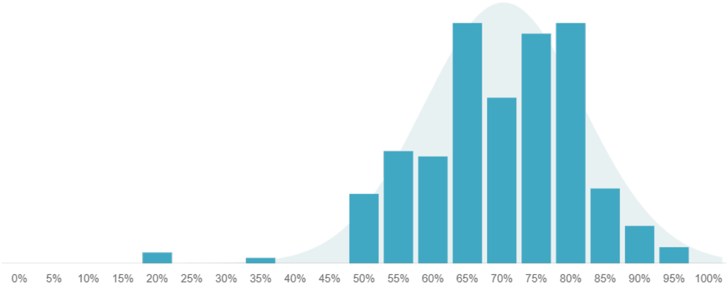

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HW3 is due on Tue (Oct 26th)

Outline

1. Decision tree
2. Boosting

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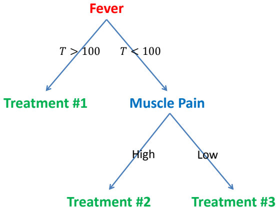
- nonlinear in general
- works for both classification and regression; we focus on classification
- one key advantage is good interpretability
- used to be very popular; ensemble of trees (i.e. "forest") can still be very effective
- not to be confused with the "tree reduction" in Lec 4

Example

Many decisions are made based on some tree structure

Medical treatment



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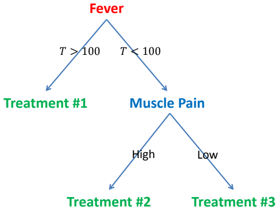
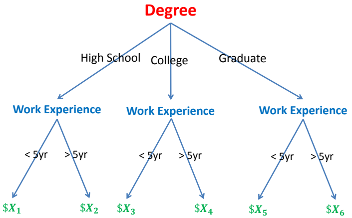
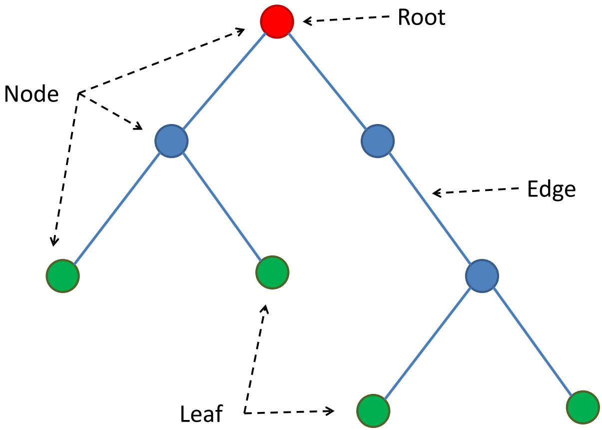


Salary in a company

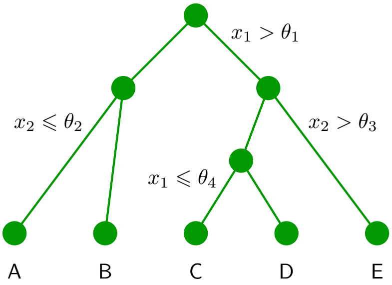


Tree terminology



A more abstract example of decision trees

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



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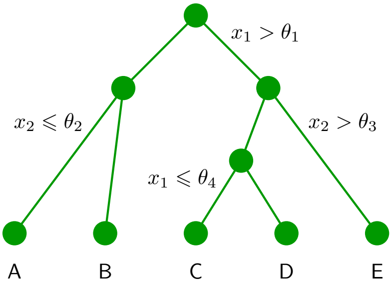

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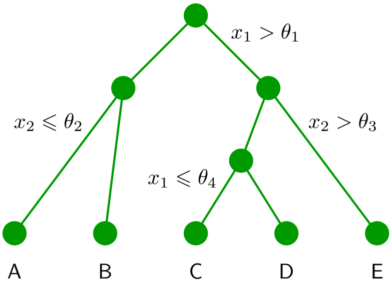

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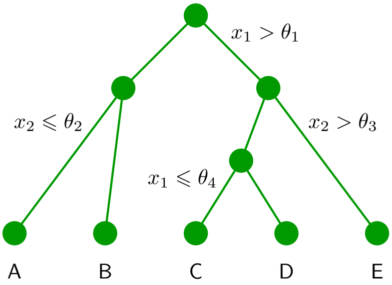

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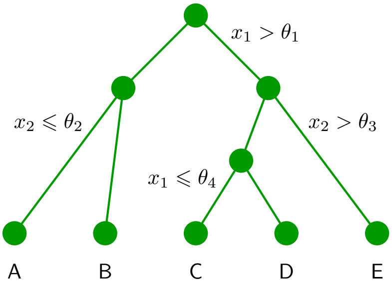

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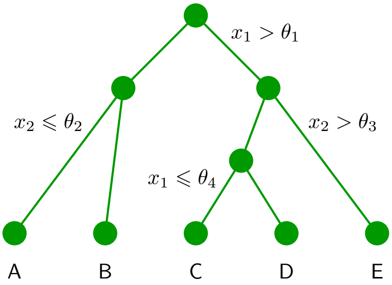

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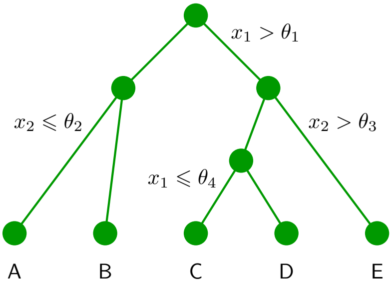

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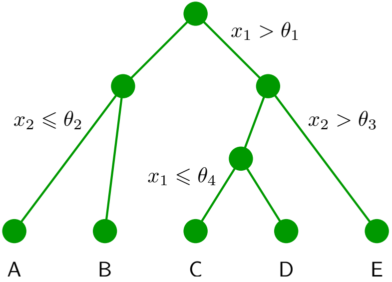
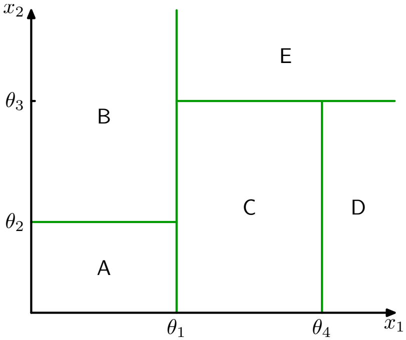
Complex to formally write down, but easy to represent pictorially or as codes.

The decision boundary

Corresponds to a classifier with boundaries:





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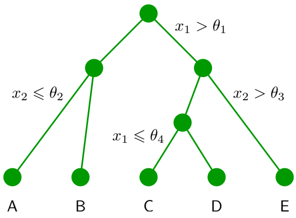

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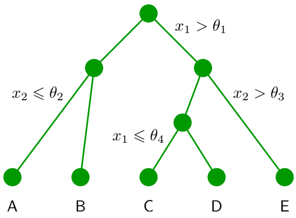

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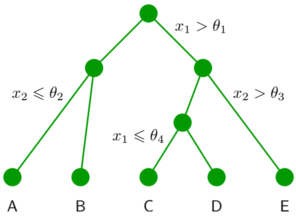

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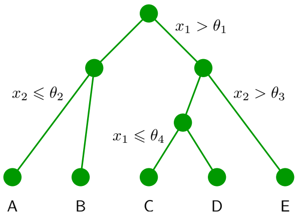

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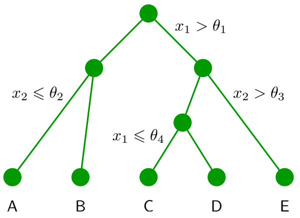

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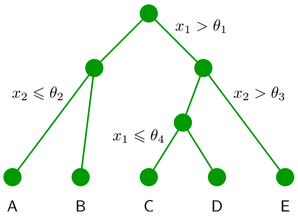

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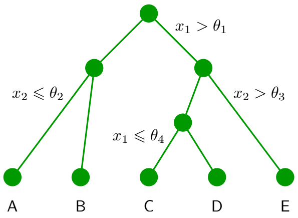

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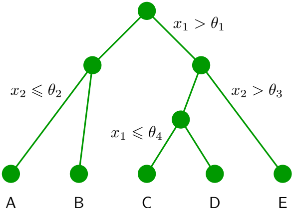

- the value/prediction of the leaves (A, B, ...)

Learning the parameters

So how do we *learn all these parameters?*

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

A running example

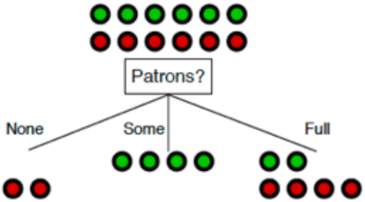
[Russell & Norvig, AIMA]

- 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	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	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

First step: how to build the root?

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



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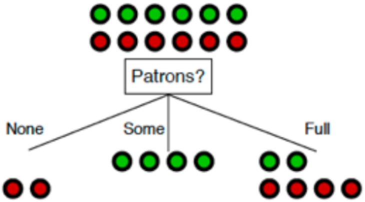

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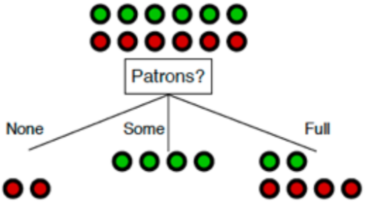

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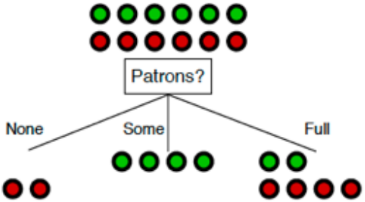

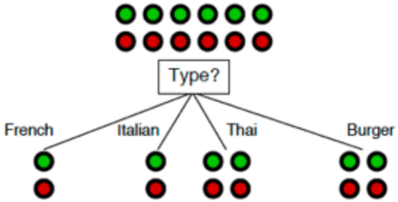

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- intuitively "patrons" is a better feature since it leads to "more pure" or "more certain" children
- how to quantify this intuition?

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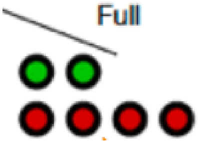

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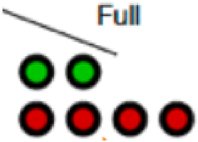

One classic uncertainty measure of a distribution is its *(Shannon) entropy*:

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

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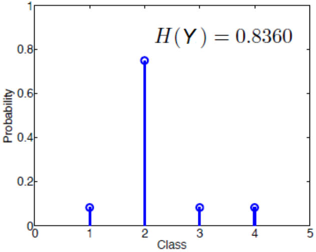
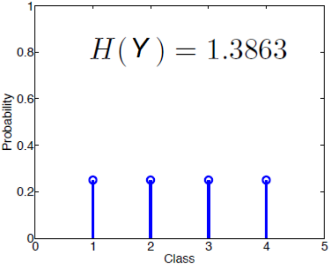
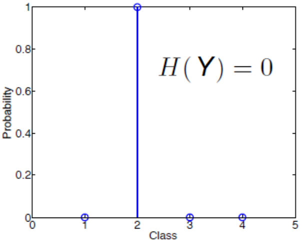
  - $0 \log 0$ is defined naturally as $\lim_{z \to 0+} z \log z = 0$

Examples of computing entropy

With base e and 4 classes:







Another example

Entropy in each child if root tests on "patrons"

For "None" branch

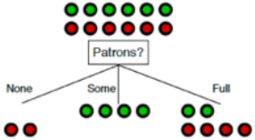
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

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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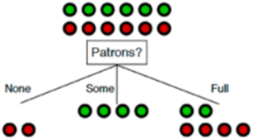

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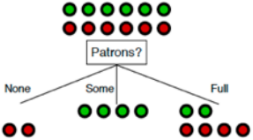

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Very naturally, we take the weighted average of entropy:

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

Measure of uncertainty of a split

Suppose we split based on a discrete feature A, the uncertainty can be measured by the **conditional entropy**:

$$H(Y \mid A)$$

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Pick the feature that leads to the smallest conditional entropy.

Deciding the root

For "French" branch

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

For "Italian" 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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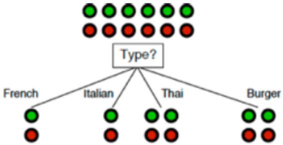

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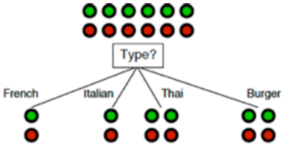

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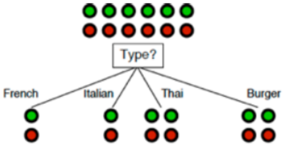

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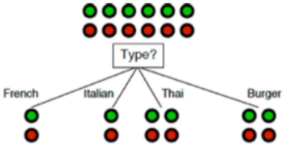

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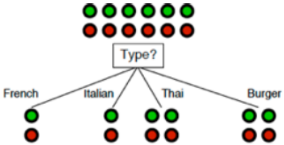

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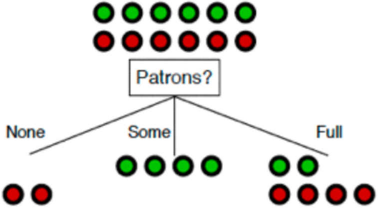
We are now done with building the root (this is also called a **stump**).

Repeat recursively

Split each child in the same way.



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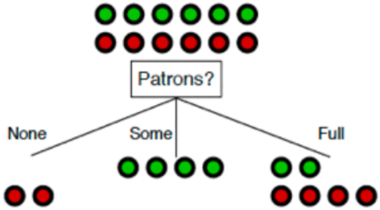
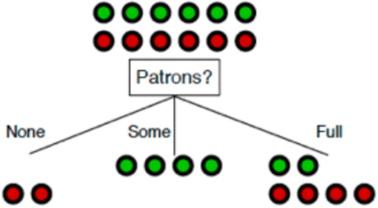


Repeat recursively

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:



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
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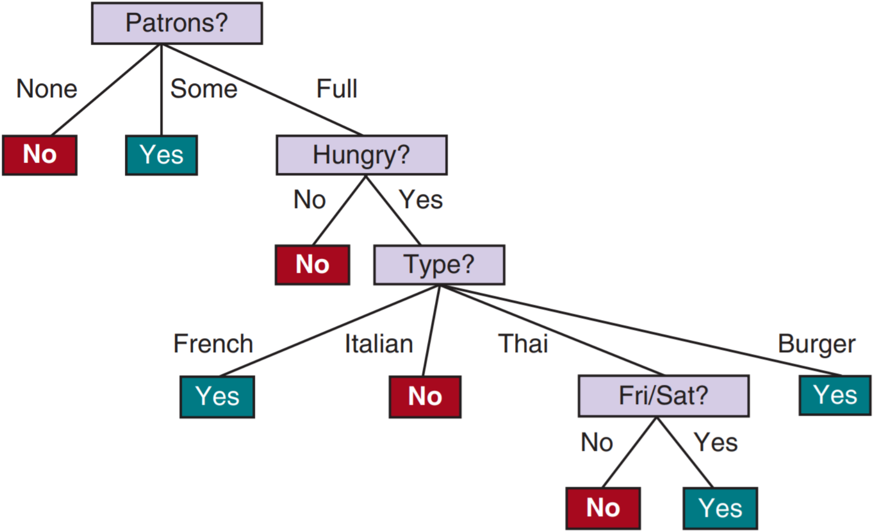
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T



Again, very easy to interpret.

Putting it together

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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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- 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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- obtain a weak classifier $h_t \leftarrow \mathcal{A}(S, D_t)$
- calculate the importance of h_t as

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

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- update distributions

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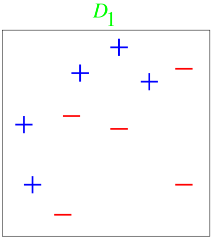
Output the final classifier $H(\boldsymbol{x}) = \text{sgn}\left(\sum_{t=1}^{T} \beta_t h_t(\boldsymbol{x}) \right)$

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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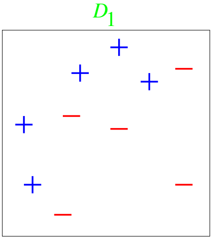

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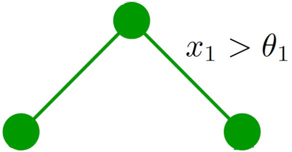

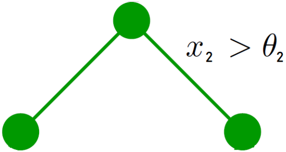

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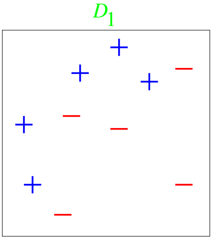

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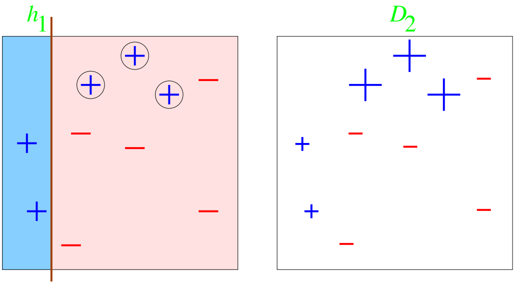
Base algorithm is decision stump:

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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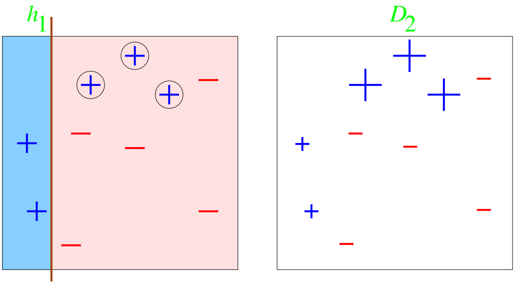

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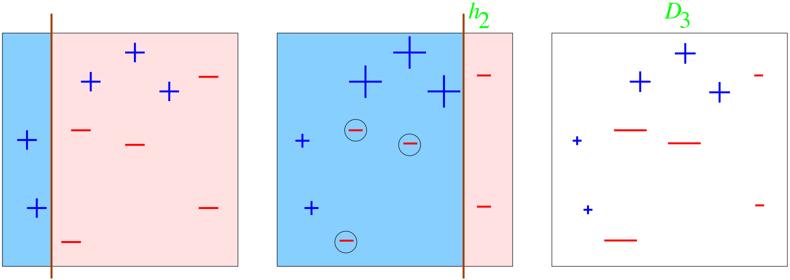

- 3 misclassified (circled): $\epsilon_2 = 0.21 \rightarrow \beta_2 = 0.65$.

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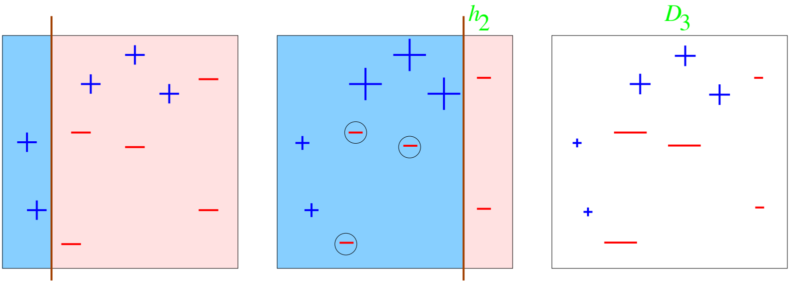

- 3 misclassified (circled): $\epsilon_2 = 0.21 \rightarrow \beta_2 = 0.65$.
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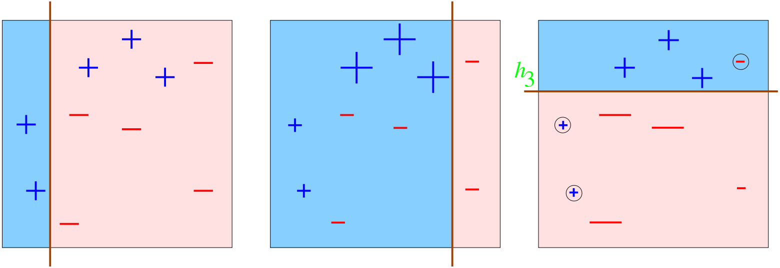
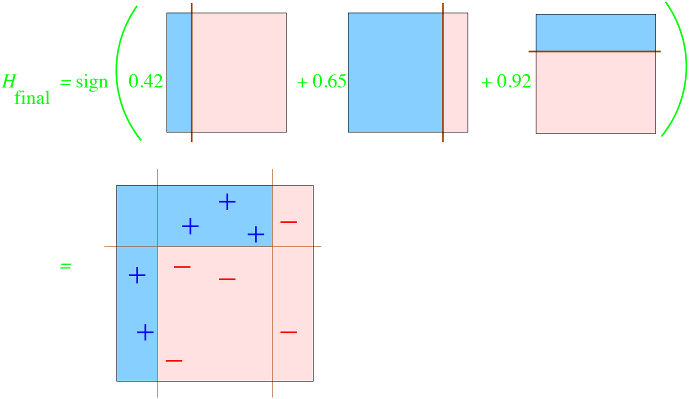


- again 3 misclassified (circled): $\epsilon_3 = 0.14 \rightarrow \beta_3 = 0.92$.

Final classifier: combining 3 classifiers



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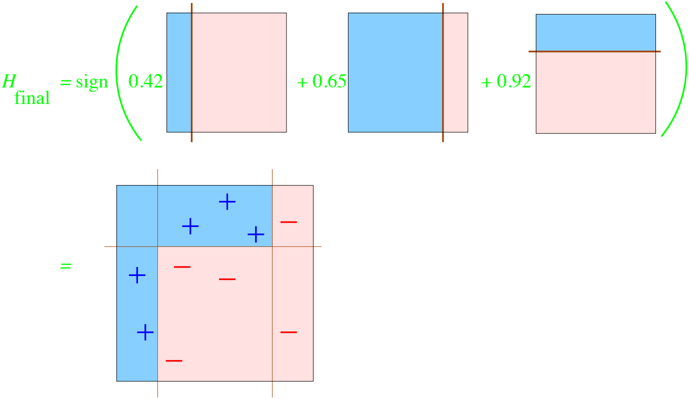

All data points are now classified correctly, even though each weak classifier makes 3 mistakes.

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When T is large, the model is very complicated and overfitting can happen

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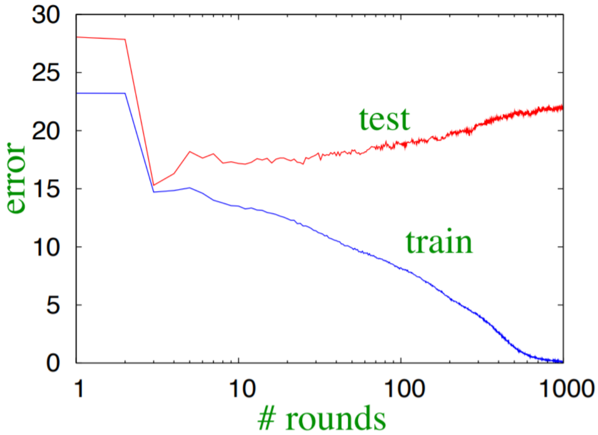

(boosting "stumps" on heart-disease dataset)

Resistance to overfitting

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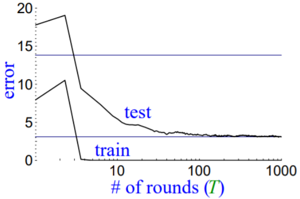

(boosting C4.5 on "letter" dataset)

- 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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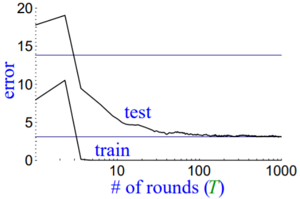

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Used to be a mystery, but by now rigorous theory has been developed to explain this phenomenon.

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

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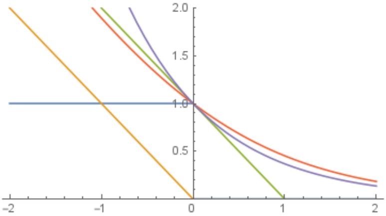

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where the last step is by the definition of weights

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

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This greedy step is abstracted out through a base algorithm.

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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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AdaBoost is often **resistant to overfitting**.

Quiz 1 Problem 5 (a)

Consider the following Gaussian/RBF kernel

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(\frac{-\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{2}\right). \tag{3}$$

It is known that there exists an infinite-dimensional nonlinear mapping $\boldsymbol{\phi}_{\text{RBF}}$ such that

$$\boldsymbol{\phi}_{\text{RBF}}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}_{\text{RBF}}(\boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}') \tag{4}$$

for any $\boldsymbol{x}$ and $\boldsymbol{x}'$. In this problem, you will investigate a way to approximate this nonlinear mapping $\boldsymbol{\phi}_{\text{RBF}}$.

(a) Consider a nonlinear mapping $\phi_{\boldsymbol{v},b} : \mathbb{R}^D \to \mathbb{R}$ constructed as follows: randomly draw a vector $\boldsymbol{v} \in \mathbb{R}^D$ from the standard Gaussian and a scalar b from the uniform distribution over $[0, \pi]$, then define $\phi_{\boldsymbol{v},b}(\boldsymbol{x}) = \sqrt{2}\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x} + b)$ for any input feature vector $\boldsymbol{x} \in \mathbb{R}^D$.

For any two feature vectors $\boldsymbol{x}$ and $\boldsymbol{x}'$, prove the following

$$\mathbb{E}\left[\phi_{\boldsymbol{v},b}(\boldsymbol{x})\phi_{\boldsymbol{v},b}(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}') \tag{5}$$

where the expectation is over the randomness of $\boldsymbol{v}$ and b, and $k(\cdot,\cdot)$ is defined in Eq. (3). You can directly use the following two identities in your proof:

- trigonometric identity: $2\cos(\alpha)\cos(\beta) = \cos(\alpha - \beta) + \cos(\alpha + \beta)$;
- integral identity: $\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{z})\right] = \exp\left(\frac{-\|\boldsymbol{z}\|_2^2}{2}\right)$ where the expectation is with respect to $\boldsymbol{v}$ randomly drawn from the standard Gaussian. (With this, you do not even need to know what the standard Gaussian is to solve this problem.)

Quiz 1 Problem 5 (a)

Plugging in the definition of $\phi_{\boldsymbol{v},b}$, we first have

$$\mathbb{E}\left[\phi_{\boldsymbol{v},b}(\boldsymbol{x})\phi_{\boldsymbol{v},b}(\boldsymbol{x}')\right] = 2\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}+b)\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}'+b)\right]. \qquad \text{(1 point)}$$

Using the given trigonometric identity, the above is equal to

$$\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{x}')) + \cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}+\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}'+2b)\right]. \qquad \text{(1 point)}$$

For the first term above, directly applying the given integral identity gives

$$\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{x}'))\right] = k(\boldsymbol{x},\boldsymbol{x}'). \qquad \text{(1 point)}$$

For the second term, fixing $\boldsymbol{v}$ and taking the expectation over b shows

$$\begin{aligned}\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}+\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}'+2b)\right] &= \frac{1}{\pi}\int_0^{\pi}\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}+\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}'+2b)db \\ &= \frac{1}{2\pi}\sin(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}+\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}'+2b)\Big|_0^{\pi} = 0. \qquad \text{(2 points)}\end{aligned}$$

This finishes the proof. (The last step can also be argued by symmetry without writing down the integral explicitly.)

Quiz 1 Problem 5 (b)

(b) Comparing Eq. (4) and Eq. (5), we see that $\phi_{\boldsymbol{v},b}$ can be used as an approximation for $\boldsymbol{\phi}_{\mathrm{RBF}}$. However, using only one sample $(\boldsymbol{v}, b)$ leads to large variance for this approximation. Based on this information, for any given dimension $M > 1$, can you come up with a random nonlinear mapping $\boldsymbol{\phi} : \mathbb{R}^D \to \mathbb{R}^M$, such that it is a better approximation of $\boldsymbol{\phi}_{\mathrm{RBF}}$ satisfying $\mathbb{E}\left[\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}')$? Write down your proposal, prove $\mathbb{E}\left[\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}')$, and finally explain why it is a better approximation (in one concise sentence). (5 points)

Proposal: $\boldsymbol{\phi}(\boldsymbol{x}) = \left(\frac{1}{\sqrt{M}}\phi_{\boldsymbol{v}_1,b_1}(\boldsymbol{x}), \ldots, \frac{1}{\sqrt{M}}\phi_{\boldsymbol{v}_M,b_M}(\boldsymbol{x})\right)$ where each $(\boldsymbol{v}_j, b_j)$ is an independent sample drawn from the distribution described in the last question.

It satisfies the claimed equality since

$$\mathbb{E}\left[\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')\right] = \mathbb{E}\left[\frac{1}{M}\sum_{j=1}^{M}\phi_{\boldsymbol{v}_j,b_j}(\boldsymbol{x})\phi_{\boldsymbol{v}_j,b_j}(\boldsymbol{x}')\right] = \frac{1}{M}\sum_{j=1}^{M}k(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}'),$$

where the second step is by Eq. (5). It is a better approximation since using multiple independent samples reduces the variance (by a factor of $1/M$ precisely).

Quiz 1 Problem 5 (c)

(c) As discussed in Lecture 5, in RBF-kernelized linear regression with training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$, we maintain a weight vector $\boldsymbol{\alpha} = (\boldsymbol{K} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y} \in \mathbb{R}^N$, where $\boldsymbol{K} \in \mathbb{R}^{N\times N}$ is the Gram matrix (such that $K_{n,m} = k(\boldsymbol{x}_n, \boldsymbol{x}_m)$), $\lambda > 0$ is the regularization coefficient, and $\boldsymbol{y} = (y_1, \ldots, y_N)^{\mathrm{T}}$ is the response vector. For a test point $\boldsymbol{x}$, we make a prediction via $\sum_{n=1}^{N} \alpha_n k(\boldsymbol{x}_n, \boldsymbol{x})$. While powerful, this method can be computationally expensive when N is huge.

Based on the nonlinear mapping you proposed in the last question for M much smaller than N, describe how you can approximate the kernelized linear regression described above with a much better time and space complexity. You only need to describe what quantities your method maintains, and how it makes a prediction for a test point. (4 points)

The method is simply what we discussed in Lectures 2 and 5: maintain a weight vector $\boldsymbol{w}^* \in \mathbb{R}^M$ as:

$$\boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y},$$

where the n-th row of $\boldsymbol{\Phi} \in \mathbb{R}^{N\times M}$ is $\boldsymbol{\phi}(\boldsymbol{x}_n)^{\mathrm{T}}$. To make a prediction for a test point $\boldsymbol{x}$, simply compute $\boldsymbol{w}^{*\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$.

Reasoning (NOT required): First, this has better time and space complexity since M is assumed to be much smaller than N. Second, based on the discussion in Lecture 5, this is equivalent to kernelized linear regression with Gram matrix $\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}}$, which is a good approximation of $\boldsymbol{K}$ according to the last question.

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- Rahimi and Recht won NeurIPS 2017 Test of Time Award for this