Big Data Computing

Master's Degree in Computer Science

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Recap from Last Lecture

- Decision Trees (DTs) highly expressive yet interpretable models both for regression and classification
- Learning the optimal DT is NP-Complete: Recursive Binary Splitting algorithm is an effective greedy training heuristic
- Regression Trees:
  - Use Residual Sum of Squares (RSS) as splitting criterion
  - At inference time, predictions are the mean of the leaf observations

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Classification Trees

- Very similar to a regression tree
- Used to predict a categorical response rather than a numerical one
- Tree building is still based on Recursive Binary Splitting algorithm but RSS cannot be used as a criterion for splitting nodes
- A natural alternative to RSS minimization is to minimize the "impurity"
- The predicted label of a test instance is the most frequent label (mode) of the instances belonging to the region where it falls

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- Several different measures to represent this notion of node "impurity":
  - Classification Error Rate
  - Gini Index
  - Entropy
- It is often convenient to refer to the information gain of a split

Classification Trees: Notation

Subset of training instances falling into region R

$$\mathcal{D}_R = \mathcal{D} \cap R = \{(\mathbf{x}_i, y_i) \in \mathcal{D} \mid \mathbf{x}_i \in R\}$$

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(*f*, *s*)-split

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$$IG(\mathcal{D}_R, f, s) = \underbrace{I(\mathcal{D}_R)}_{\text{parent node's impurity}} - \underbrace{\left[\frac{|\mathcal{D}_{R_{\text{left}}(f,s)}|}{|\mathcal{D}_R|} I(\mathcal{D}_{R_{\text{left}}(f,s)}) + \frac{|\mathcal{D}_{R_{\text{right}}(f,s)}|}{|\mathcal{D}_R|} I(\mathcal{D}_{R_{\text{right}}(f,s)})\right]}_{\text{children nodes' impurity}}$$

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- Other 2 measures are preferable: Gini Index and Entropy

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- Measures the variance across the K classes

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- A small value indicates that a node contains predominantly observations from a single class

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- Alternative, yet similar to Gini

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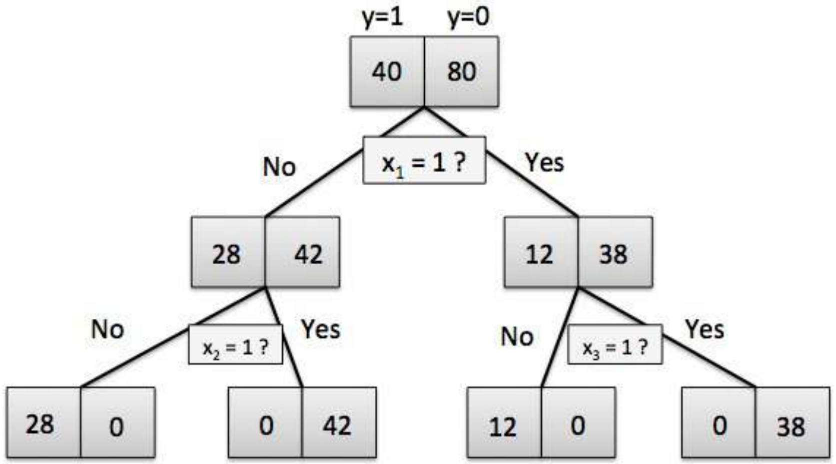
- Like Gini, a small value of entropy is obtained whenever all the proportions are either close to 1 or to 0
- In practice, both entropy and Gini can be used to grow a tree

Classification Error Rate vs. Entropy (Gini)

Consider this decision tree which perfectly separates positive ($y=1$) from negative ($y=0$) samples using 3 splits on 3 binary features x_1, x_2, x_3



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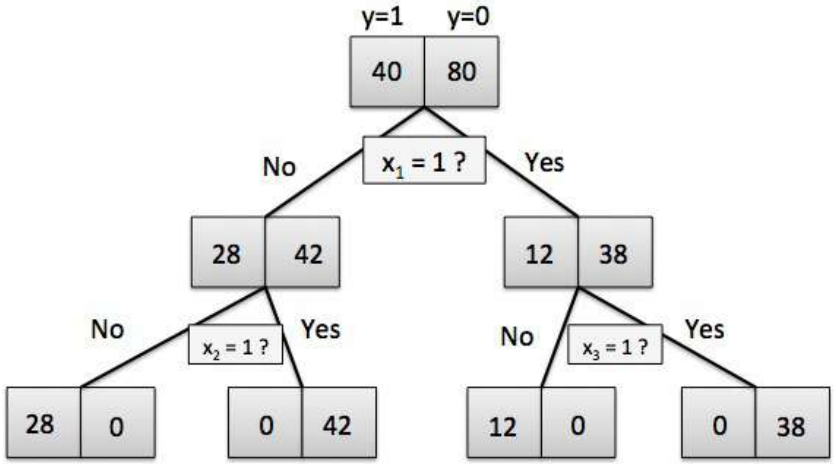
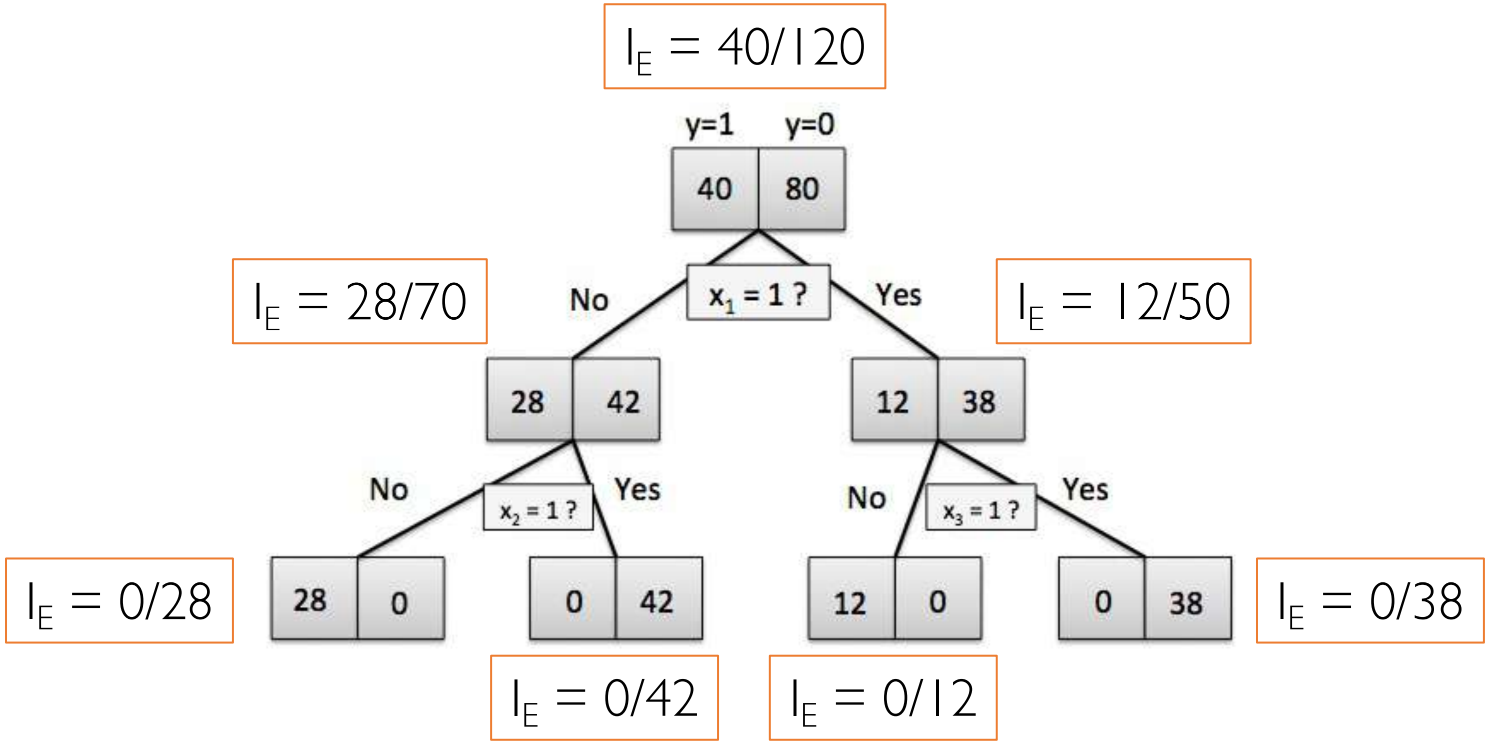


Question

Would we be able to learn the tree above using classification error rate as splitting criterion?

Classification Error Rate vs. Entropy (Gini)

Node impurity using I_E

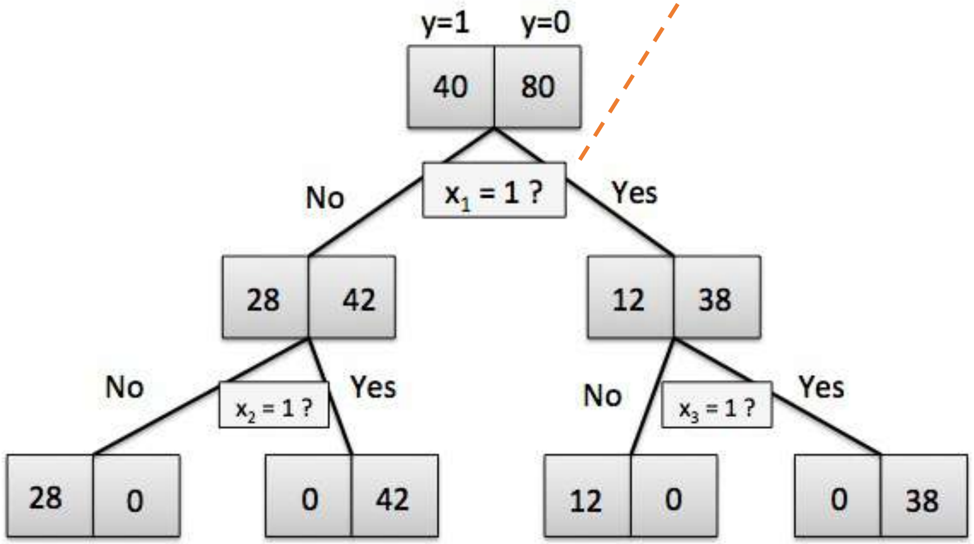


source: https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html

Classification Error Rate vs. Entropy (Gini)

Compute IG of the first split using I_E

$I_E = 40/120$



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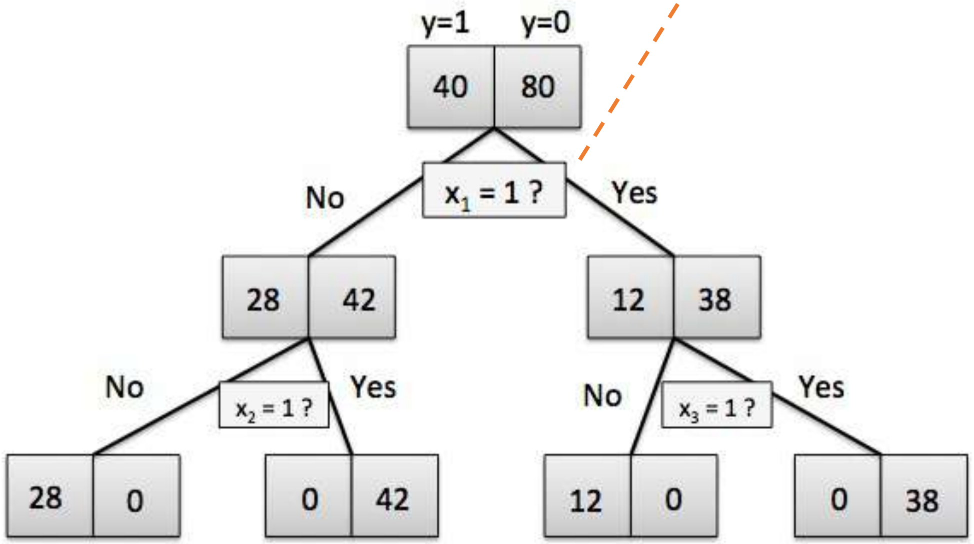

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$40/120 - [(70/120 * 28/70) + (50/120 * 12/50)]$

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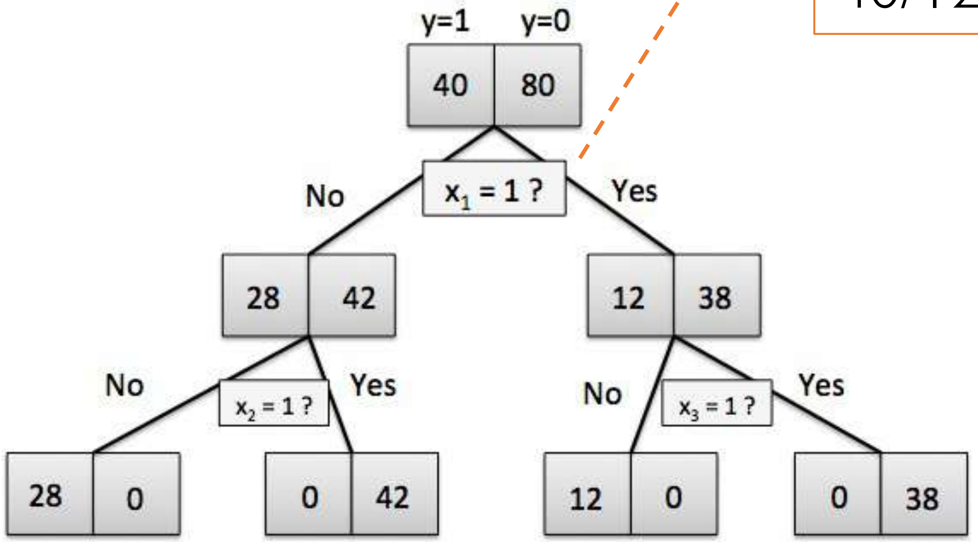

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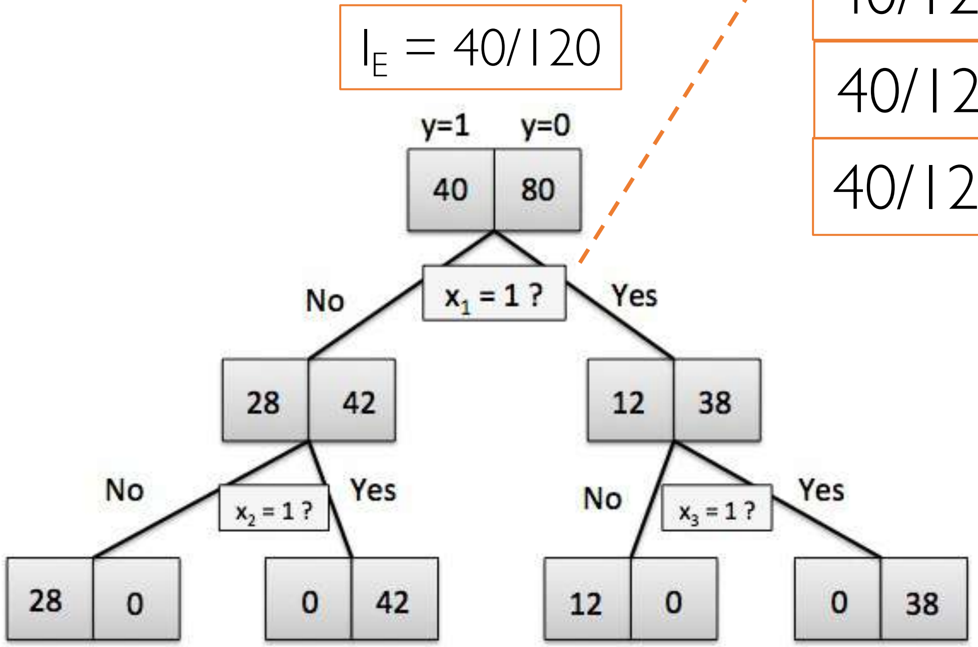

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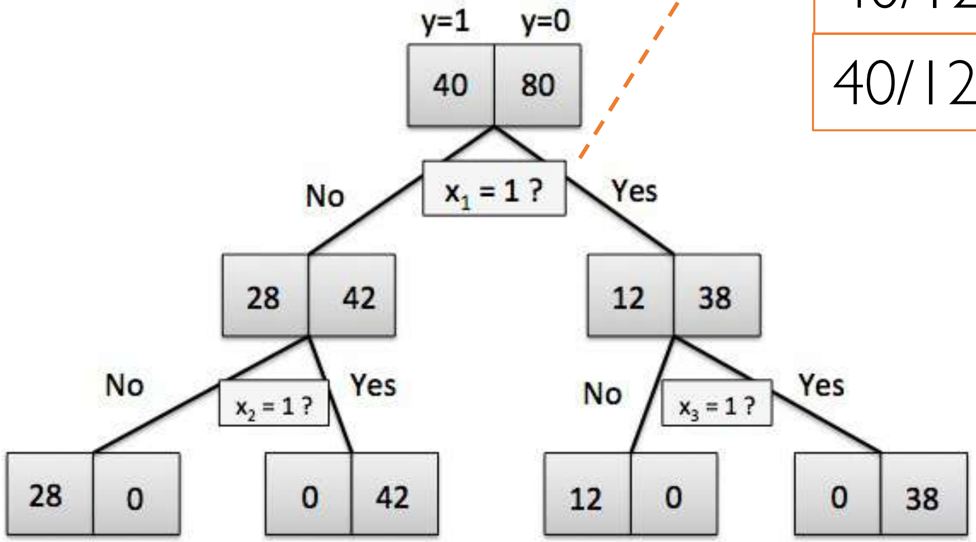

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the sum of I_E of the 2 child nodes is equal to that of the parent (40/120)

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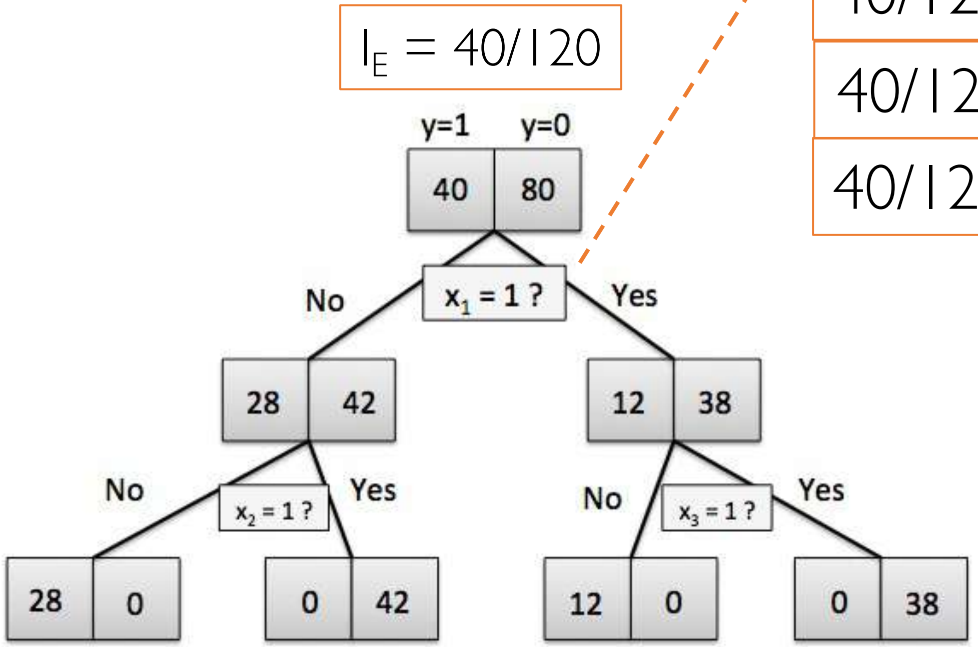

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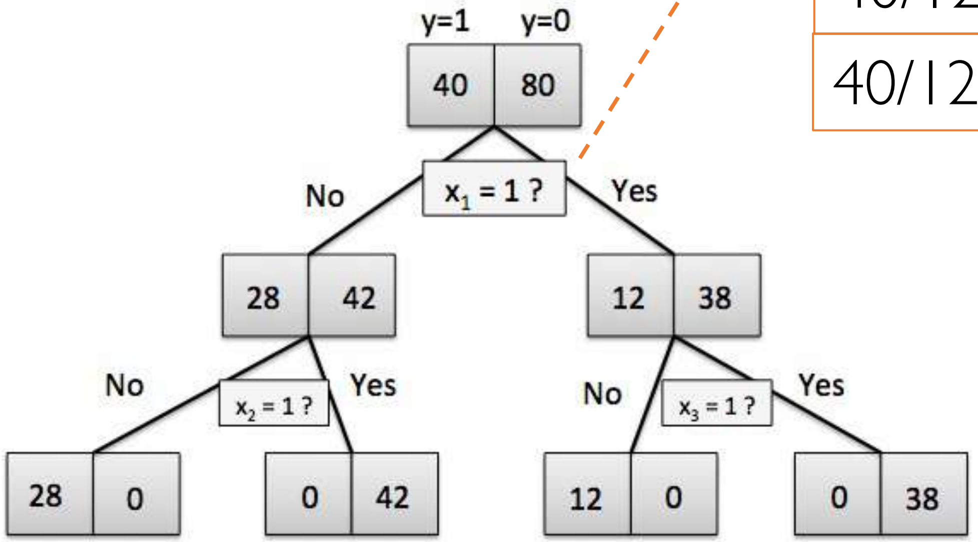

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The tree learning algorithm would stop at this point

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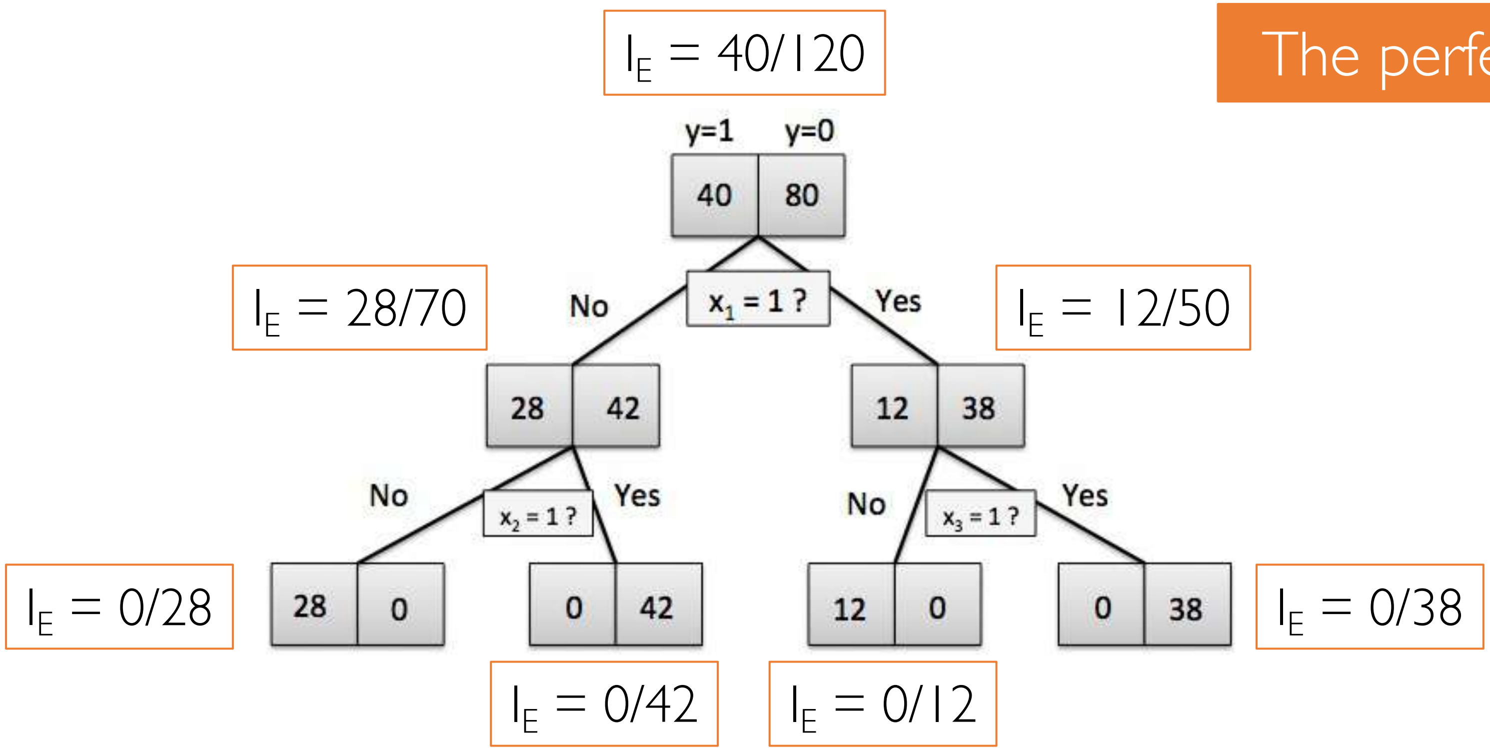

The perfect tree cannot be built using I_E

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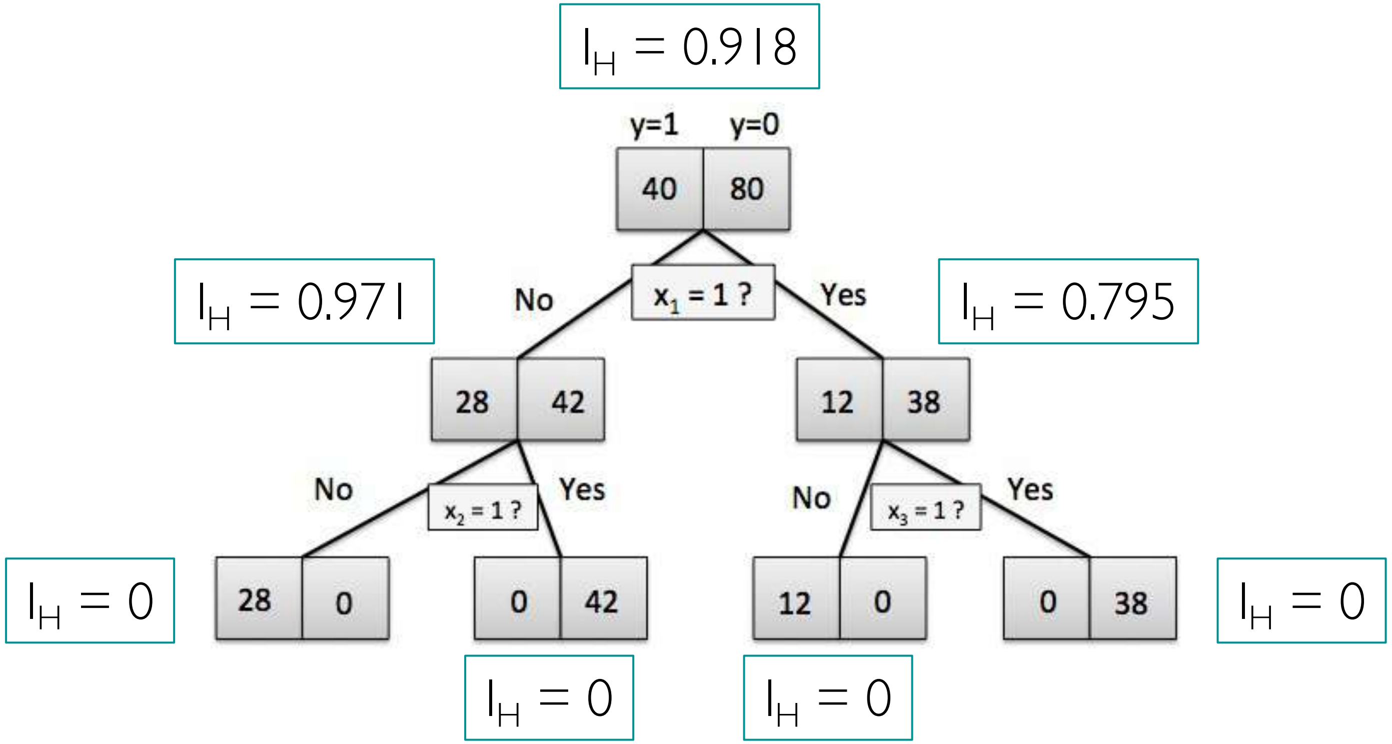
Classification Error Rate vs. Entropy (Gini)

Node impurity using I_H



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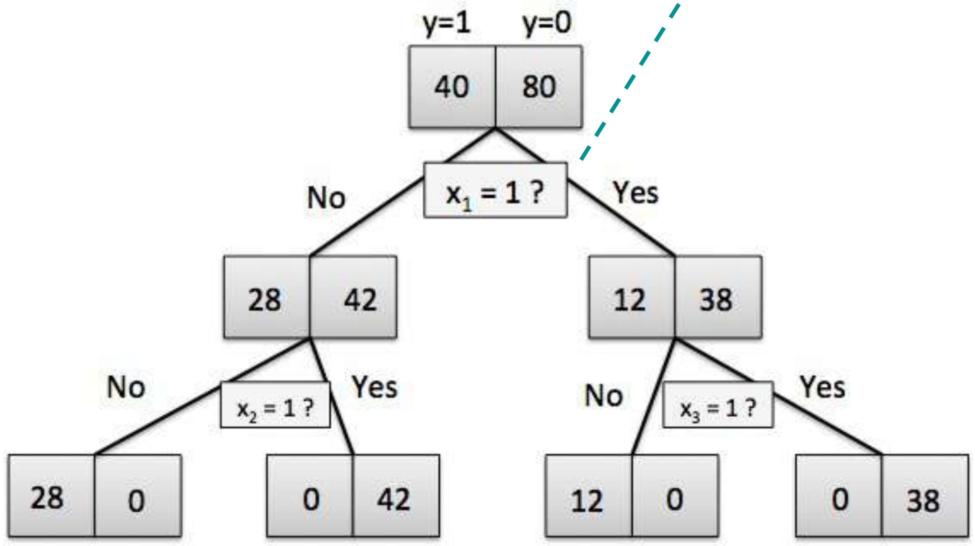
Classification Error Rate vs. Entropy (Gini)

Compute IG of the first split using I_H

$I_H = 0.918$



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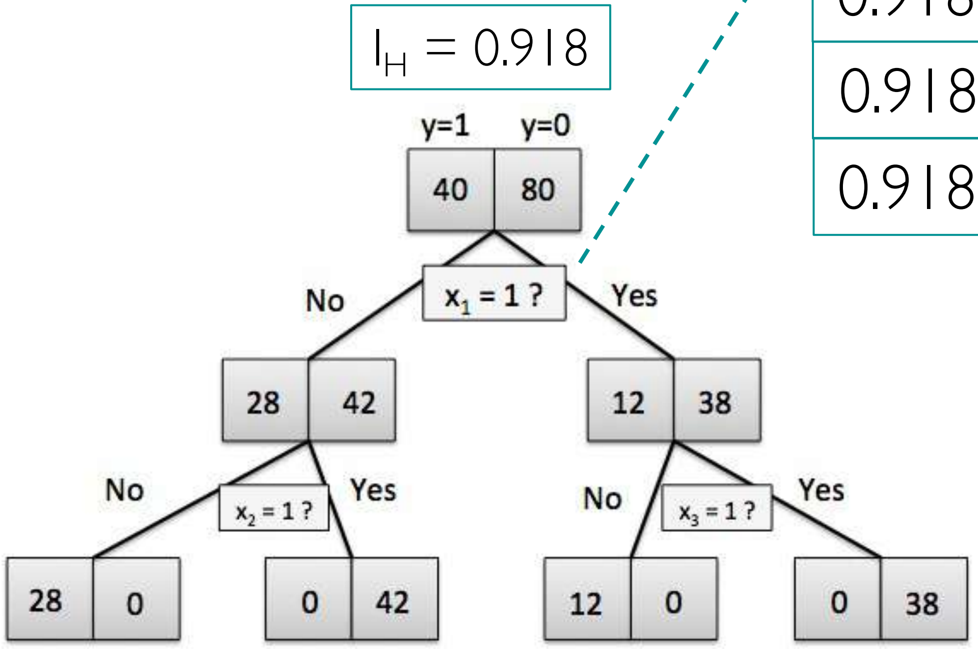

Compute IG of the first split using I_H

0.918 - [(70/120 * 0.971) + (50/120 * 0.795)]

0.918 - [0.566 + 0.331]

0.918 - 0.897 = 0.021

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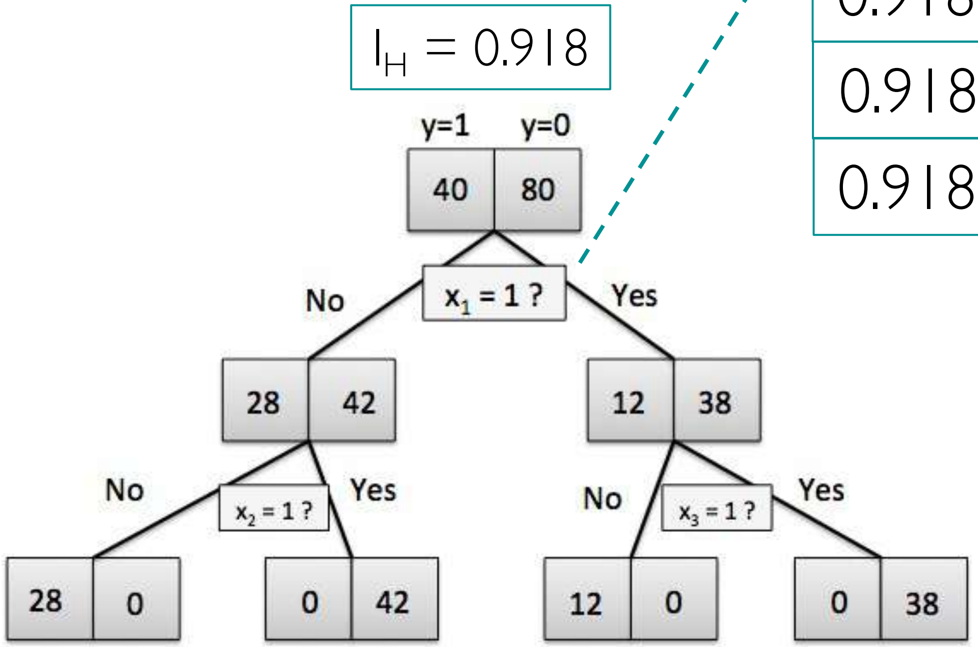

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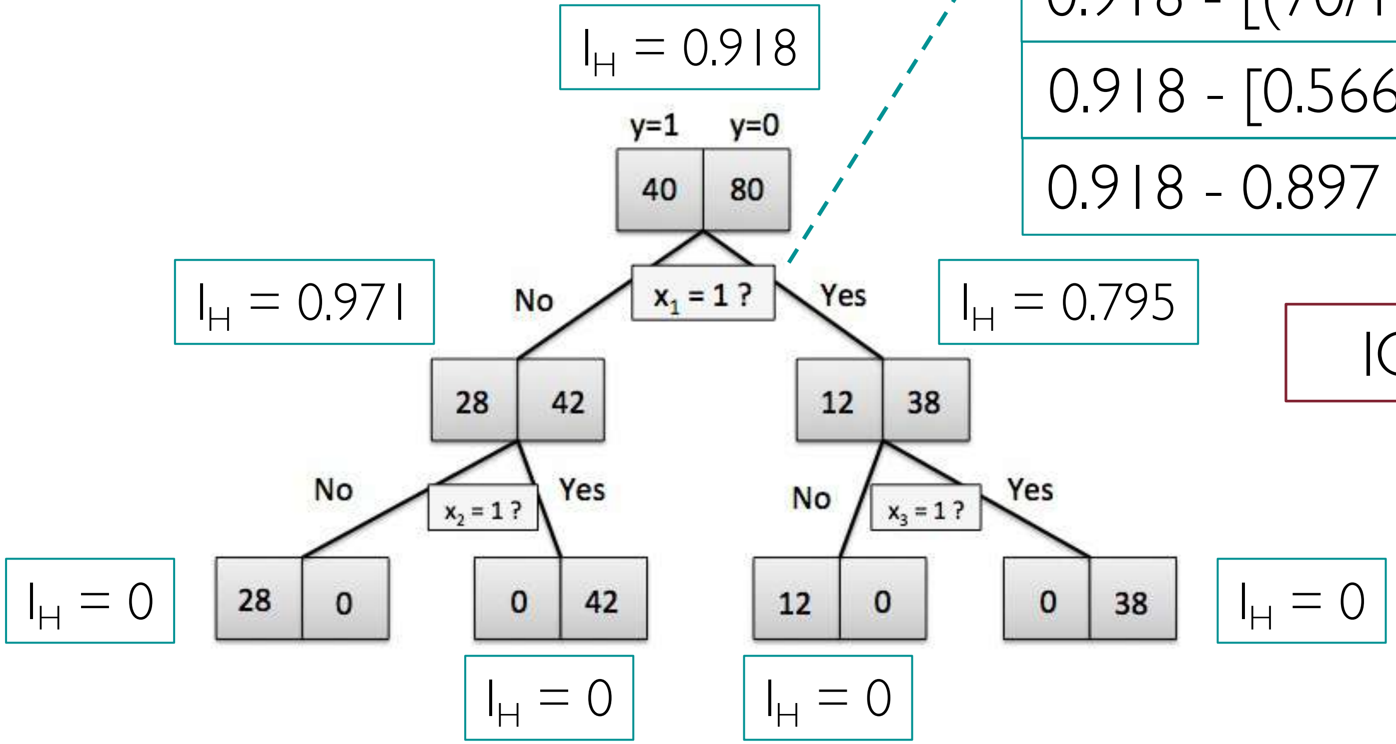

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The splitting rule would continue until the child nodes are pure

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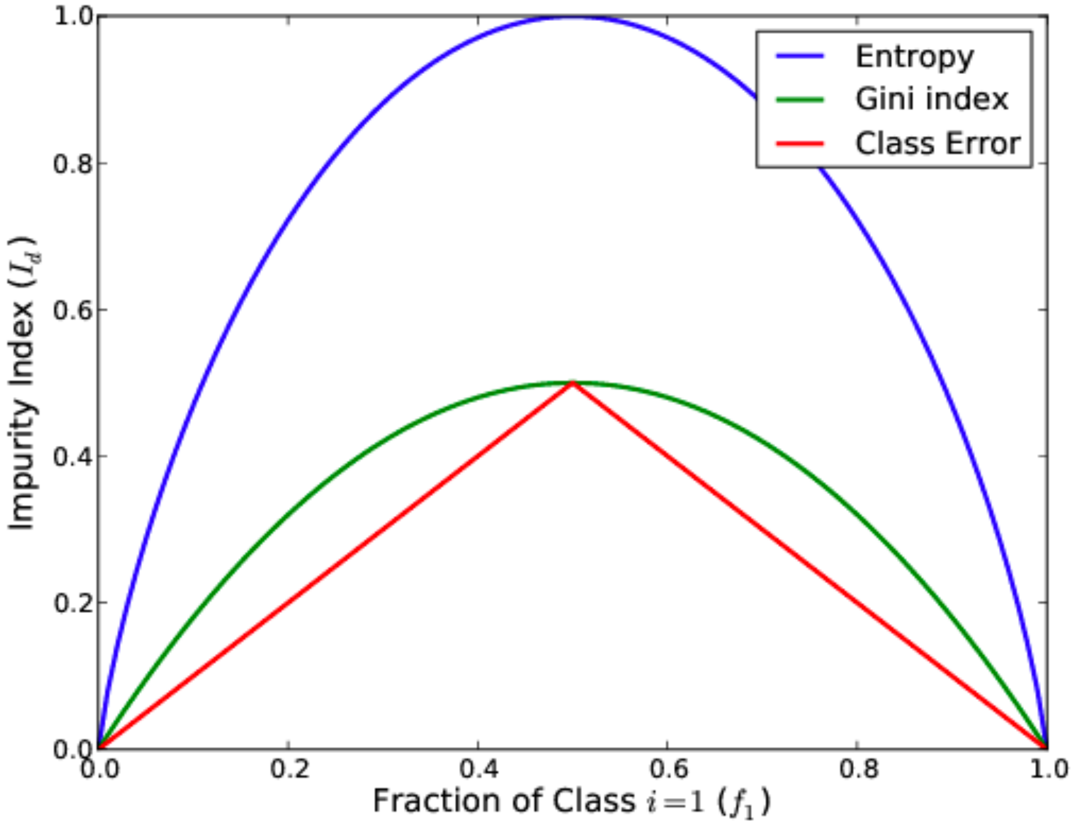

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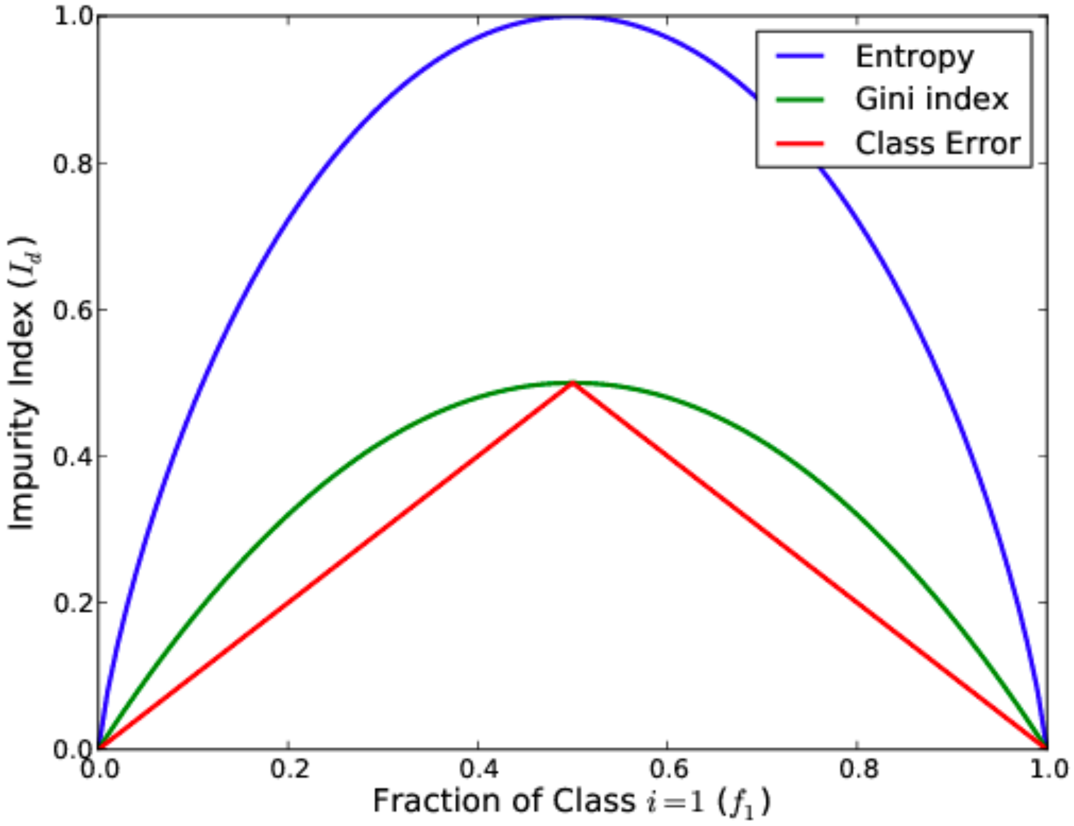

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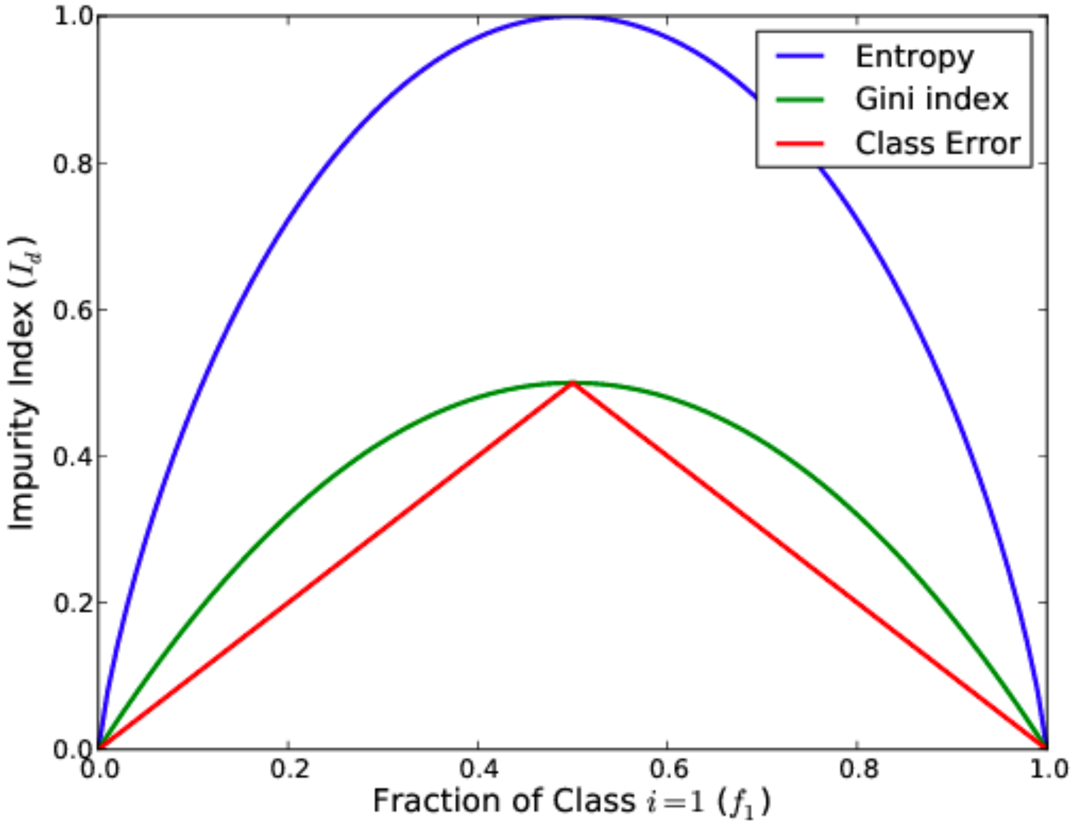

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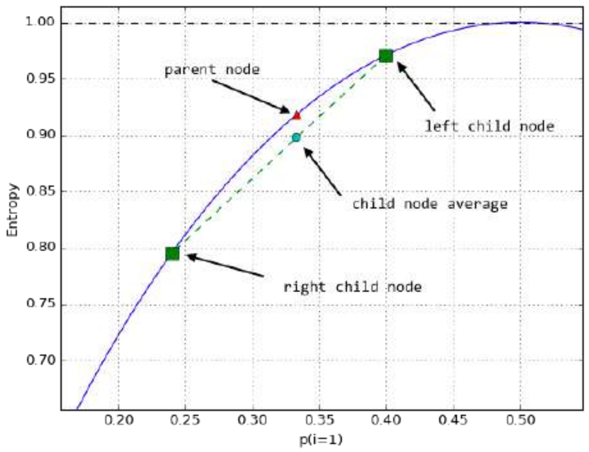

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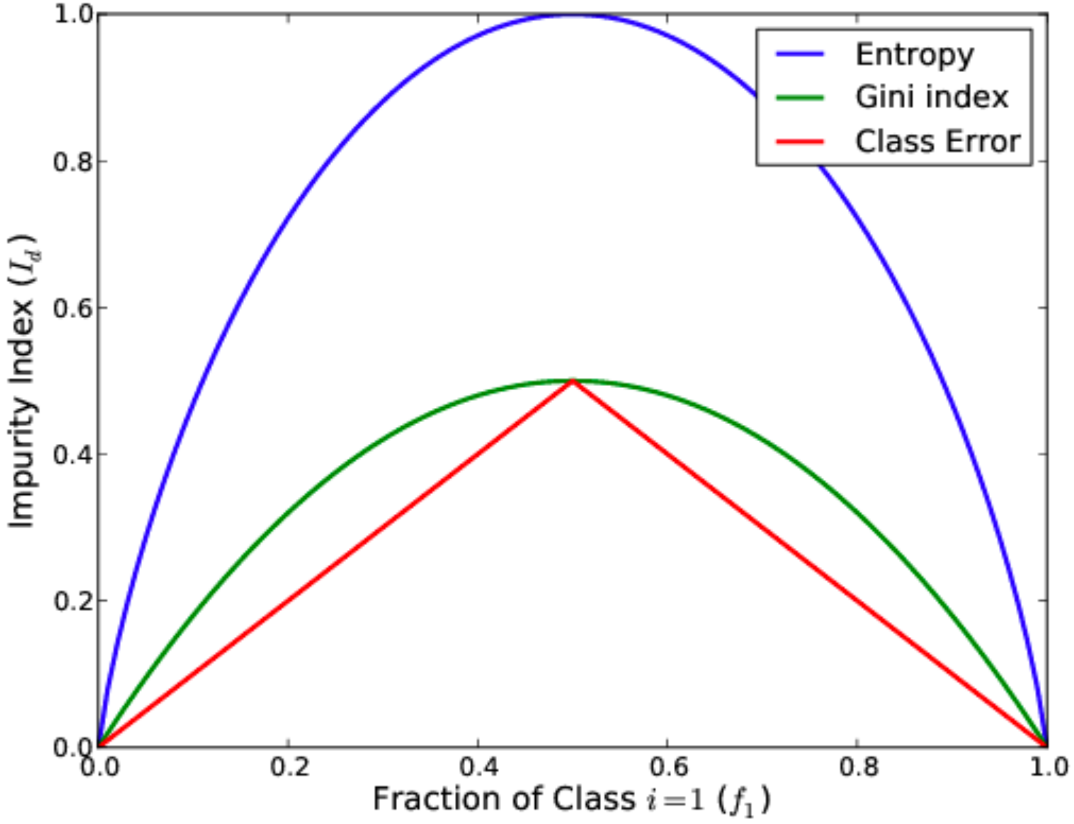

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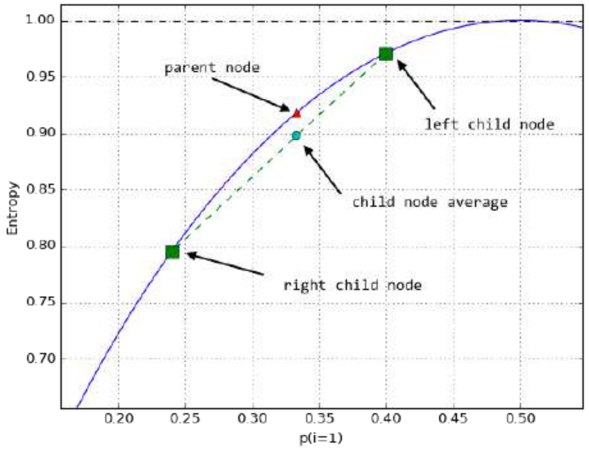

If the parent's entropy sits between children's entropy, it will always be larger than the weighted averaged children's entropy due to its "bell shape"

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- We define the ratio $p = N^+/N$ and $q = N^-/N$
- The entropy is defined as:

$$H = -\Big[p\log_2(p) + q\log_2(q)\Big] = -\frac{N^+}{N}\log_2\left(\frac{N^+}{N}\right) - \frac{N^-}{N}\log_2\left(\frac{N^-}{N}\right)$$

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- H is maximum (i.e., H=1) when N^+ = N^- = N/2
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Since each x_i takes on a binary value (K=2), H ranges in [0, 1], in general it ranges in [0, +infinity]

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- The worst split will occur if the two resulting children nodes will both contain half +/half - examples
  - In such a case, each child node will still have entropy = 1
- To account for the number of elements, the weighted average of children entropies are computed

$$H_{\text{split}} = \frac{N_{\text{left}}}{N} H_{\text{left}} + \frac{N_{\text{right}}}{N} H_{\text{right}}$$

Evolution of Entropy in Tree Splitting

- Suppose we start with a node whose entropy is 1 (half +/half -)
- The worst split will occur if the two resulting children nodes will both contain half +/half - examples
  - In such a case, each child node will still have entropy = 1
- To account for the number of elements, the weighted average of children entropies are computed

splitting can't do worst!

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Linear Models vs. Decision Trees

Linear Models

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \theta_0 + \sum_{i=1}^{n} \theta_i x_i$$

Decision Trees

$$h(\mathbf{x}) = \sum_{j=1}^{J} c_j \cdot \mathbf{1}_{R_j}(\mathbf{x})$$

Learned hypothesis is constant within a region

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If there is a strong linear relationship between input and output

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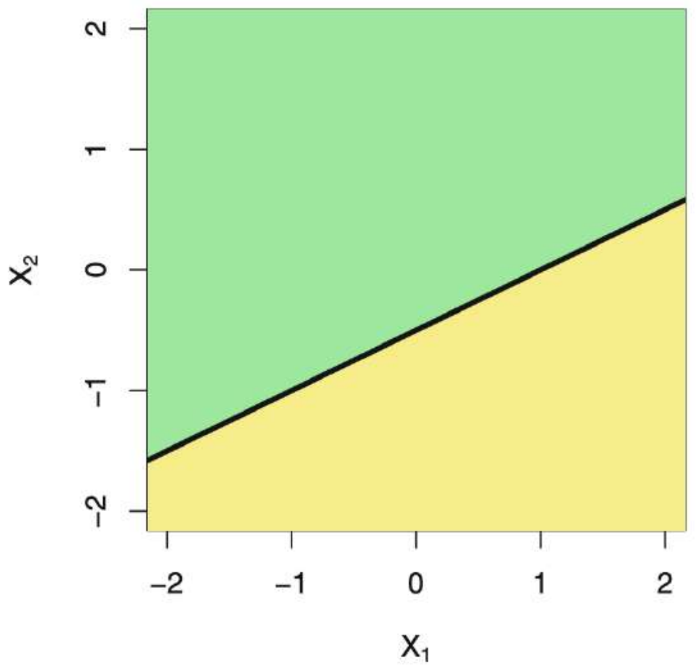
Which one is better?

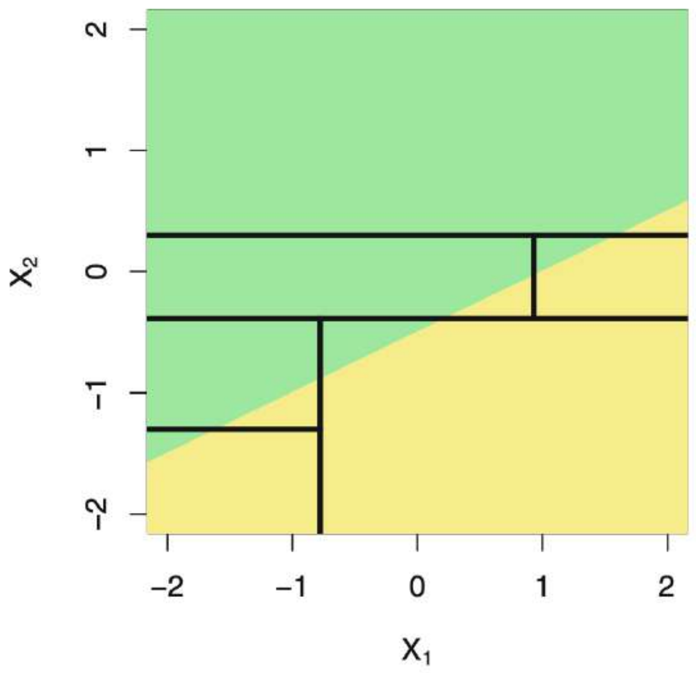
If there is a highly non-linear relationship between input and output

Linear Models vs. Decision Trees: Example

Linear Regression



Decision Tree



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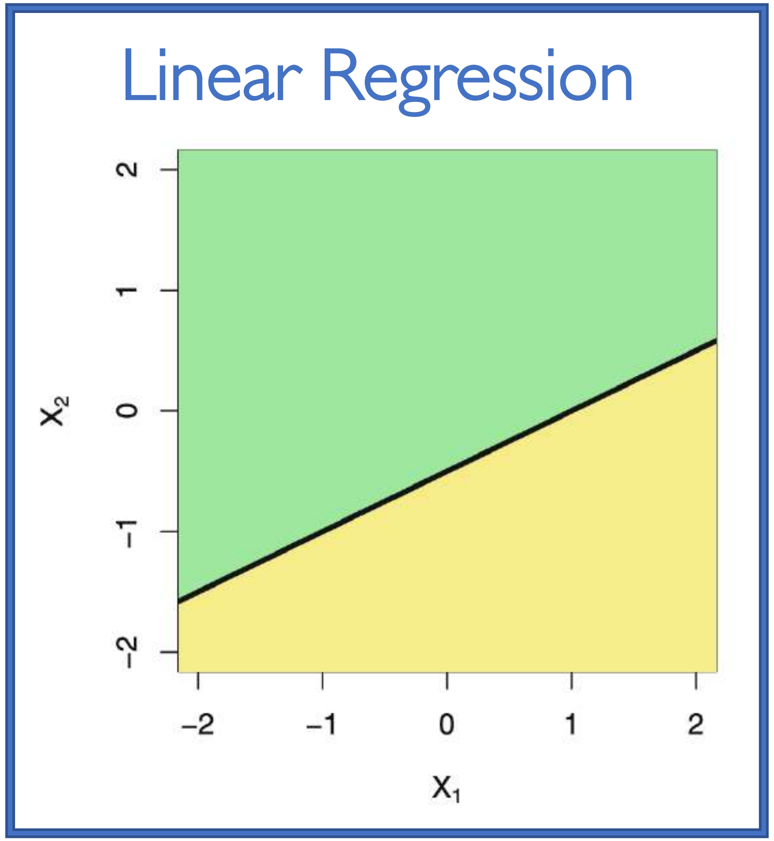

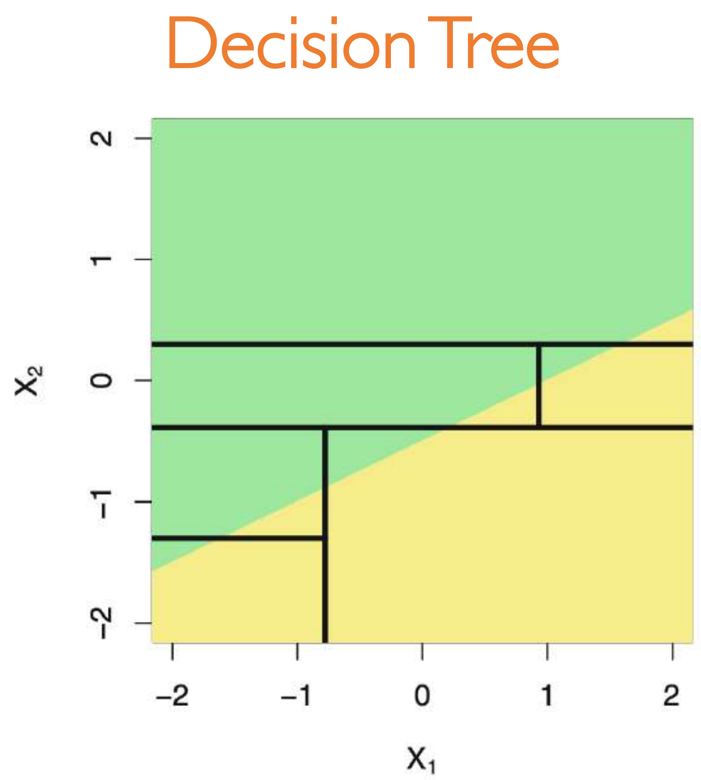

Nice linear decision boundary

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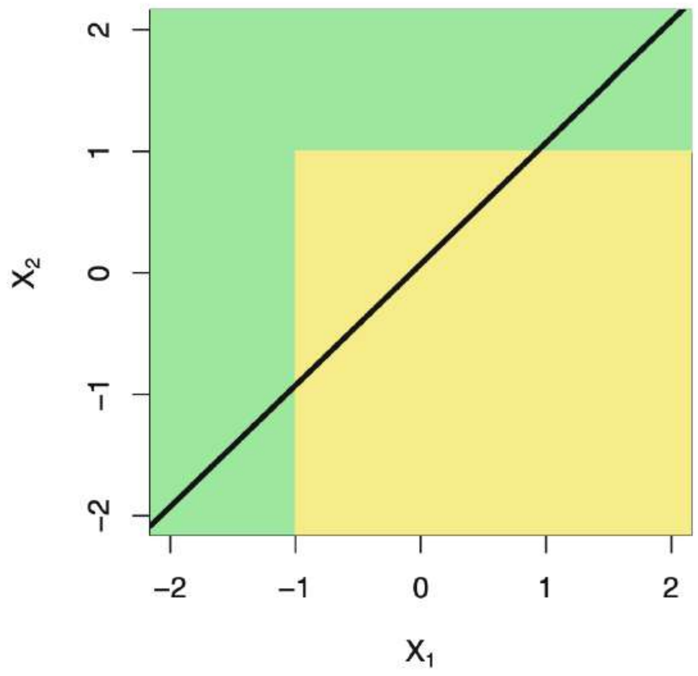

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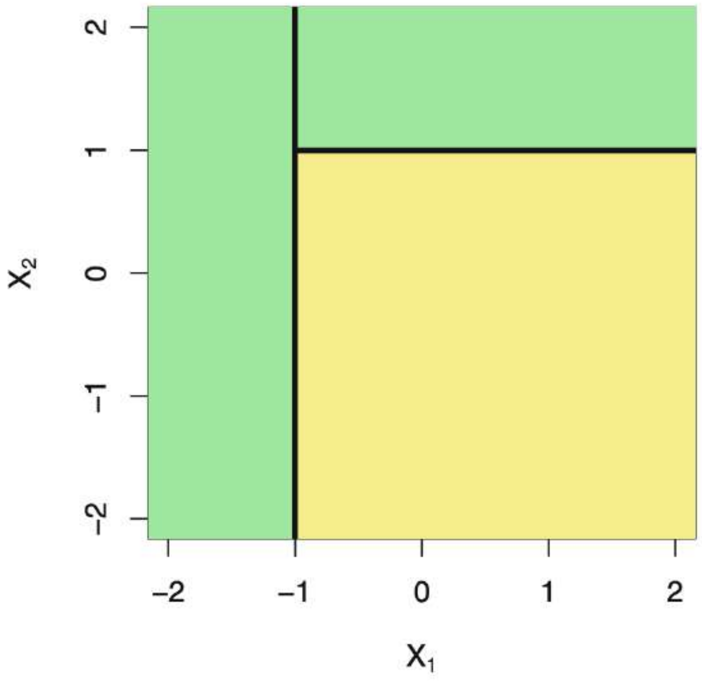

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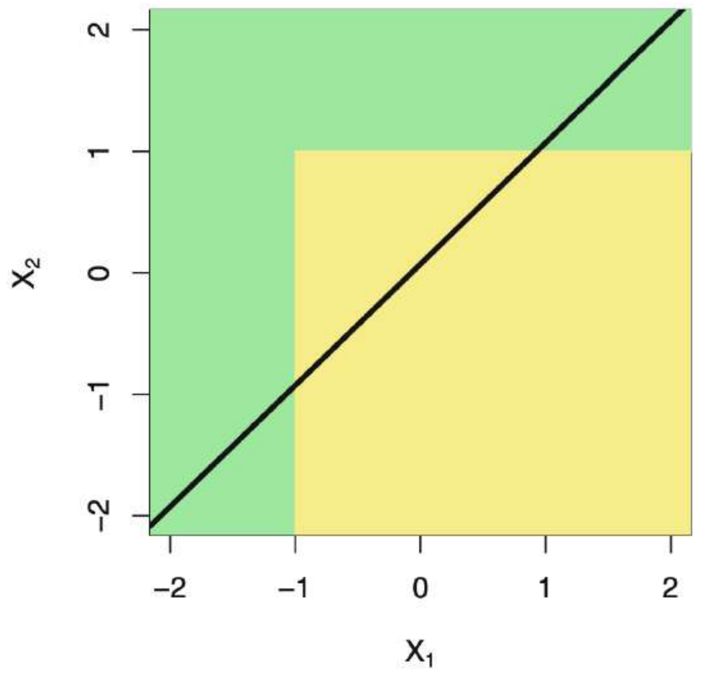

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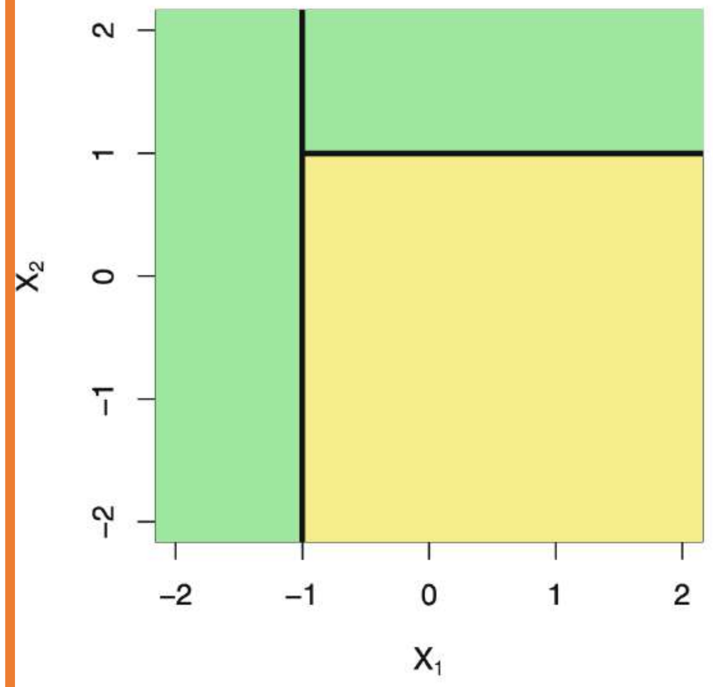

Non-linear decision boundary

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Intuitively, by selecting the subtree with the smalles test error!

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Cost Complexity Pruning (a.k.a. Weakest Link Pruning)

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- We can select a value of α using a validation set or cross-validation

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- Trees can easily handle categorical features without the need to create dummy variables (i.e., one-hot encoding)

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Bagging | Random Forest | Boosting

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- Low-variance approaches, instead, are less sensitive to different training sets
- Bootstrap aggregation (Bagging) is a general-purpose method to lower the variance of a statistical learning method

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Averaging a set of observations reduces variance!

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Bootstrap

Taking repeated samples from the same training set

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Generate B different bootstrapped samples from the original training set

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$$\boxed{h_{\text{bagging}}(\mathbf{x}) = \frac{1}{B}\sum_{b=1}^{B} h^{b*}(\mathbf{x})}$$

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- It can be used in combination with *any* model
- When used with classification trees the final prediction is typically obtained via majority voting
  - The overall prediction is just the most common across the B models

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- Still, one can obtain an overall summary of the importance of each feature using RSS (regression) or Gini index/Entropy (classification)
- Add up the total RSS/Gini index reduction obtained splitting on a certain feature and take the average over all the B trees

Tree Ensemble: Random Forests

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- Each split is allowed to use only one of those k features

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- This may sound crazy, but it has a clever rationale

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Lower variance reduction

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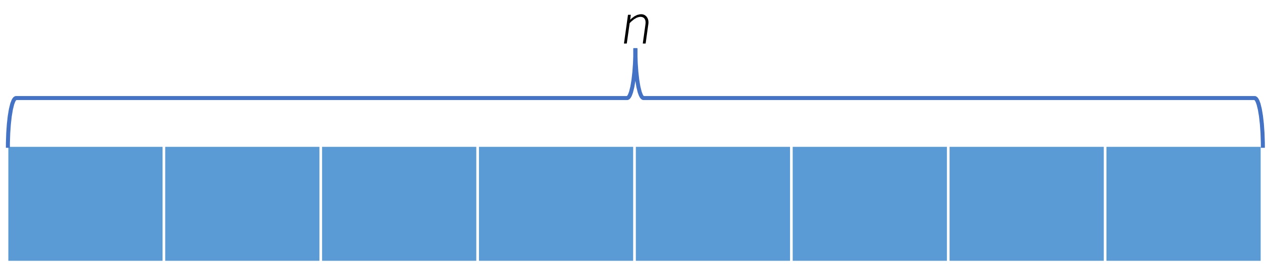
- As with bagging, random forests will not overfit if we increase B

Why k/n?



Randomly choose k features out of n, each with uniform probability $p = 1/n$

What is the probability that the highly predictive feature f is contained in the k-sized random sample?

Why *k*/*n*? – Approach 1.a.

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$$\textbf{OR} \left[P(f \text{ is } \textbf{NOT} \text{ extracted as 1st } \textbf{AND } \dots \textbf{ AND } f \text{ is } \textbf{NOT} \text{ extracted as } k-1\text{-th } \textbf{AND } f \text{ is extracted as } k\text{-th})\right]$$

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Why *k/n*? – Approach 1.b.

It might be easier to compute the following:

$$1 - P(f \text{ is } \textbf{NOT} \text{ extracted as 1st } \textbf{AND } f \text{ is } \textbf{NOT} \text{ extracted as 2nd } \textbf{AND } \dots \textbf{ AND } f \text{ is } \textbf{NOT} \text{ extracted as } k\text{-th})$$

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$$\boxed{1 - \frac{n-k}{n} = \frac{k}{n}}$$

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Combinations of *k* out of *n* elements "*n choose k*"

$$= \frac{\frac{(n-1)!}{(k-1)!(n-1-(k-1))!}}{\frac{n!}{k!(n-k)!}} = \frac{(n-1)!}{(k-1)!(n-k)!} * \frac{k!(n-k)!}{n!} = \boxed{\frac{k}{n}}$$

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Tree Ensemble: Boosting

- Again, general approach that can be applied to many statistical learning methods for regression or classification
- In bagging, each tree is built on a bootstrap data set, independent of the other trees
- Boosting works in a similar way, except that the trees are grown sequentially using information from previously grown trees
- Boosting does not involve bootstrap sampling; instead each tree is fit on a modified version of the original data set

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- Unlike fitting a single large decision tree to the data, potentially leading to overfitting, the boosting approach instead learns slowly
- Consider boosting regression trees:
  1. Fit the tree to the current residuals rather than the actual response Y
  2. Add this new decision tree into the fitted function so as to update the residuals
  3. Each of these trees can be rather small, with just a few terminal nodes, determined by a model's hyperparameter (d)
  4. The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals

Boosting: Algorithm

Algorithm 8.2 *Boosting for Regression Trees*

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   (a) Fit a tree $\hat{f}^b$ with d splits ($d+1$ terminal nodes) to the training data (X, r).
   (b) Update $\hat{f}$ by adding in a shrunken version of the new tree:
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x). \tag{8.10}$$
   (c) Update the residuals,
   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i). \tag{8.11}$$
3. Output the boosted model,
   $$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x). \tag{8.12}$$

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- Boosting has 3 tuning hyperparameters:
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- Tuning done via validation or cross-validation

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- Decision Trees (DTs) highly expressive yet interpretable models both for regression and classification

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- Decision Trees (DTs) highly expressive yet interpretable models both for regression and classification
- Learning the optimal DT is NP-Complete: Recursive Binary Splitting algorithm is an effective greedy heuristic
- DTs tend to overfit and have a low prediction accuracy
- Pruning and Ensembling techniques overcome both issues