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# Large-Scale Machine Learning (1): Decision Trees

CS246: Mining Massive Datasets  
Jure Leskovec, Stanford University  
<http://cs246.stanford.edu>



# New Topic: ML!

## High dim. data

Locality  
sensitive  
hashing

Clustering

Dimensional  
ity  
reduction

## Graph data

PageRank,  
SimRank

Community  
Detection

Spam  
Detection

## Infinite data

Filtering  
data  
streams

Web  
advertising

Queries on  
streams

## Machine learning

Decision  
Trees

Random  
Forest,  
GBDT

Neural  
Networks,  
GNNs

## Apps

Recommen  
der systems

Association  
Rules

Duplicate  
document  
detection

# Supervised Learning

## Given some data:

- “Learn” a function to map from the **input** to the **output**

- **Given:**

Training examples  $(x_i, y_i = f(x_i))$  for some unknown function  $f$

- **Find:**

A good approximation to  $f$

# Many Other ML Paradigms

- **Supervised:**

- Given “labeled data”  $\{x, y\}$ , learn  $f(x) = y$

- **Unsupervised:**

- Given only “unlabeled data”  $\{x\}$ , learn  $f(x)$

- **Semi-supervised:**

- Given some labeled  $\{x, y\}$  and some unlabeled data  $\{x\}$ , learn  $f(x) = y$

- **Active learning:**

- When we predict  $f(x) = y$ , we then receive true  $y^*$

- **Transfer learning:**

- Learn  $f(x)$  so that it works well on new domain  $f(z)$

# Supervised Learning

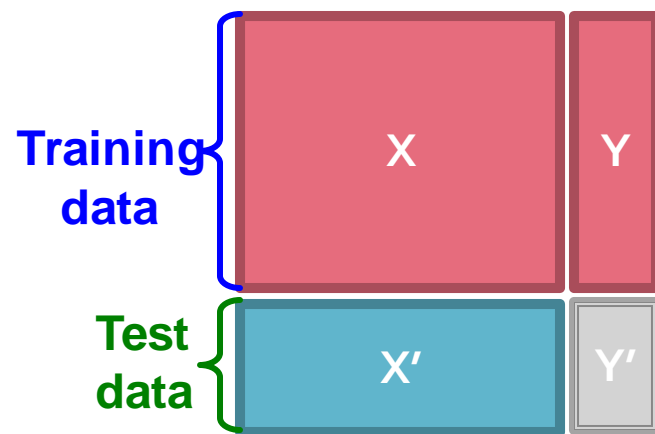
- Would like to do **prediction**:  
**estimate** a function  $f(x)$  so that  $y = f(x)$
- Where  $y$  can be:
  - **Real number**: Regression
  - **Categorical**: Classification
  - **Complex object**:
    - Ranking of items, Parse tree, etc.
- Data is **labeled**:
  - Have many pairs  $\{(x, y)\}$ 
    - $x$  ... vector of binary, categorical, real valued features
    - $y$  ... class, or a real number

# Supervised Learning

- **Task:** Given data  $(X, Y)$  build a model  $f()$  to predict  $Y'$  based on  $X'$

- **Strategy:** Estimate  $y = f(x)$  on  $(X, Y)$

Hope that the same  $f(x)$  also works to predict unknown  $Y'$



- The “hope” is called **generalization**
  - **Overfitting:** If  $f(x)$  predicts well  $Y$  but is unable to predict  $Y'$
- **We want to build a model that generalizes well to unseen data**

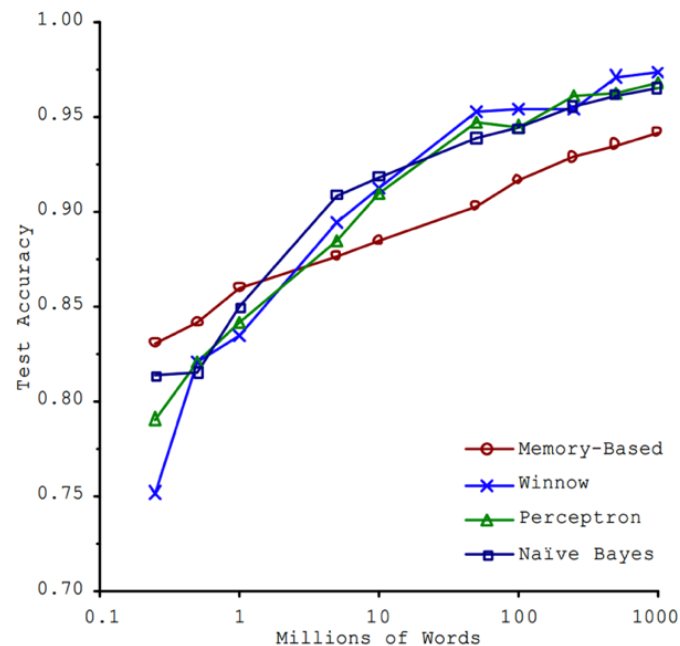
# Why Large-Scale ML?

## ■ Brawn or Brains?

- In 2001, Microsoft researchers ran a test to evaluate 4 of different approaches to ML-based language translation

## ■ Findings:

- **Size of the dataset** used to train the model **mattered more** than the model itself
- As the dataset grew large, **performance difference between the models became small**



Banko, M. and Brill, E. (2001), "[Scaling to Very Very Large Corpora for Natural Language Disambiguation](#)"

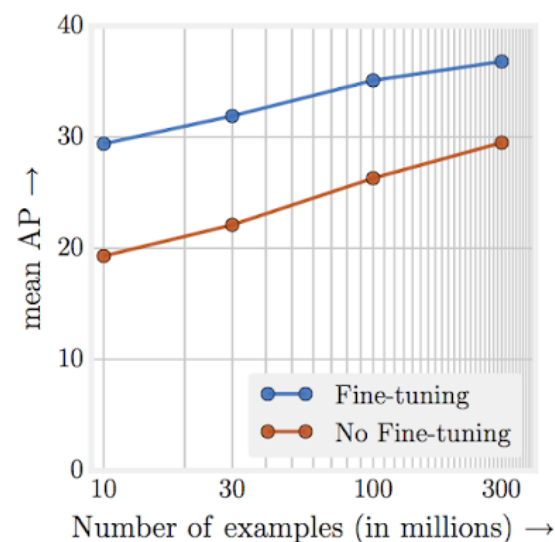
# Why Large-Scale ML?

## ■ The Unreasonable Effectiveness of Data

- In 2017, Google revisited the same type of experiment with the latest Deep Learning models in computer vision

## ■ Findings:

- Performance increases logarithmically based on volume of training data
- Complexity of modern ML models (i.e., deep neural nets) allows for even further performance gains



## ■ Large datasets + large ML models => amazing results!!

“Revisiting Unreasonable Effectiveness of Data in Deep Learning Era”: <https://arxiv.org/abs/1707.02968>



# Why Worry About Non-Deep Models?

## A few reasons why this is important:

- Classical tasks in NLP and Vision are getting commoditized (you take pretrained model and fine tune it), but there are many other unique ML tasks.
- Deep models are often hard to scale and require lots and lots of data. Traditional models allow you to encode prior knowledge better and give you more control.
- Personally, if I am working on a well understood problem I'd use deep learning, but if I am the first person to work on a new problem/classifier I'd use techniques we'll discuss here.

# Decision Trees, Random Forests and GBDTs

# Preface: Decision Trees

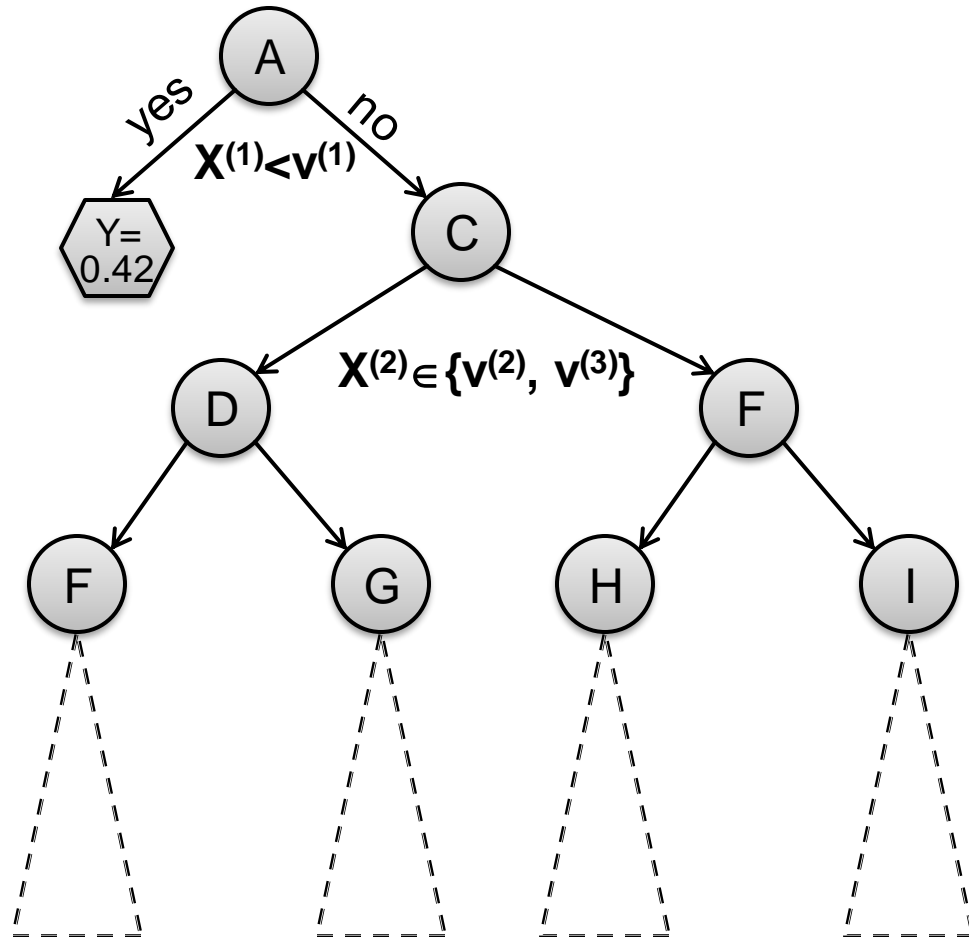
- **Decision trees are part of ML since 1980s**
  - Introduced by Leo Breiman in 1984
  - Notable algorithms: ID3, C4.5
- **More recent innovations include:**
  - Boosted decision trees (gradient boosted DT)
  - Random forest
- Even though DTs are old, hand-engineered and heuristic, they are a method of choice for tabular data and for Kaggle competitions. 😊

# Decision Tree Learning

- Given one attribute (e.g., lifespan), try to predict the value of new people's lifespans by means of some of the other available attribute
- **Input attributes:**
  - $d$  features/attributes:  $x^{(1)}, x^{(2)}, \dots, x^{(d)}$
  - Each  $x^{(j)}$  has **domain**  $O_j$ 
    - **Categorical:**  $O_j = \{red, blue\}$
    - **Numerical:**  $H_j = (0, 10)$
  - $Y$  is output variable with domain  $O_Y$ :
    - **Categorical:** Classification, **Numerical:** Regression
- **Data D:**
  - $n$  examples  $(x_i, y_i)$  where  $x_i$  is a  $d$ -dim feature vector,  $y_i \in O_Y$  is output variable
- **Task:**
  - Given an input data vector  $x$  predict output label  $y$

# Decision Trees

- A **Decision Tree** is a tree-structured plan of a set of attributes to test in order to predict the output



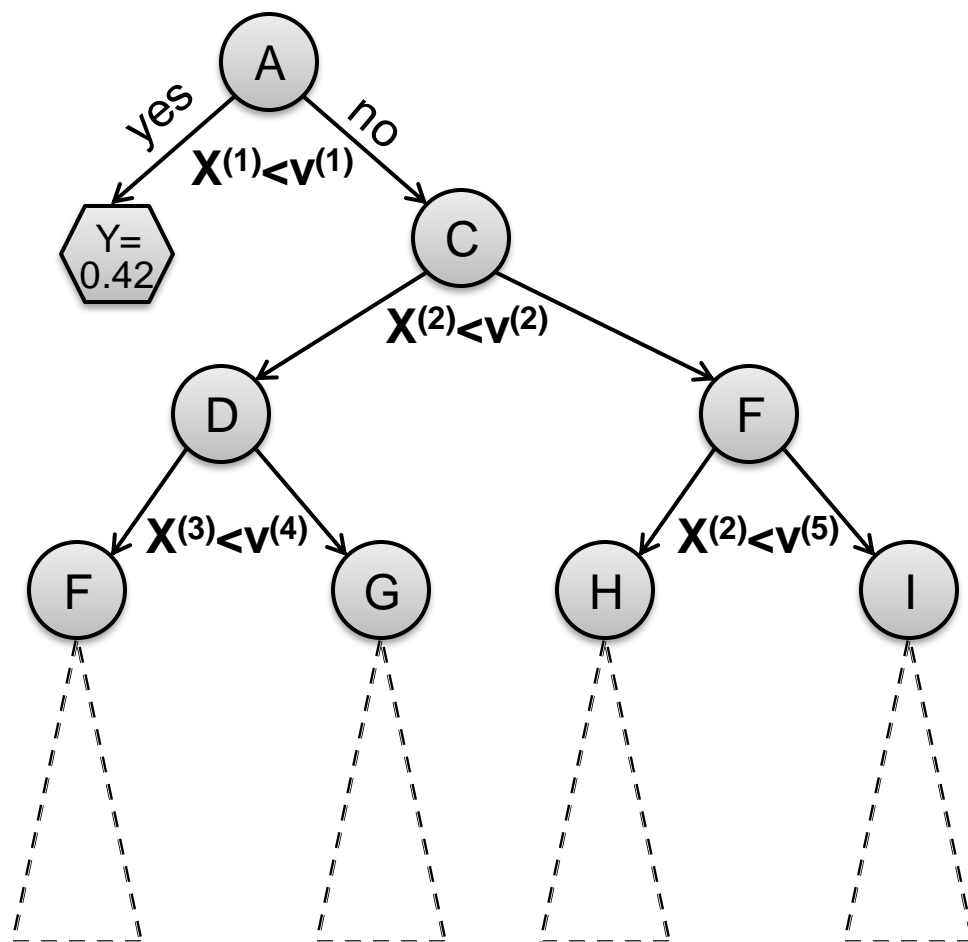
# Decision Trees

## ■ Decision trees:

- Split the data at each internal node
- Each leaf node makes a prediction

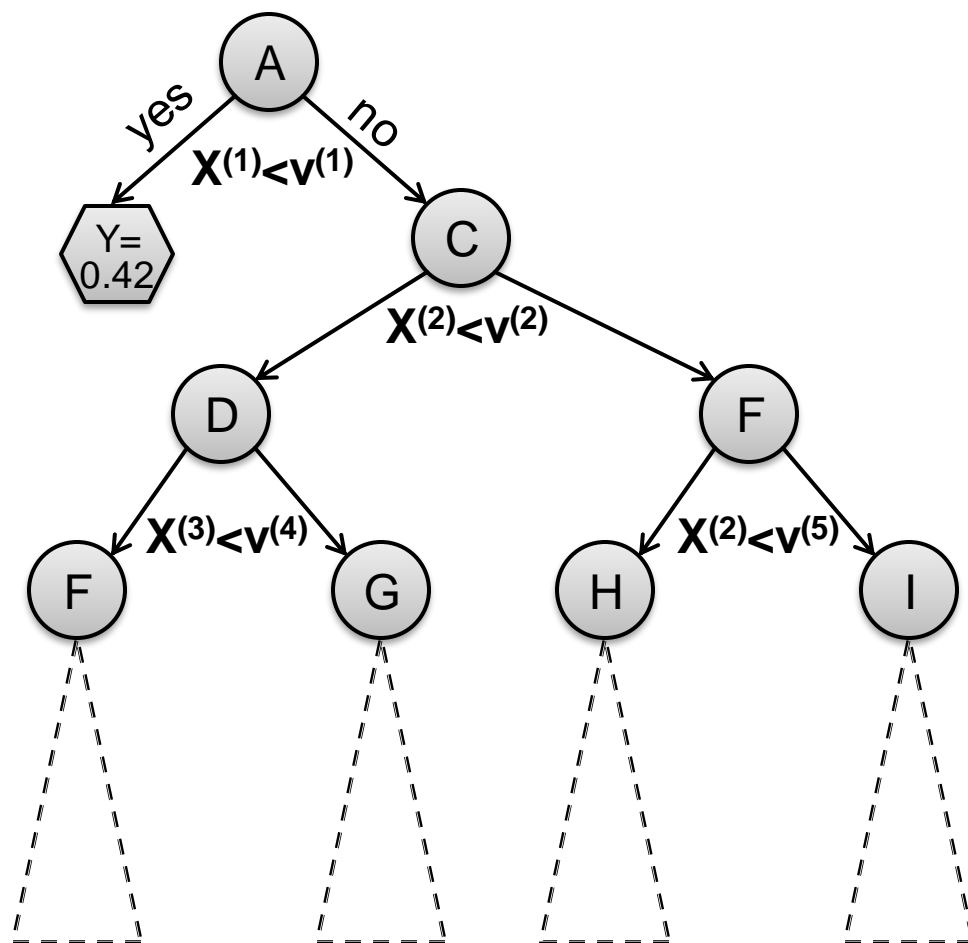
## ■ Lecture today:

- Binary splits:  $X^{(j)} < v$
- Numerical attributes
- Regression



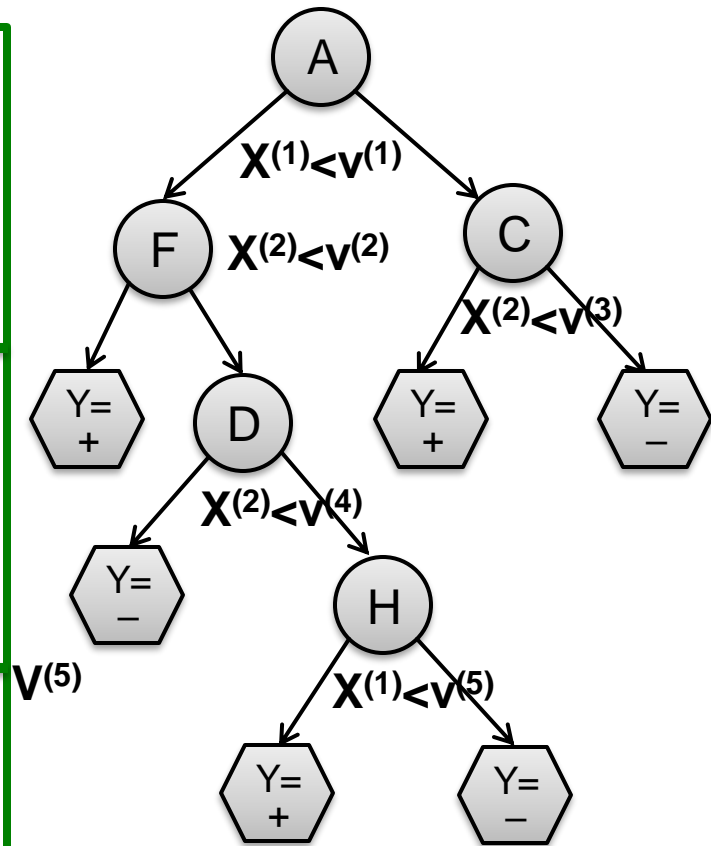
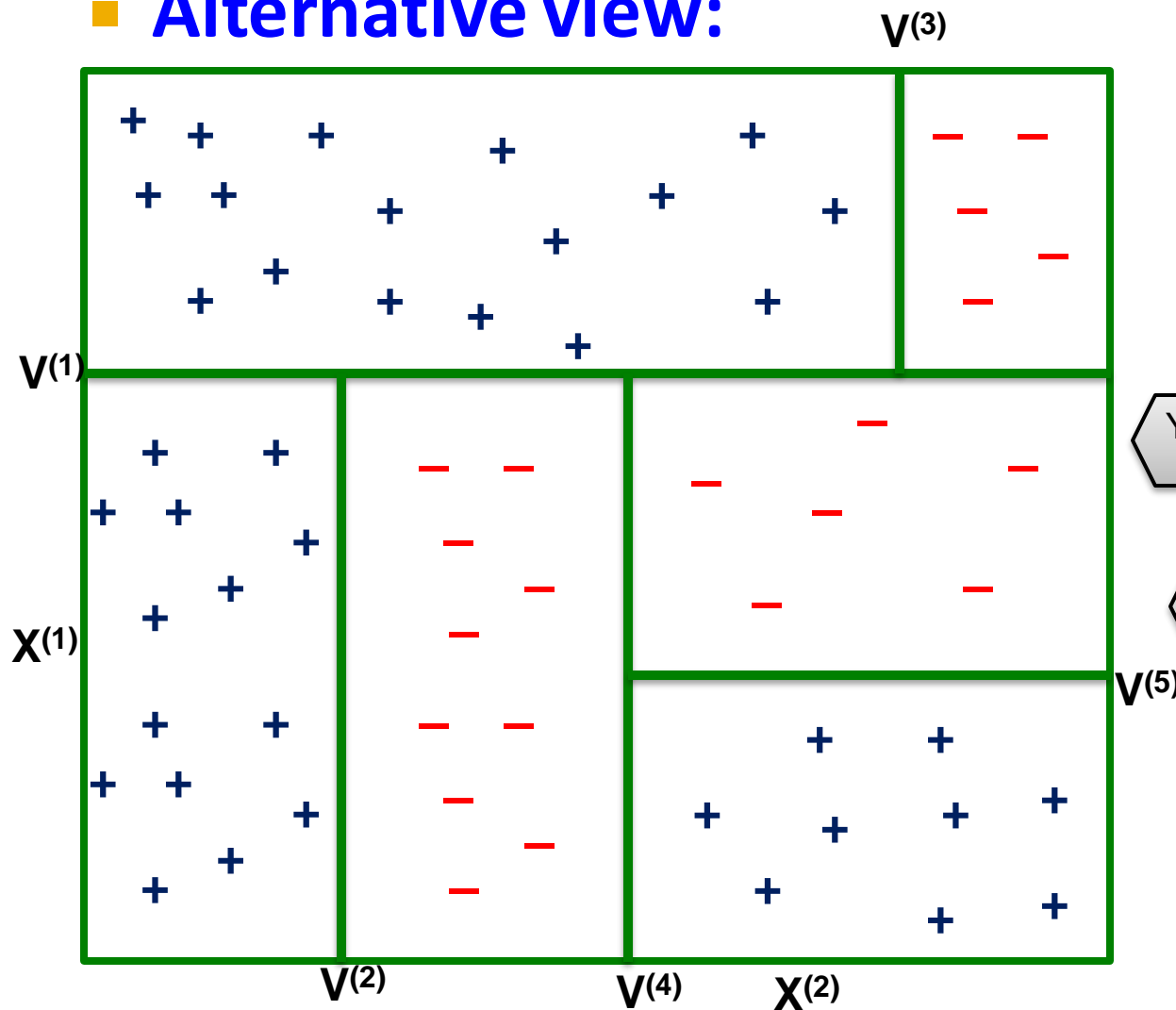
# How to make predictions?

- **Input:** Example  $x_i$
- **Output:** Predicted  $\hat{y}_i$
- “Drop”  $x_i$  down the tree until it hits a leaf node
- Predict the value stored in the leaf that  $x_i$  hits



# Decision Trees: feature space

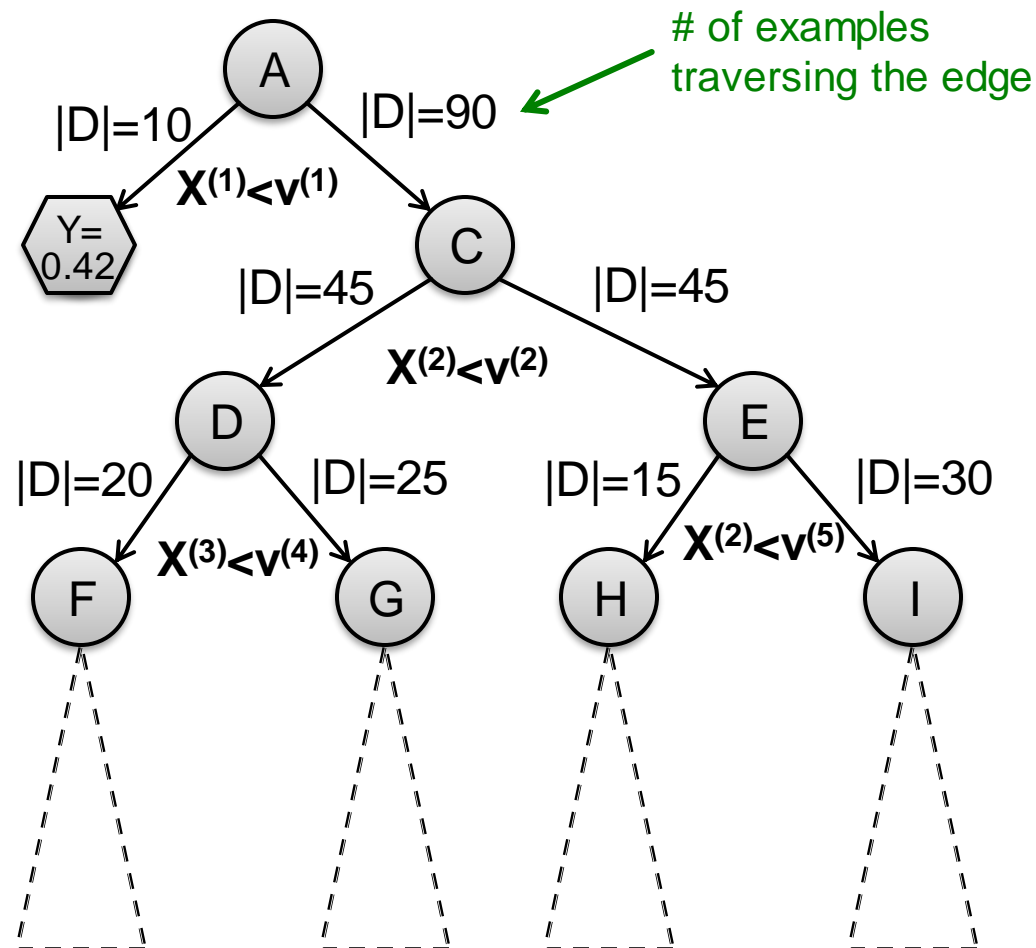
## ■ Alternative view:





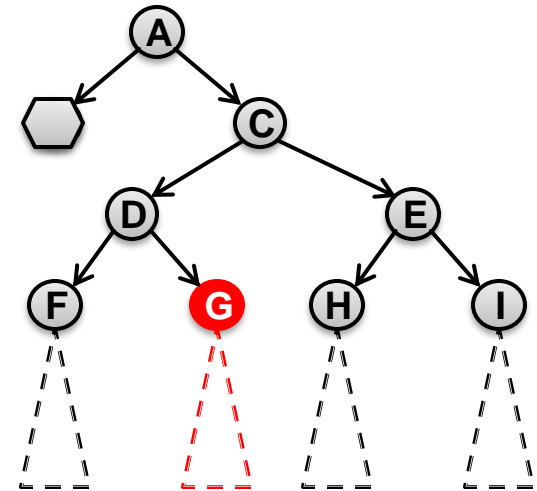
# How to construct a tree?

- Training dataset  $D^*$ ,  $|D^*| = 100$  examples



# How to construct a tree?

- Imagine we are currently at some node ***G***
  - Let  $D_G$  be the data that reaches ***G***
- **There is a decision we have to make: Do we continue building the tree?**
  - **If yes**, which variable and which value do we use for a **split**?
    - Continue building the tree recursively
  - **If not**, how do we make a prediction?
    - We need to build a “**predictor node**”



# 3 steps in constructing a tree

## Algorithm 1 BuildSubtree

Require: Node  $n$ , Data  $D \subseteq D^*$

1:  $(n \rightarrow \text{split}, D_L, D_R) = \text{FindBestSplit}(D)$  (1)

2: if  $\text{StoppingCriteria}(D_L)$  then (2)

3:    $n \rightarrow \text{left\_prediction} = \text{FindPrediction}(D_L)$  (3)

4: else

5:         **BuildSubtree** ( $n \rightarrow \text{left}, D_L$ )

6: if  $\text{StoppingCriteria}(D_R)$  then

7:    $n \rightarrow \text{right\_prediction} = \text{FindPrediction}(D_R)$

8: else

9:         **BuildSubtree** ( $n \rightarrow \text{right}, D_R$ )

- Requires at least a single pass over the data!

# How to construct a tree?

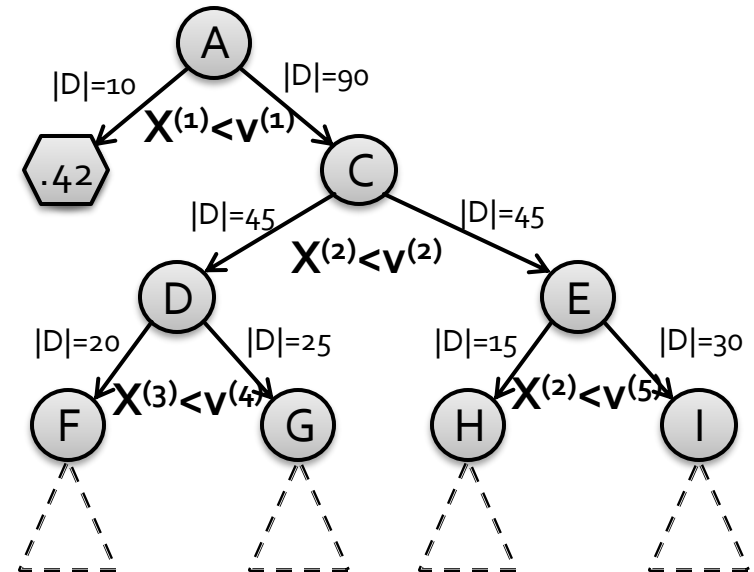
(1) How to split? Pick attribute & value that optimizes some criterion

- Regression: Purity

- Find split  $(X^{(i)}, v)$  that creates  $D, D_L, D_R$ : parent, left, right child datasets and maximizes:

$$|D| \cdot \text{Var}(D) - (|D_L| \cdot \text{Var}(D_L) + |D_R| \cdot \text{Var}(D_R))$$

- $\text{Var}(D) = \frac{1}{|D|} \sum_{i \in D} (y_i - \bar{y})^2$  ... variance of  $y_i$  in  $D$



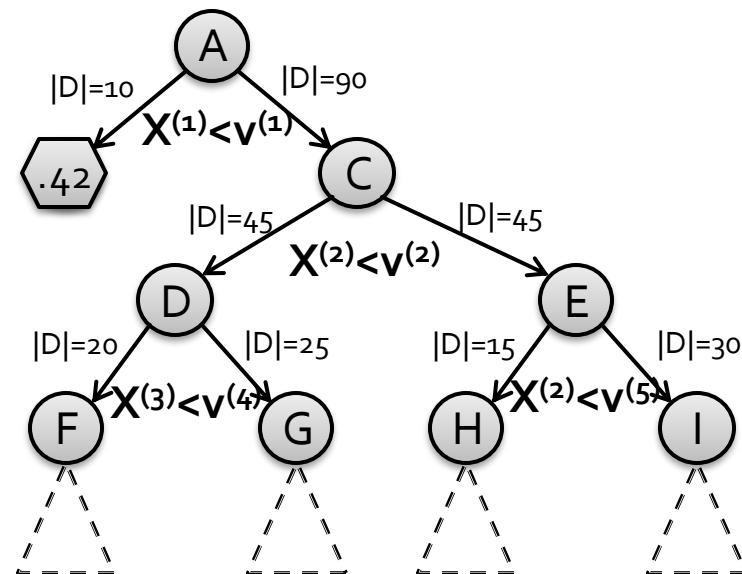
# How to construct a tree?

**(1) How to split?** Pick attribute & value that optimizes some criterion

- Classification:

**Information Gain**

- Measures how much a given attribute  $X$  tells us about the class  $Y$
- $IG(Y | X)$  : We must transmit  $Y$  over a binary link. How many bits on average would it save us if both ends of the line knew  $X$ ?

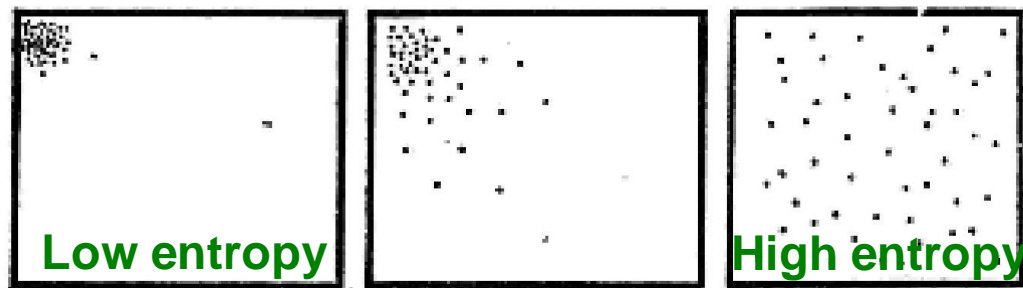


# Why Information Gain? Entropy

**Entropy:** What's the smallest possible number of bits, on average, per symbol, needed to transmit a stream of symbols drawn from  $X$ 's distribution?

**The entropy of  $X$ :**  $H(X) = -\sum_{j=1}^m p(X_j) \log p(X_j)$

- **“High Entropy”:**  $X$  is from a uniform (boring) distribution
  - A histogram of the frequency distribution of values of  $X$  is **flat**
- **“Low Entropy”:**  $X$  is from a varied (peaks/valleys) distrib.
  - A histogram of the frequency distribution of values of  $X$  would have many lows and one or two highs



# Why Information Gain? Entropy

- Suppose I want to predict  $Y$  and I have input  $X$ 
  - $X$  = College Major
  - $Y$  = Likes “Casablanca”

$X$	$Y$
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
Math	Yes
History	No

- From this data we estimate
  - $P(Y = \text{Yes}) = 0.5$
  - $P(X = \text{Math} \ \& \ Y = \text{No}) = 0.25$
  - $P(X = \text{Math}) = 0.5$
  - $P(Y = \text{Yes} \mid X = \text{History}) = 0$
- Note:
  - $H(Y) = -\frac{1}{2}\log_2(\frac{1}{2}) - \frac{1}{2}\log_2(\frac{1}{2}) = 1$
  - $H(X) = 1.5$

# Why Information Gain? Entropy

- Suppose I want to predict  $Y$  and I have input  $X$ 
  - $X$  = College Major
  - $Y$  = Likes “Casablanca”

$X$	$Y$
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
Math	Yes
History	No

- Def: **Specific Conditional Entropy**
  - $H(Y | X = v)$  = The entropy of  $Y$  among only those records in which  $X$  has value  $v$
  - **Example:**
    - $H(Y|X = \textit{Math}) = 1$
    - $H(Y|X = \textit{History}) = 0$
    - $H(Y|X = \textit{CS}) = 0$



# Why Information Gain?

- Suppose I want to predict  $Y$  and I have input  $X$ 
  - $X$  = College Major
  - $Y$  = Likes “Casablanca”

$X$	$Y$
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
Math	Yes
History	No

- **Def: Conditional Entropy**

- $H(Y | X)$  = The average specific conditional entropy of  $Y$ 
  - = if you choose a record at random what will be the conditional entropy of  $Y$ , conditioned on that row's value of  $X$
  - = Expected number of bits to transmit  $Y$  if both sides knew the value of  $X$
  - $= \sum_j P(X = v_j) H(Y | X = v_j)$

# Why Information Gain?

- Suppose I want to predict  $Y$  and I have input  $X$

- $H(Y | X)$  = The average specific conditional entropy of  $Y$

$$= \sum_j P(X = v_j) H(Y | X = v_j)$$

- Example:

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
Math	Yes
History	No

$v_j$	$P(X=v_j)$	$H(Y X=v_j)$
Math	0.5	1
History	0.25	0
CS	0.25	0

- So:  $H(Y | X) = 0.5 * 1 + 0.25 * 0 + 0.25 * 0 = 0.5$

# Why Information Gain?

- Suppose I want to predict  $Y$  and I have input  $X$

- **Def: Information Gain**

- $IG(Y|X)$  = I must transmit  $Y$ . **How many bits on average would it save me if both ends of the line knew  $X$ ?**

$$IG(Y|X) = H(Y) - H(Y|X)$$

- **Example:**

- $H(Y) = 1$
  - $H(Y|X) = 0.5$
  - Thus  $IG(Y|X) = 1 - 0.5 = 0.5$

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
Math	Yes
History	No

# What is Information Gain used for?

- Suppose you are trying to predict whether someone is going to live past 80 years
- From historical data you might find:
  - $IG(LongLife \mid HairColor) = 0.01$
  - $IG(LongLife \mid Smoker) = 0.4$
  - $IG(LongLife \mid Gender) = 0.25$
  - $IG(LongLife \mid LastDigitOfSSN) = 0.00001$
- IG tells us how much information about  $Y$  is contained in  $X$ 
  - So attribute  $X$  that has high  $IG(Y|X)$  is a good split!

# 3 steps in constructing a tree

## Algorithm 1 BuildSubtree

Require: Node  $n$ , Data  $D \subseteq D^*$

1:  $(n \rightarrow \text{split}, D_L, D_R) = \text{FindBestSplit}(D)$  (1)

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4: else

5:         **BuildSubtree** ( $n \rightarrow \text{left}, D_L$ )

6: if  $\text{StoppingCriteria}(D_R)$  then

7:    $n \rightarrow \text{right\_prediction} = \text{FindPrediction}(D_R)$

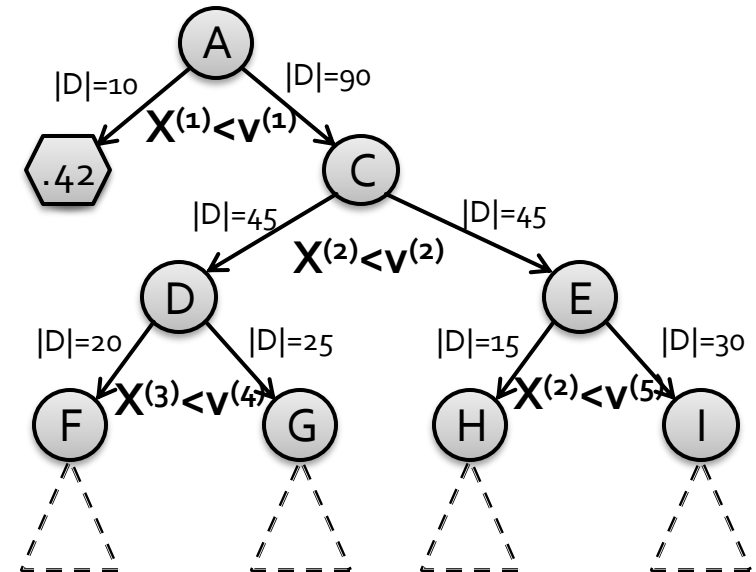
8: else

9:         **BuildSubtree** ( $n \rightarrow \text{right}, D_R$ )

# When to stop?

## (2) When to stop?

- Many different heuristic options
- **Two ideas:**
  - **(1) When the leaf is “pure”**
    - The target variable does not vary too much:  $Var(y) < \varepsilon$
  - **(2) When # of examples in the leaf is too small**
    - For example,  $|D| \leq 100$



# How to predict?

## (3) How to predict?

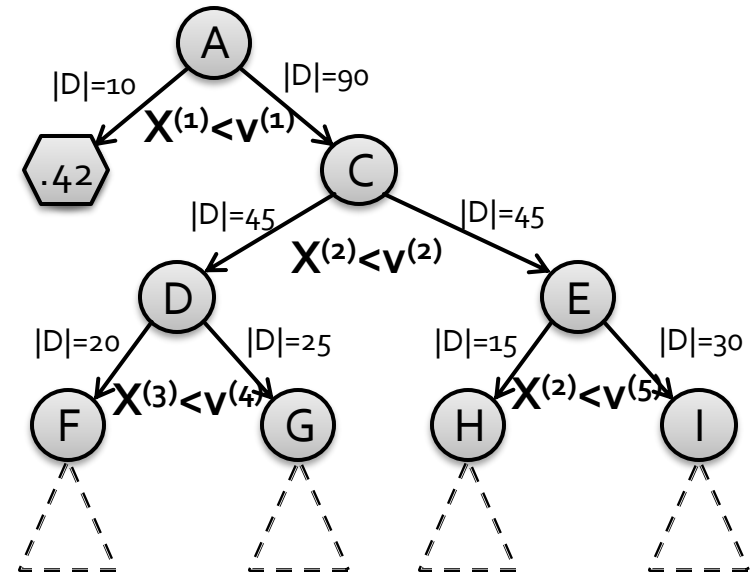
### ■ Many options

#### ■ Regression:

- Predict average  $y_i$  of the examples in the leaf
- Build a linear regression model on the examples in the leaf

#### ■ Classification:

- Predict most common  $y_i$  of the examples in the leaf



# Decision Trees

## ■ Characteristics

### ■ Classification & Regression

- Multiple (~10) classes

### ■ Real valued and categorical features

### ■ Few (hundreds) of features

### ■ Usually dense features

### ■ Complicated decision boundaries

- Early stopping to avoid overfitting!

## ■ Example applications

### ■ User profile classification

### ■ Landing page bounce prediction



# Decision Trees

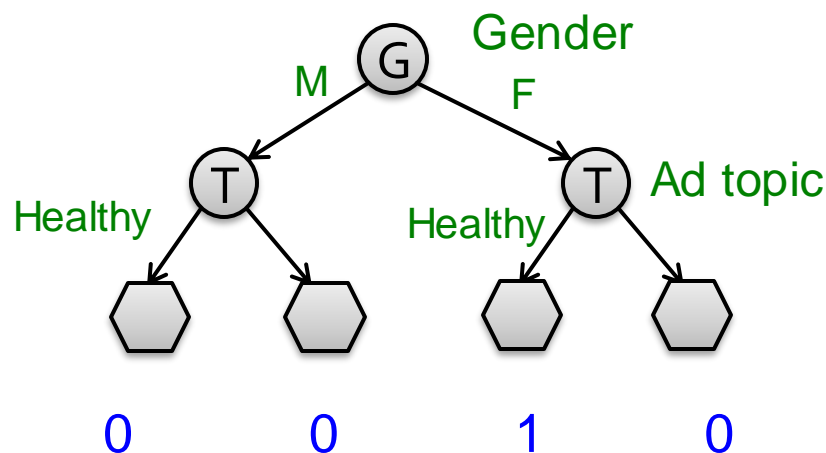
- **Decision trees are the single most popular data mining tool:**
  - Easy to understand
  - Easy to implement
  - Easy to use
  - Computationally cheap
  - It's possible to mitigate overfitting (i.e., with ensemble methods)
  - **They do classification as well as regression!**

# Benefit: Feature Transforms

- **Problem:** Many times we want to predict association between a user  $u$  and an item  $x$ 
  - For example, how much will user  $u$  like movie  $x$ ; how likely is  $u$  to click on an ad  $x$ .
- **Issue:** Many sparse features:
  - User: Demographics, interests, prior activity, ...
  - Movie/ad: Keywords, actors, director, ...
- **Goal:** Build  $f(u, x)$
- **Notice:**
  - Linear model that concatenates features ( $w \cdot [u, x]$ ) is not able to learn that women like healthy food ads.
  - We need to “**cross**” features:  $u \times x$ 
    - Create new feature: (gender, ad topic)
    - E.g., (man, healthy food), (woman, healthy food)
  - **Issue:** Number of features explodes!

# Feature Transforms

- **Solution:** Build Feature Transforms using decision trees:

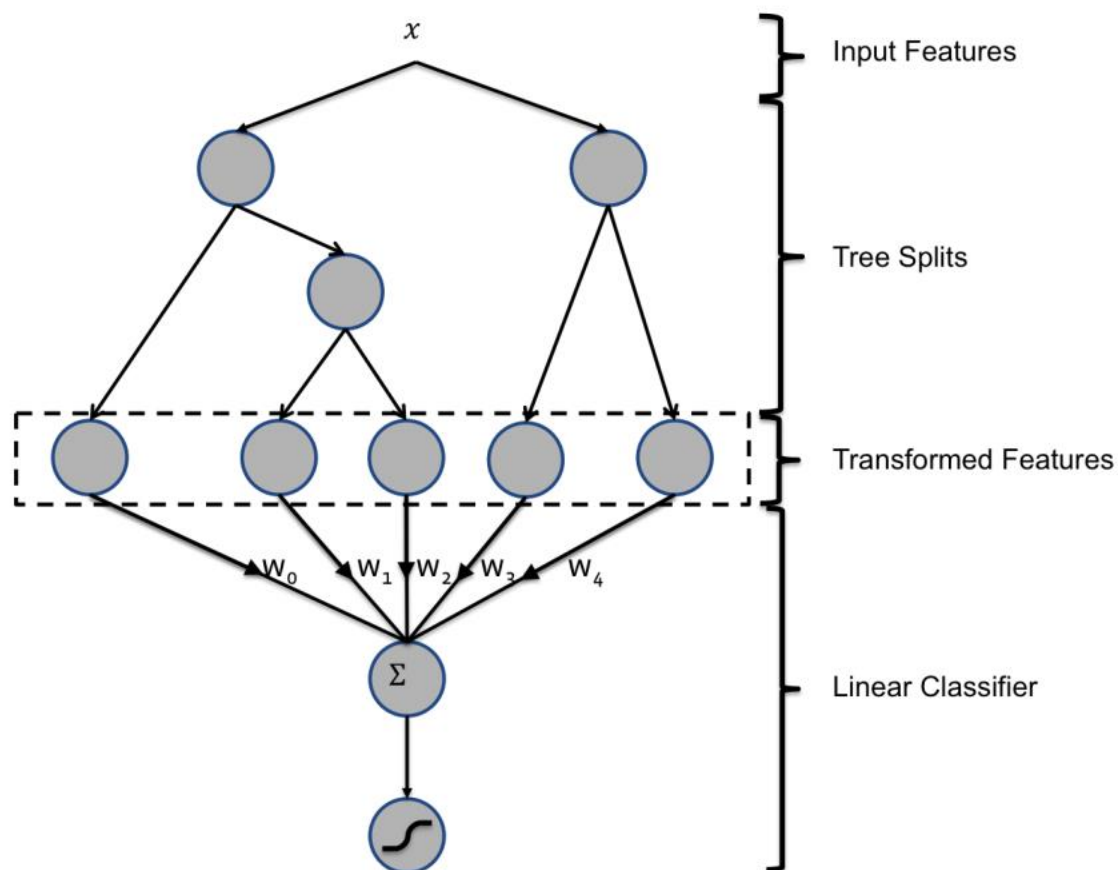


(Female, Healthy)  
is encoded as:

- Drop the example into the tree and use 1-hot encoding to denote the leaf it ends at.
- Use these 1-hot vectors as inputs to a linear classifier

# Feature Transforms

## ■ Overall architecture:

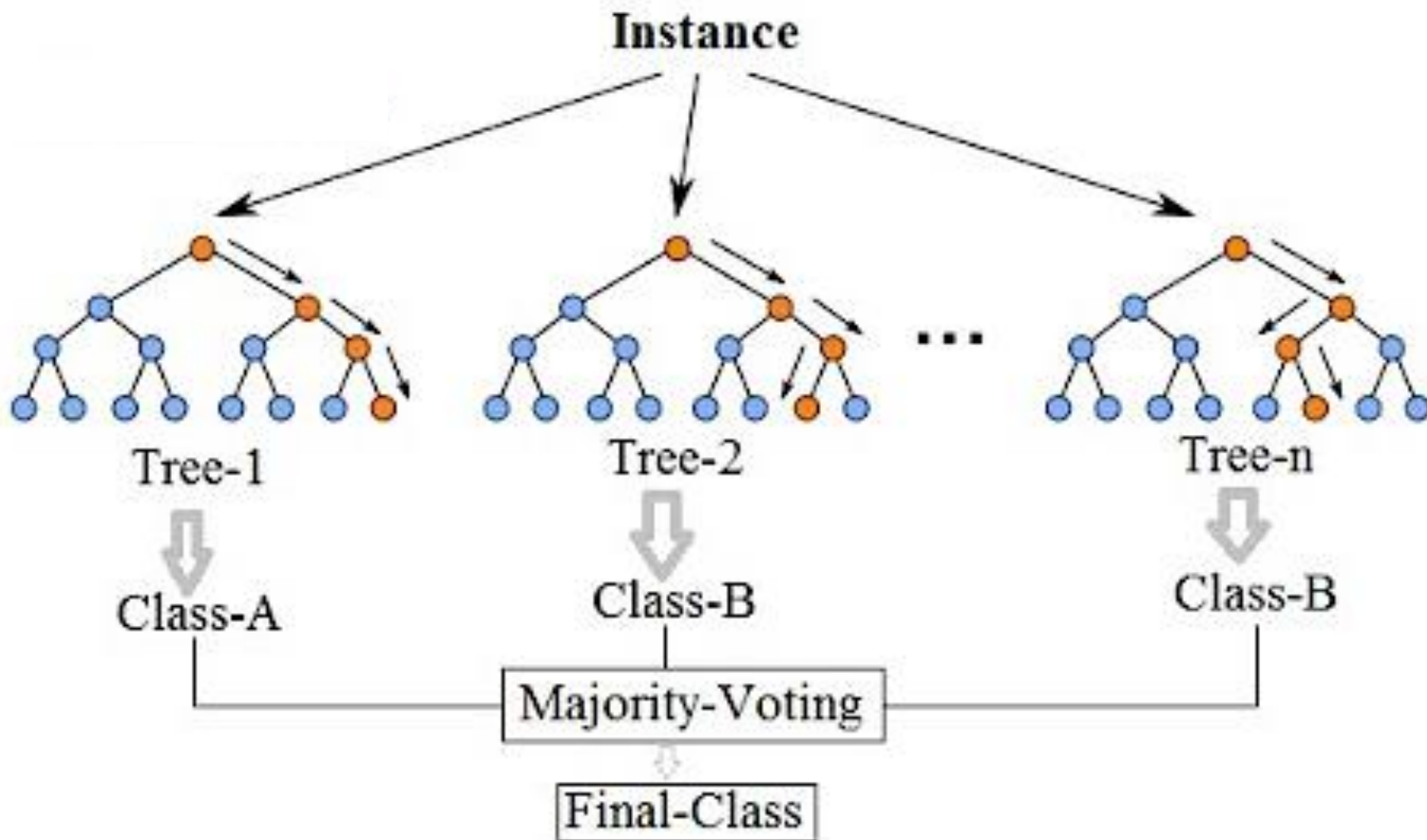


# Decision Trees: Learning Ensembles

# Learning Ensembles

- Learn multiple trees and combine their predictions
  - Gives better performance in practice
- **Bagging:**
  - Learns multiple trees over independent samples of the training data
    - For a dataset  $\mathbf{D}$  on  $n$  data points: Create dataset  $\mathbf{D}'$  of  $n$  points but sample from  $\mathbf{D}$  with replacement:
      - 33% points in  $\mathbf{D}'$  will be duplicates, 66% will be unique
  - Predictions from each tree are averaged to compute the final model prediction

# (1): Bagging Decision Trees



# (1): Bagged Decision Trees

- **How to create random samples of  $D$ ?**
  - Compute a hash of a training record's id and tree id
  - Use records that hash into a particular range to learn a tree
  - This way the same sample is used for all nodes in a tree
  - **Note:** This is sampling  $D$  without replacement (but samples of  $D$  should be created with replacement)

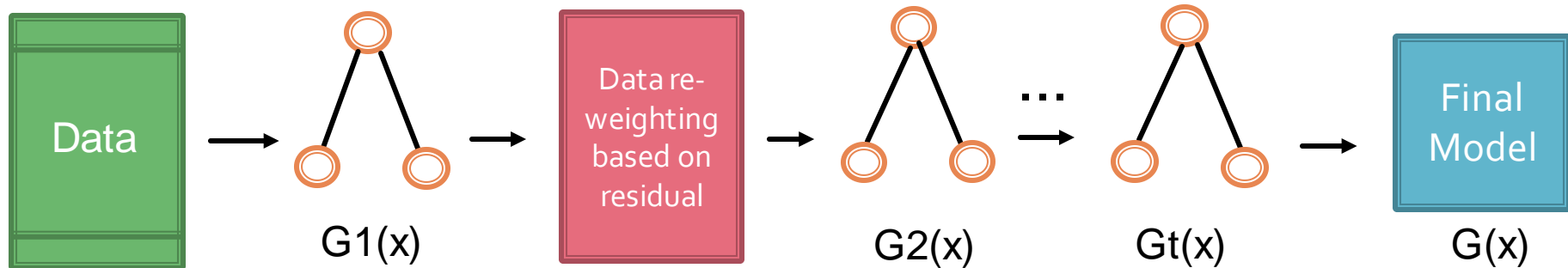


## (2) Improvement: Random Forests

- Train a **Bagged Decision Tree**
- But use a modified tree learning algorithm that selects (at each candidate split) **a random subset of features**
  - If we have  $d$  features, consider  $\sqrt{d}$  random features
- **This is called: Feature bagging**
  - **Benefit:** Breaks correlation between trees
    - If one feature is very strong predictor, then every tree will select it, causing trees to be correlated.
- **Random Forests achieve state-of-the-art results in many classification problems!**

# (3): Boosting

- **Boosting: Another ensemble learning algorithm**
  - Combines the outputs of many “weak” classifiers to produce a powerful “committee”
  - Learns multiple trees sequentially, each trying to improve upon its predecessor
  - Final classifier is weighted sum of the individual classifiers



Residual: Difference between prediction and ground truth

# (3): Boosting

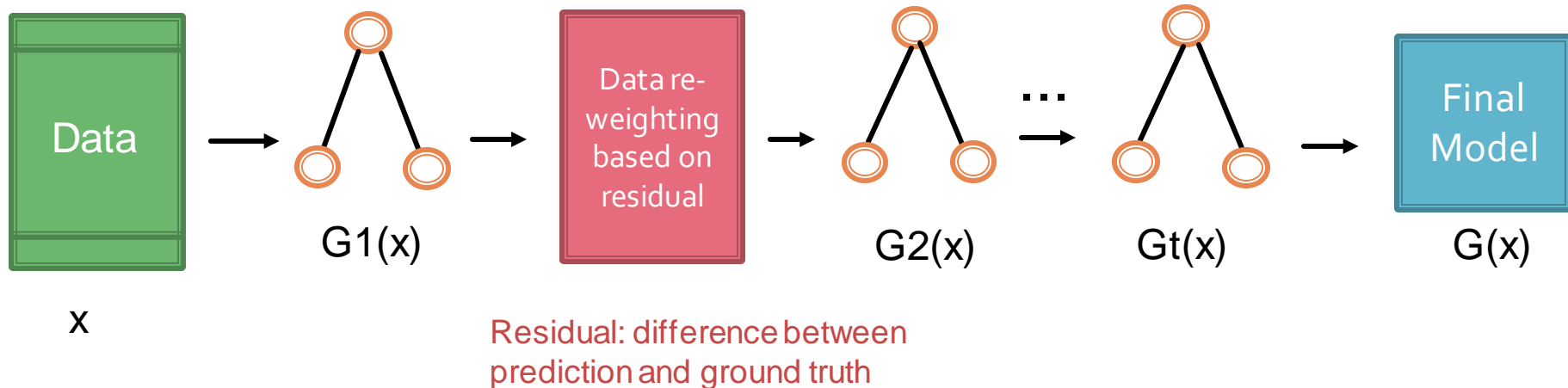
## ■ We will show 2 examples:

### ■ Example 1: AdaBoost

- Where each  $G_t(x)$  is a one-level decision tree

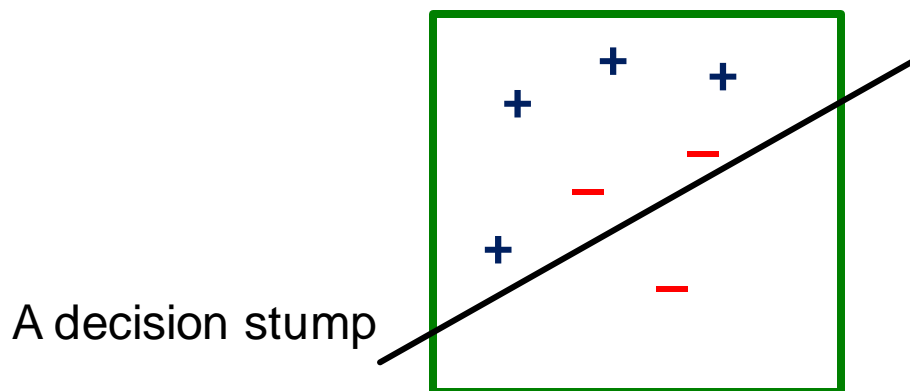
### ■ Example 2: Gradient Boosted Decision Trees

- Where each  $G_t(x)$  is a multi-level decision tree



# AdaBoost: Weak learner

- **Decision “stumps”:**
  - 1-level decision tree
  - A decision boundary based on one feature
    - E.g.: If someone is not a smoker, then predict them to live past 80 years old
  - Building blocks of AdaBoost algorithm
  - **Decision stump is a weak learner**



**Boosting theory:**  
if weak learners have  
>50% accuracy then  
we can learn a perfect  
classifier.

# Build Decision Trees with AdaBoost

Suppose we have training data  $\{(x_i, y_i)\}_{i=1}^N$ ,  $y_i \in \{1, -1\}$

- Initialize equal weights for all observations  $w_i = 1/N$
- At each iteration  $t$ :
  1. Train a stump  $G_t$  using data weighted by  $w_i$
  2. Compute the misclassification error adjusted by  $w_i$
  3. Compute the weight of the current tree  $\alpha_t$
  4. Reweight each observation based on prediction accuracy

# Training One Decision Tree

- **How to split?**

- Apply weighting to the splitting criterion function and optimize the function to find the best split
- We'll use information gain as an example

- Recall :

- **Information gain**  $IG(Y|X) = H(Y) - H(Y|X)$

- **where**

$$H(X) = - \sum_{i=1}^N p(X_i) \log(P(X_i))$$

- After weighting:

$$H_w(X) = \frac{- \sum_{i=1}^N w_i p(X_i) \log(P(X_i))}{\sum_{i=1}^N w_i}$$

# Update Step

- Calculate the weighted misclassification error

$$err_t = \frac{\sum_{i=1}^N w_i I(y_i \neq G_t(x_i))}{\sum_{i=1}^N w_i}$$

- Use the error score to weight the current tree in the final classifier:

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

A classifier with 50% accuracy is given a weight of zero;

- Use misclassification error and tree weight to reweight the training data:

$$w_i \leftarrow w_i \exp[\alpha_t I(y_i \neq G_t(x_i))]$$

Harder to classify training instances get higher weight

# Final Prediction

- Final prediction is a weighted sum of the predictions from each stump:

$$G(x) = \text{sign} \left[ \sum_{t=1}^T \alpha_t G_t(x) \right]$$

- More accurate trees are weighted higher in the final model



# AdaBoost: Summary

1. Initialize the observation weights  $w_i = 1/N$ ,  $i = 1, 2, \dots, N$ .

2. For  $m = 1$  to  $M$ :

(a) Fit a classifier  $G_m(x)$  to the training data using weights  $w_i$ .

(b) Compute (1) Train a stump

$$\text{err}_m = \frac{\sum_{i=1}^N w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^N w_i}.$$

(2) Compute error

(c) Compute  $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$ . (3) Compute tree weight

(d) Set  $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))]$ ,  $i = 1, 2, \dots, N$ .

3. Output  $G(x) = \text{sign} \left[ \sum_{m=1}^M \alpha_m G_m(x) \right]$ . (4) Reweight data

# AdaBoost Conclusion

- Iteratively train weak learners (decision stumps) to form a strong model:
  - Trees with high accuracy are given more weights in the final model
  - Misclassified data get higher weights in the next iteration
- AdaBoost is the equivalent to additive training with the exponential loss (Friedman et al. 2000)
- We will talk about additive training in more general scenarios next!

# Gradient Boosted Decision Trees

## ■ Idea: Additive training:

- Start from constant prediction, **add a new decision tree  $f_i$  each time:**

- Here  $f_i$  can be multi-level!

$$\hat{y}_i^{(0)} = 0$$

$$\hat{y}_i^{(1)} = f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i)$$

$$\hat{y}_i^{(2)} = f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i)$$

...

$$\hat{y}_i^{(t)} = \sum_{k=1}^t f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i).$$

Prediction at  
training round  $t$

Keep predictions  
from previous rounds

New model

# How to decide which $f$ to add?

- **Prediction at round  $t$  is:**  $\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + f_t(x_i)$ 
  - Where we need to decide what  $f_t()$  to add
- **Goal: Find tree  $f_t(\cdot)$  that minimizes loss  $l()$ :**  
$$\sum_i l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t)$$
  - $y_i$ : The ground-truth label
  - $\hat{y}_i^{(t-1)} + f_t(x_i)$ : The prediction made at round  $t$
  - $\Omega(f_t)$ : The model complexity

# How to decide which $f$ to add?

- $Obj = \sum_i l(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)) + \Omega(f_t)$

- Take Taylor expansion of the objective:

- $g(x + \Delta) \approx g(x) + g'(x)\Delta + \frac{1}{2}g''(x)\Delta^2$

- So, we get the approximate objective:

$$\sum_{i=1}^n \left[ \underline{l(y_i, \hat{y}_i^{(t-1)})} + g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t)$$

We can ignore this part, since we are optimizing over  $f_t$

- where:

$$g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial_{\hat{y}^{(t-1)}}^2 l(y_i, \hat{y}^{(t-1)})$$

# How to decide which $f$ to add?

- **Example: The square loss (L2 loss)**

- **The approximate objective:**

$$\sum_{i=1}^n \left[ g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t)$$

where  $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$ ,  $h_i = \partial_{\hat{y}^{(t-1)}}^2 l(y_i, \hat{y}^{(t-1)})$

- **Derive  $g$  and  $h$  for square loss:**

$$g_i = \partial_{\hat{y}^{(t-1)}} (\hat{y}^{(t-1)} - y_i)^2 = 2(\hat{y}^{(t-1)} - y_i) \quad h_i = \partial_{\hat{y}^{(t-1)}}^2 (\hat{y}^{(t-1)} - y_i)^2 = 2$$

# Our New Goal

- **Our new goal: Find tree  $f_t$  that:**

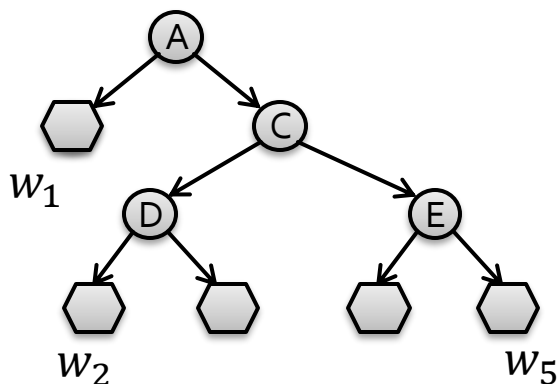
$$\sum_{i=1}^n \left[ g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t)$$

where  $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$ ,  $h_i = \partial_{\hat{y}^{(t-1)}}^2 l(y_i, \hat{y}^{(t-1)})$

- **Why spending s much efforts to derive the objective, why not just grow trees ...**
  - **Theoretical benefit:** Know what we are learning
  - **Engineering benefit:**
    - $g$  and  $h$  comes from definition of loss function
    - Learning  $f_t$  only depends on the objective via  $g$  and  $h$
    - We can now directly learn trees that optimize the loss (rather than using some heuristic procedure)

# Define a Tree

- Every leaf  $j$  have a weight  $w_j$ 
  - We will predict  $w_j$  for any data belongs to leaf  $j$



$$f_t(x) = w_{\underline{q(x)}}$$

$q(x)$  indicate the leaf node that data point  $x$  belongs to

- Define complexity of tree  $f$  as:

$$\Omega(f) = \gamma * T + \frac{1}{2} \lambda \sum_j^T w_j^2$$

$T$ ... number of leaves of tree  $f$

$\gamma$ ... cost adding a leaf to the tree  $f$



# Revisiting the Objective

- **Define:** The set of examples in the leaf  $j$ :

$$I_j = \{i | q(x_i) = j\}$$

$q(x)$  denotes the leaf that data point  $x$  belongs to

- **Reorder the objective from slide 55 by leaf:**

$$\begin{aligned} &\simeq \sum_{i=1}^n \left[ g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t) \\ &= \sum_{i=1}^n \left[ g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2 \right] + \gamma T + \lambda \frac{1}{2} \sum_{j=1}^T w_j^2 \\ &= \sum_{j=1}^T \underbrace{\left[ \left( \sum_{i \in I_j} g_i \right) w_j + \frac{1}{2} \left( \sum_{i \in I_j} h_i + \lambda \right) w_j^2 \right]}_{\text{Associated with leaf node } j} + \gamma T \end{aligned}$$

- Notice this is a sum of  $T$  quadratic functions, each function is associated with a leaf node  $j$

# Finding the Optimal $w_j^*$

- Two facts about single var. quadratic function:

$$\operatorname{argmin}_x Gx + \frac{1}{2}Hx^2 = -\frac{G}{H}, \quad H > 0 \quad \min_x Gx + \frac{1}{2}Hx^2 = -\frac{1}{2}\frac{G^2}{H}$$

- We can use the facts to derive optimal  $w_j$ :

Let us define  $G_j = \sum_{i \in I_j} g_i$   $H_j = \sum_{i \in I_j} h_i$

$$\begin{aligned} Obj^{(t)} &= \sum_{j=1}^T \left[ (\sum_{i \in I_j} g_i)w_j + \frac{1}{2}(\sum_{i \in I_j} h_i + \lambda)w_j^2 \right] + \gamma T \\ &= \sum_{j=1}^T \left[ G_j w_j + \frac{1}{2}(H_j + \lambda)w_j^2 \right] + \gamma T \end{aligned}$$

- So, for a fixed tree the optimal  $w_j$  and  $Obj$  are:

$$w_j^* = -\frac{G_j}{H_j + \lambda} \quad Obj = -\frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T$$

# How to find a single tree $f_t$

Given a tree  $f_t$ , we know how to

- Calculate the score for  $f$ :

$$Obj = -\frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T$$

- And then set optimal weights for the chosen  $f$ :

$$w_j^* = -\frac{G_j}{H_j + \lambda}$$

In principle we could:

- Enumerate possible tree structures  $f$  and take the one that minimizes  $Obj$

# How to find a single tree $f_t$

- In practice we grow tree greedily:
  - Start with tree with depth 0
  - For each leaf node in the tree, try to add a split
  - The change of the objective after adding a split is:

$$Gain = \frac{1}{2} \left[ \underbrace{\frac{G_L^2}{H_L + \lambda}}_{\text{Score of left child}} + \underbrace{\frac{G_R^2}{H_R + \lambda}}_{\text{Score of right child}} - \underbrace{\frac{(G_L + G_R)^2}{H_L + H_R + \lambda}}_{\text{Score if we do not split}} \right] - \gamma$$

- Take the split that gives best gain
- **Next: How to find the best split?**

# How to Find the Best Split?

- **For each node, enumerate over all features**
  - For each feature, sort the instances by feature value
  - Use a linear scan to decide the best split along that feature
  - Take the best split solution along all the features
- **Pre-stopping:**
  - Stop split if the best split have negative gain
  - But maybe a split can benefit future splits..
- **Post-Pruning:**
  - Grow a tree to maximum depth, recursively prune all the leaf splits with negative gain.

# Summary: GBDT Algorithm

- Add a new tree  $f_t(x)$  in each iteration

- Compute necessary statistics for our objective

$$g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial_{\hat{y}^{(t-1)}}^2 l(y_i, \hat{y}^{(t-1)})$$

- Greedily grow the tree that minimizes the objective:

$$Obj = -\frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T$$

- Add  $f_t(x)$  to our ensemble model

$$y^{(t)} = y^{(t-1)} + \epsilon f_t(x_i)$$

$\epsilon$  is called step-size or shrinkage,  
usually set around 0.1

**Goal:** prevent overfitting

- Repeat until we use  $M$  ensemble of trees

# XGBoost

- **XGBoost: eXtreme Gradient Boosting**
  - A highly scalable implementation of gradient boosted decision trees with regularization

Widely used by data scientists and provides state-of-the-art results on many problems!

- System optimizations:
  - **Parallel tree constructions** using column block structure
  - **Distributed Computing** for training very large models using a cluster of machines.
  - **Out-of-Core Computing** for very large datasets that don't fit into memory.

# Summary of the Lecture

- Basics of supervised learning
- **Decision Trees**
  - **Key idea:** split data at each internal node, make prediction at each leaf node
  - **How to construct a tree:** Information Gain
- **Ensemble of decision trees:**
  - **Bagging:** Random forests
  - **Boosting:** Boosted decision trees