ECS171: Machine Learning

Lecture 15: Tree-based Algorithms

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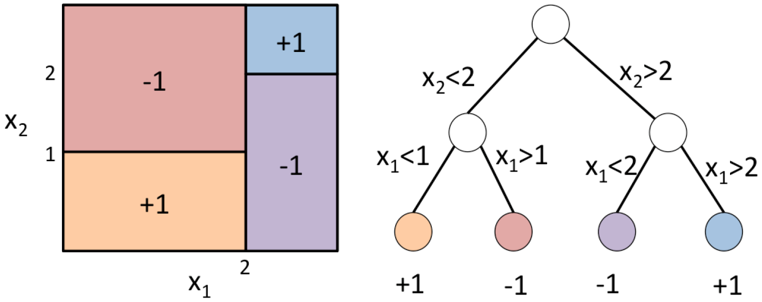
Outline

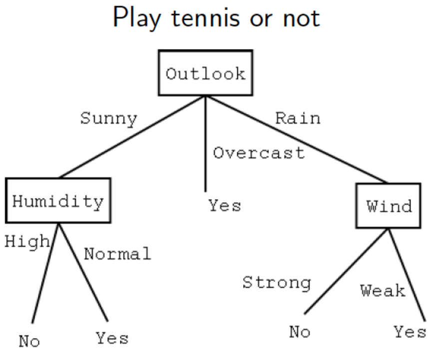
- Decision Tree
- Random Forest
- Gradient Boosted Decision Tree (GBDT)

Decision Tree

- Each node checks one feature x_i:
  - Go left if $x_i <$ threshold
  - Go right if $x_i \geq$ threshold



A real example



Decision Tree

- Strength:
  - It's a nonlinear classifier
  - Better interpretability
  - Can naturally handle categorical features

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- Strength:
  - It's a nonlinear classifier
  - Better interpretability
  - Can naturally handle categorical features
- Computation:
  - Training: slow
  - Prediction: fast

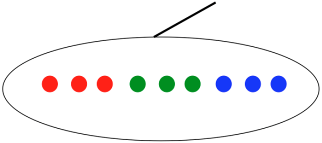
    h operations (h: depth of the tree, usually ≤ 15)

Splitting the node

- Classification tree: Split the node to maximize entropy
- Let S be set of data points in a node, $c = 1, \cdots, C$ are labels:

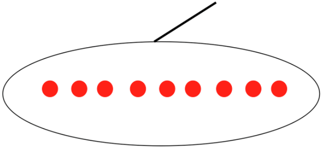
$$\text{Entroy} : H(S) = -\sum_{c=1}^{C} p(c) \log p(c),$$

where $p(c)$ is the proportion of the data belong to class c.
  - Entropy$=0$ if all samples are in the same class
  - Entropy is large if $p(1) = \cdots = p(C)$



Entropy:
-(1/3)*log(1/3) – (1/3)*log(1/3) – (1/3) * log(1/3)
= 1.58

Bad split



Entropy:
-1*log*(1) = 0

Good split

Information Gain

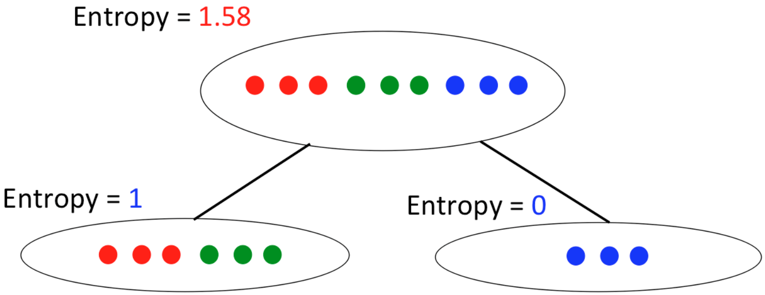
- The averaged entropy of a split $S \to S_1, S_2$

$$\frac{|S_1|}{|S|} H(S_1) + \frac{|S_2|}{|S|} H(S_2)$$

- Information gain: measure how good is the split

$$H(S) - \Big((|S_1|/|S|) H(S_1) + (|S_2|/|S|) H(S_2) \Big)$$

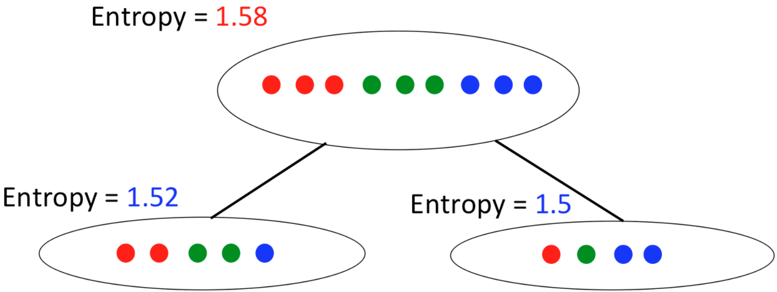
Information Gain



Averaged entropy: 2/3*1 + 1/3*0 = 0.67

Information gain: 1.58 – 0.67 = 0.91

Information Gain



Averaged entropy: 1.51

Information gain: 1.58 – 1.51 = 0.07

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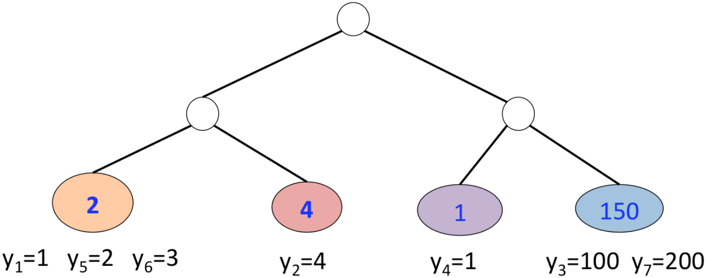
    Compute the information gain after the split

    Choose the best one (maximal information gain)
- For n samples and d features: need $O(nd)$ time

Regression Tree

- Assign a real number for each leaf
- Usually averaged y values for each leaf (minimize square error)



Regression Tree

- Objective function:

$$\min_F \frac{1}{n}\sum_{i=1}^{n}(y_i - F(\boldsymbol{x}_i))^2 + (\text{Regularization})$$

- The quality of partition $S = S_1 \cup S_2$ can be computed by the objective function:

$$\sum_{i \in S_1}(y_i - y^{(1)})^2 + \sum_{i \in S_2}(y_i - y^{(2)})^2,$$

where $y^{(1)} = \frac{1}{|S_1|}\sum_{i \in S_1} y_i$, $y^{(2)} = \frac{1}{|S_2|}\sum_{i \in S_2} y_i$

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- Find the best split:

  Try all the features & thresholds and find the one with minimal objective function

Parameters

- Maximum depth: (usually ~ 10)
- Minimum number of nodes in each node: (10, 50, 100)

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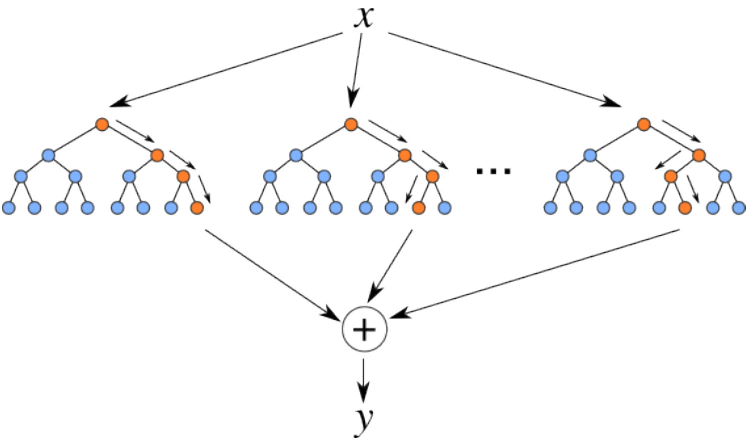
- Minimum number of nodes in each node: (10, 50, 100)
- Single decision tree is not very powerful$\cdots$
- Can we build multiple decision trees and ensemble them together?

Random Forest

Random Forest

- Random Forest (Bootstrap ensemble for decision trees):
  - Create T trees
  - Learn each tree using a subsampled dataset S_i and subsampled feature set D_i
  - Prediction: Average the results from all the T trees
- Benefit:
  - Avoid over-fitting
  - Improve stability and accuracy
- Good software available:
  - R: "randomForest" package
  - Python: sklearn

Random Forest



Gradient Boosted Decision Tree

Boosted Decision Tree

- Minimize loss $\ell(y, F(x))$ with $F(\cdot)$ being ensemble trees

$$F^* = \operatorname*{argmin}_F \sum_{i=1}^{n} \ell(\mathbf{y}_i, F(\boldsymbol{x}_i)) \quad \textbf{with} \quad F(\boldsymbol{x}) = \sum_{m=1}^{T} f_m(\boldsymbol{x})$$

(each f_m is a decision tree)

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  (each f_m is a decision tree)
- Direct loss minimization: at each stage m, find the best function to minimize loss
  - solve $f_m = \operatorname{argmin}_{f_m} \sum_{i=1}^{N} \ell(y_i, F_{m-1}(\boldsymbol{x}_i) + f_m(\boldsymbol{x}_i))$
  - update $F_m \leftarrow F_{m-1} + f_m$
- $F_m(\boldsymbol{x}) = \sum_{j=1}^{m} f_j(\boldsymbol{x})$ is the prediction of $\boldsymbol{x}$ after m iterations.

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- Two problems:
  - Hard to implement for general loss
  - Tend to overfit training data

Gradient Boosted Decision Tree (GBDT)

- Approximate the current loss function by a quadratic approximation:

$$\begin{aligned}\sum_{i=1}^{n} \ell_i(\hat{y}_i + f_m(\boldsymbol{x}_i)) &\approx \sum_{i=1}^{n} \left(\ell_i(\hat{y}_i) + g_i f_m(\boldsymbol{x}_i) + \frac{1}{2} h_i f_m(\boldsymbol{x}_i)^2\right) \\ &= \sum_{i=1}^{n} \frac{h_i}{2} \| f_m(\boldsymbol{x}_i) - g_i/h_i \|^2 + \text{constant}\end{aligned}$$

  where $g_i = \partial_{\hat{y}_i} \ell_i(\hat{y}_i)$ is gradient,
  $h_i = \partial^2_{\hat{y}_i} \ell_i(\hat{y}_i)$ is second order derivative

Gradient Boosted Decision Tree

- Finding $f_m(\boldsymbol{x}, \theta_m)$ by minimizing the loss function:

$$\operatorname*{argmin}_{f_m} \sum_{i=1}^{N} [f_m(\boldsymbol{x}_i, \theta) - g_i/h_i]^2 + R(f_m)$$

  - Reduce the training of any loss function to regression tree (just need to compute g_i for different functions)
  - $h_i = \alpha$ (fixed step size) for original GBDT.
  - XGboost shows computing second order derivative yields better performance

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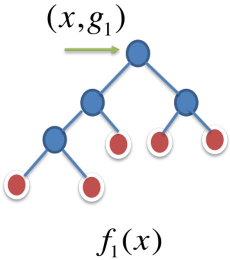
  - XGboost shows computing second order derivative yields better performance
- Algorithm:
  - Computing the current gradient for each $\hat{y}_i$.
  - Building a base learner (decision tree) to fit the gradient.
  - Updating current prediction $\hat{y}_i = F_m(\boldsymbol{x}_i)$ for all i.

Gradient Boosted Decision Trees (GBDT)

- Key idea:
  - Each base learner is a decision tree
  - Each regression tree approximates the functional gradient $\frac{\partial \ell}{\partial F}$



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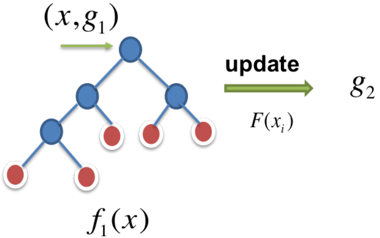

$$F_{m-1}(x_i) = \sum_{j=1}^{m-1} f_j(x_i) \qquad g_m(x_i) = \frac{\partial \ell(y_i, F(x_i))}{\partial F(x_i)}\bigg|_{F(x_i)=F_{m-1}(x_i)}$$

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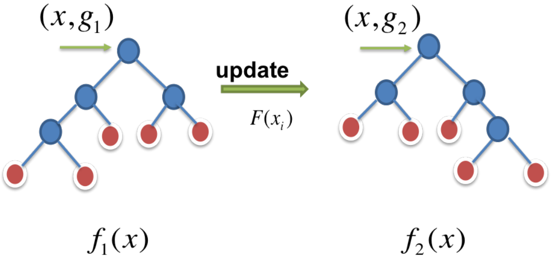

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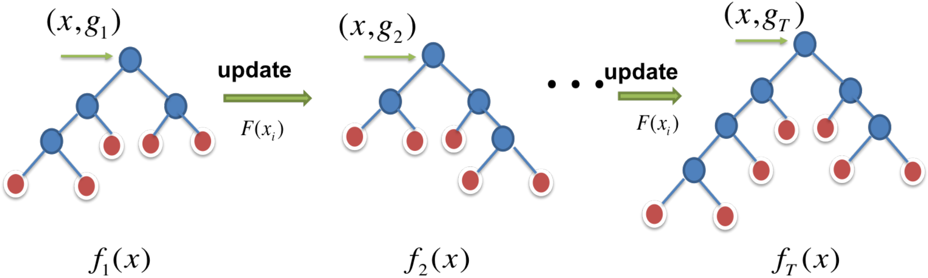

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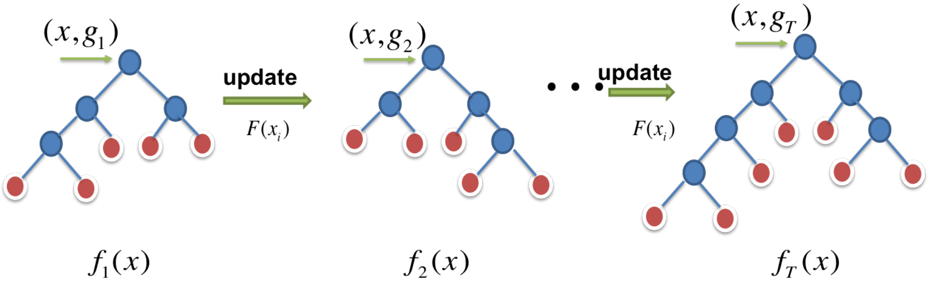

Final prediction $F(x_i) = \sum_{j=1}^{T} f_j(x_i)$

Conclusions

- Next class: Matrix factorization, word embedding

Questions?