COMP5211: Machine Learning

Lecture 11

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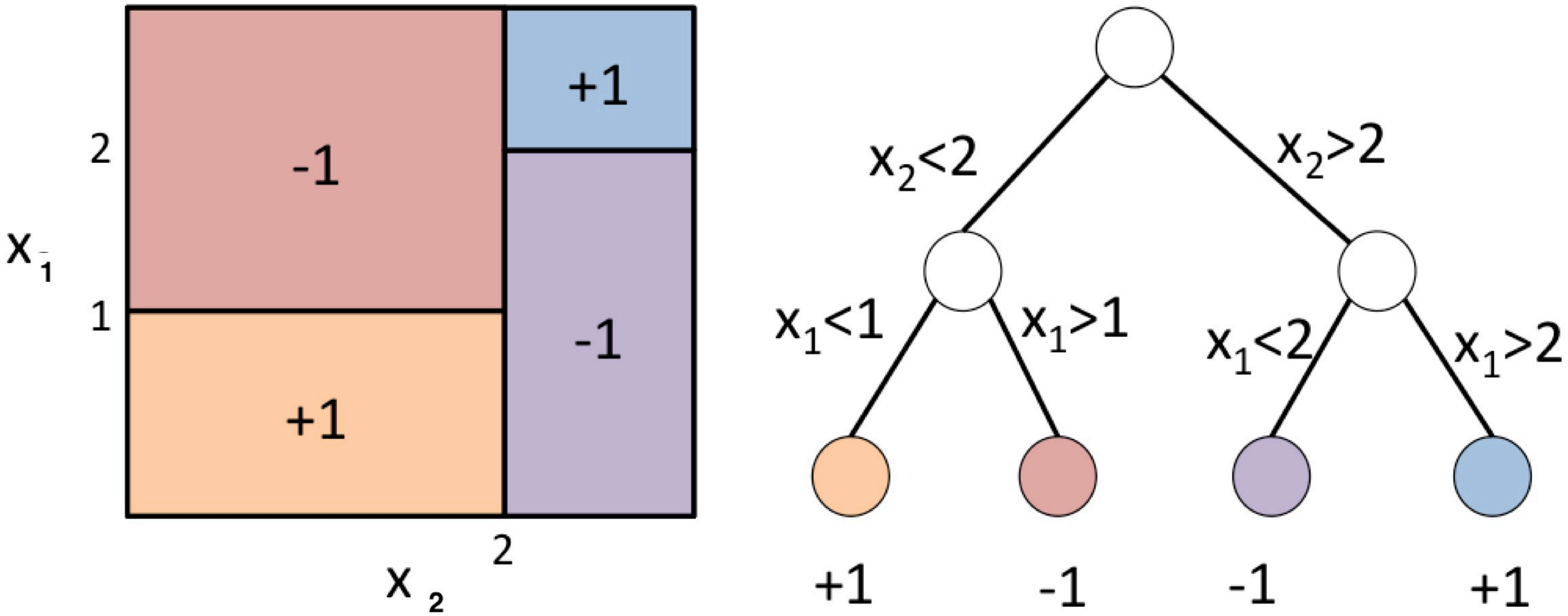
Decision Tree

Illustration

- Each node checks on feature x_i:
  - Go left if $x_i <$ threshold
  - Go right if $x_i >$ threshold



Decision Tree

A real example

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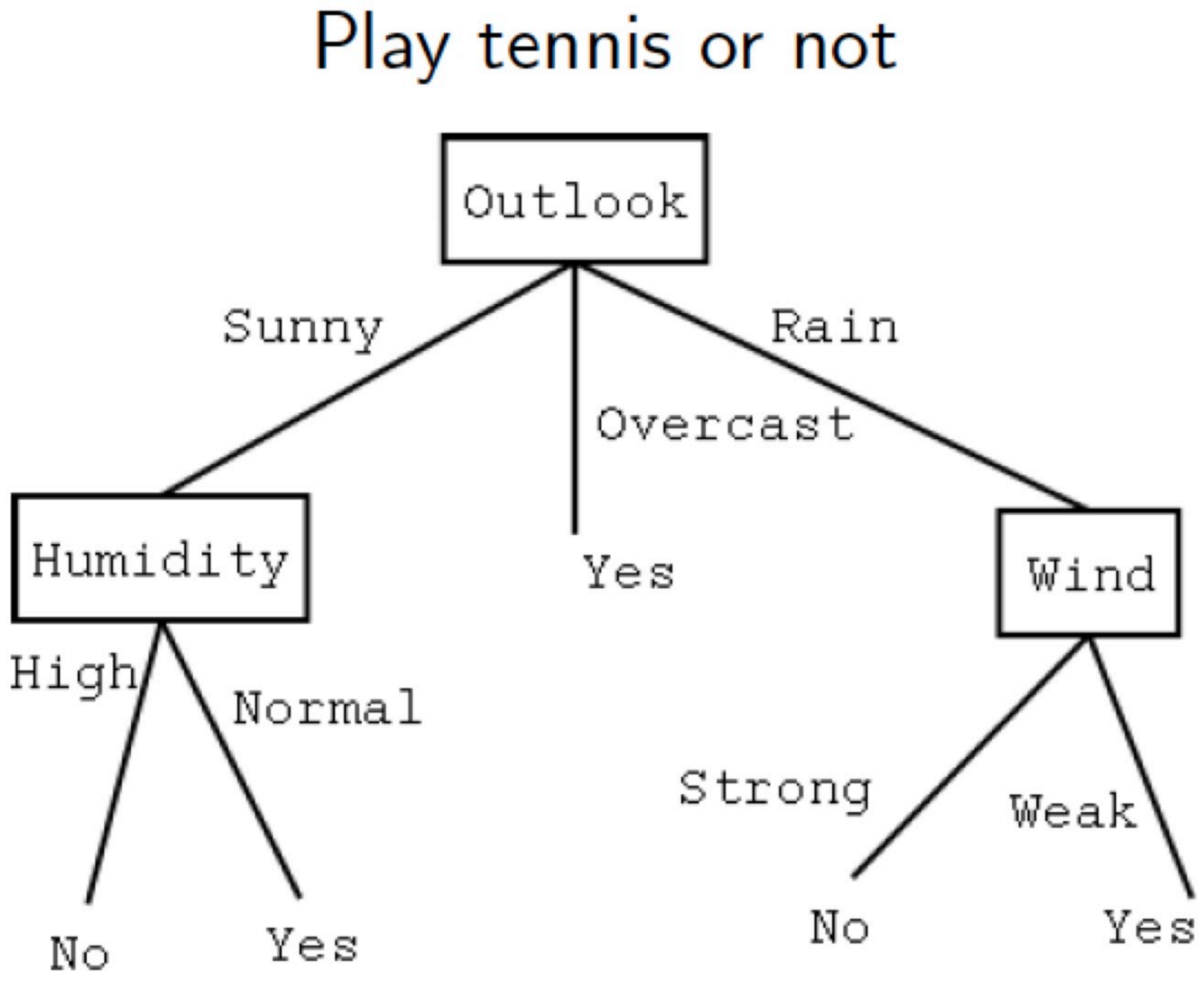


Decision Tree

Pros

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

Decision Tree

Pros

- 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)

Decision Tree

Splitting the node

- Classification tree: Split the node to maximize entropy

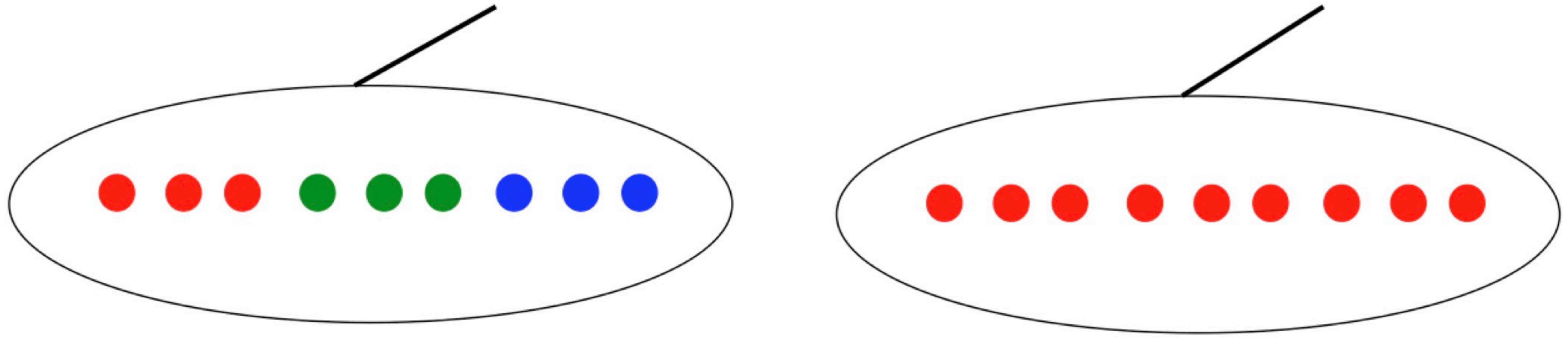
- Let S be set of data points in a node, $c = 1,\ldots,C$ are labels:

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

    - 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 $p(1) = \ldots = p(C)$



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

Decision Tree

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

Decision Tree

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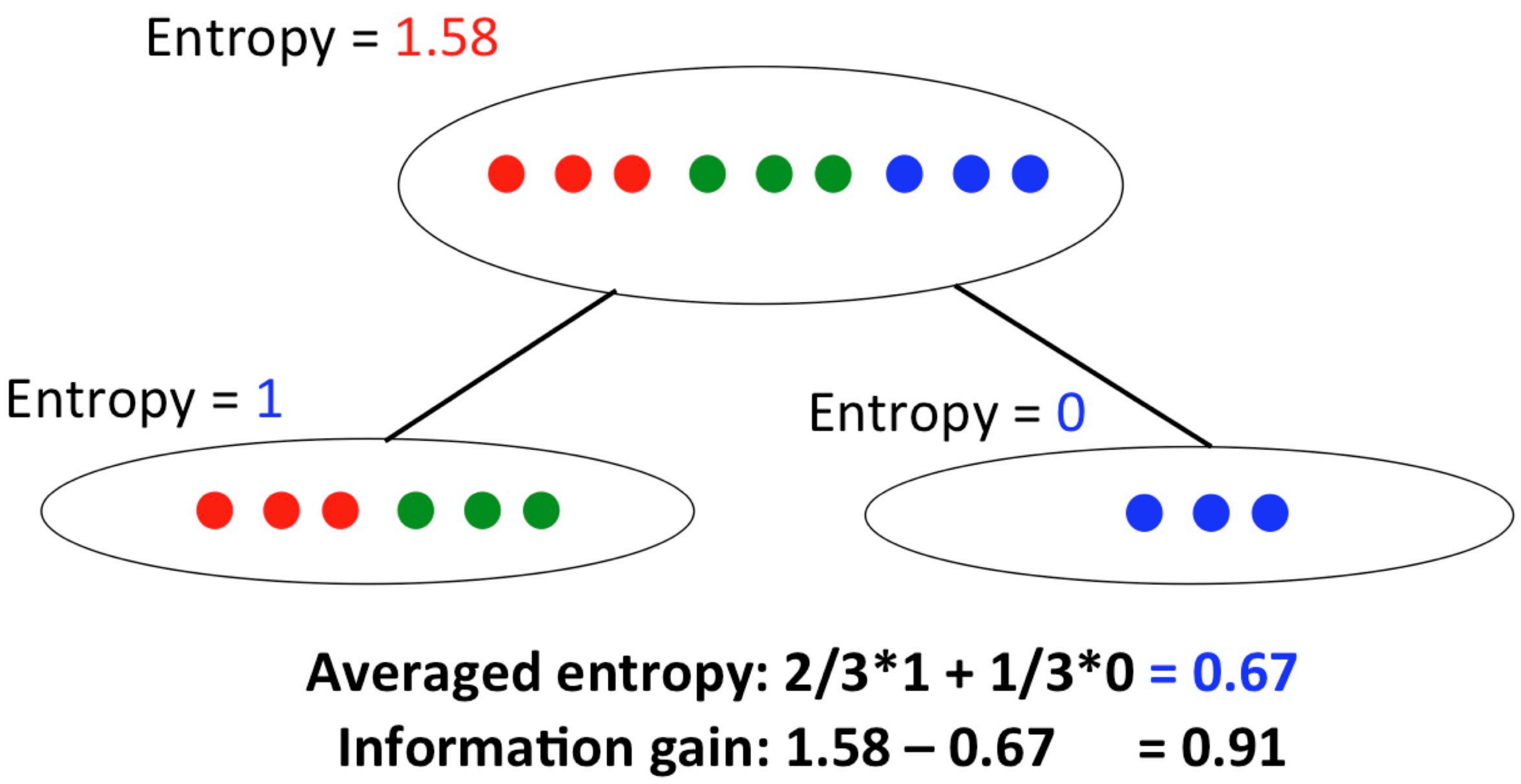

Decision Tree
Information Gain

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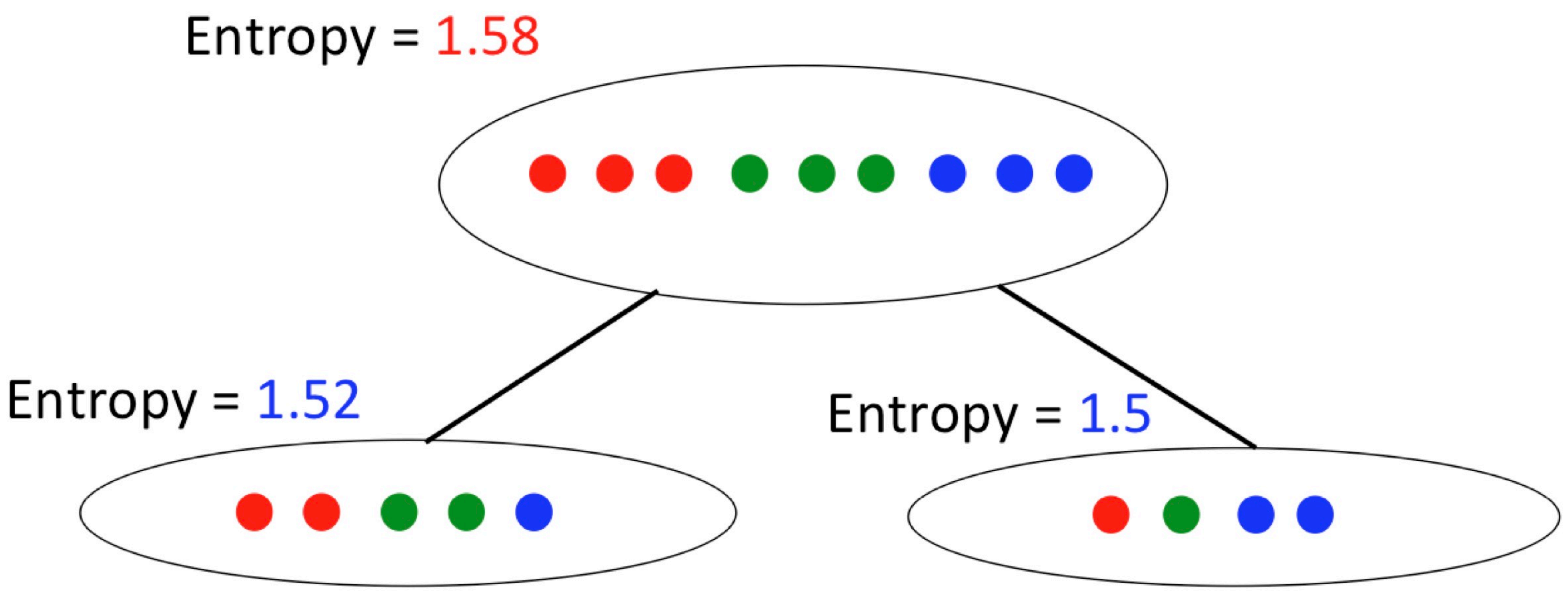

Averaged entropy: 1.51
Information gain: 1.58 – 1.51 = 0.07

Decision Tree

Splitting the node

- Given the current note, how to find the best split?

Decision Tree

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- For all the features and all the threshold
    - Compute the information gain after the split
    - Choose the best one (maximal information gain)

Decision Tree

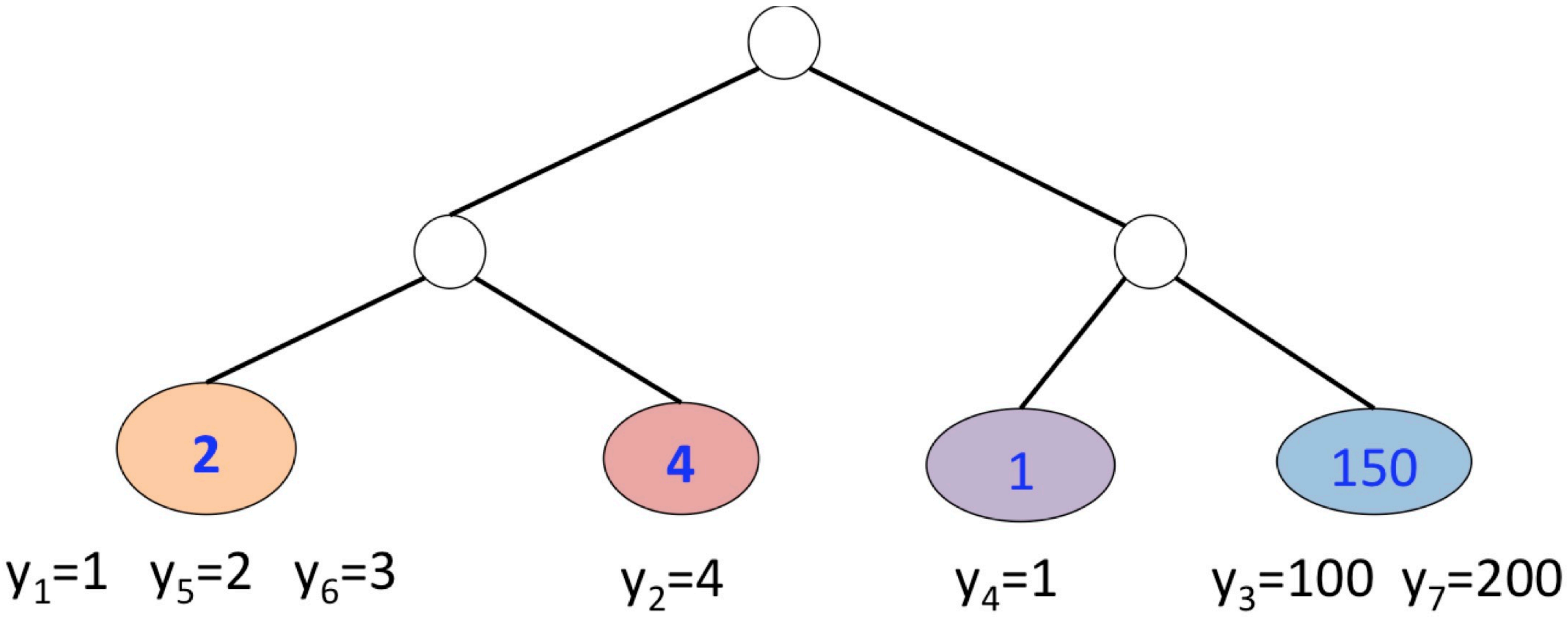
Splitting the node

- Given the current note, how to find the best split?
- For all the features and all the threshold
    - Compute the information gain after the split
    - Choose the best one (maximal information gain)
- For n samples and d features: need $O(nd)$ time

Decision Tree

Regression Tree

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



Decision Tree

Regression Tree

- Objective function:
    - $\min_F \frac{1}{n} \sum_{i=1}^{n} (y_i - F(x_i))^2 +$ (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

Decision Tree

Parameters

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

Decision Tree

Parameters

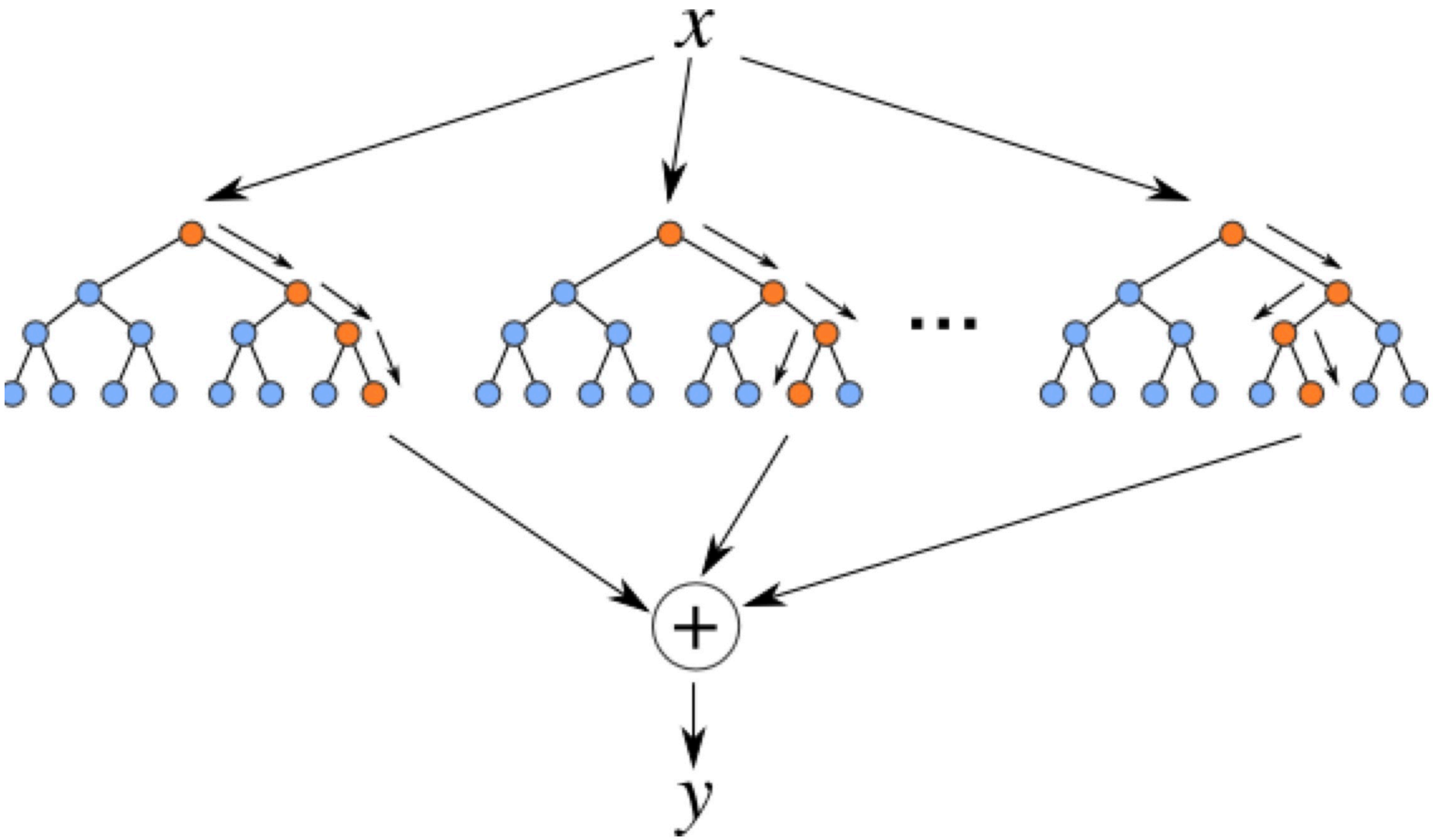
- Maximum depth: (usually ≈ 10)
- Minimum number of nodes in each node: (10, 50, 100)
- Single decision tree is not very powerful …
- Can we build multiple decision trees and ensemble them together?

Random Forest
Definition

- 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

Definition



Gradient Boosted Decision Tree

Boosted Decision Tree

- Minimize loss $\ell(y, F(x))$ with $F(\cdot)$ being ensemble trees
  - $F^* = \arg\min_F \sum_{i=1}^{n} \ell(y_i, F(x_i))$ with $F(x) = \sum_{m=1}^{T} f_m(x)$
  - (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 $f_m = \arg\min_{f_m} \sum_{i=1}^{N} \ell(y_i, F_{m-1}(x_i) + f_m(x_i))$
  - Update $F_m \leftarrow F_{m-1} + f_m$
- $F_m(x) = \sum_{j=1}^{m} f_j(x)$ is the prediction of 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

Gradient Boosted Decision Tree (GBDT)

- Approximate the current loss function by a quadratic approximation

$$\sum_{i=1}^{n} \ell(\hat{y}_i, F_{m-1}(x_i) + f_m(x_i)) \approx \sum_{i=1}^{n} (\ell_i(\hat{y}_i + g_i f_m(x_i) + \frac{1}{2} h_i f_m(x_i)^2)$$

- $$= \sum_{i=1}^{n} \frac{h_i}{2} \| f_m(x_i) - g_i / h_i \|^2 + \text{constant}$$

- 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

Gradient Boosted Decision Tree (GBDT)

- Finding $f_m(x, \theta_m)$ by minimizing the loss function:
- $$\arg\min_{f_m} \sum_{i=1}^{N} [f_m(x_i, \theta) - g_i/h_i]^2 + R(f_m)$$
    - 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 derivate yields better performance

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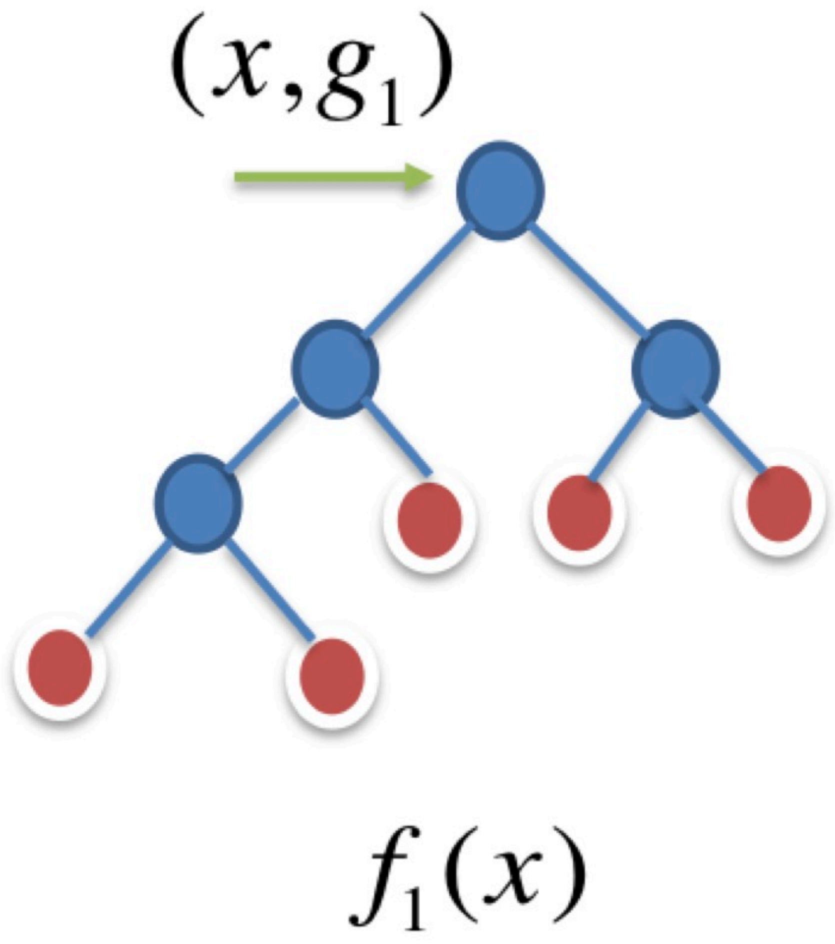
    - XGboost shows computing second order derivate yields better performance
- Algorithm:
  - Computing the current gradient for each $\hat{y}_i$
  - Building a base learner (decision tree) to fit the gradient
  - Updating current prediction $\hat{y}_i = F_m(x_i)$ for all i

Gradient Boosted Decision Tree

Gradient Boosted Decision Tree (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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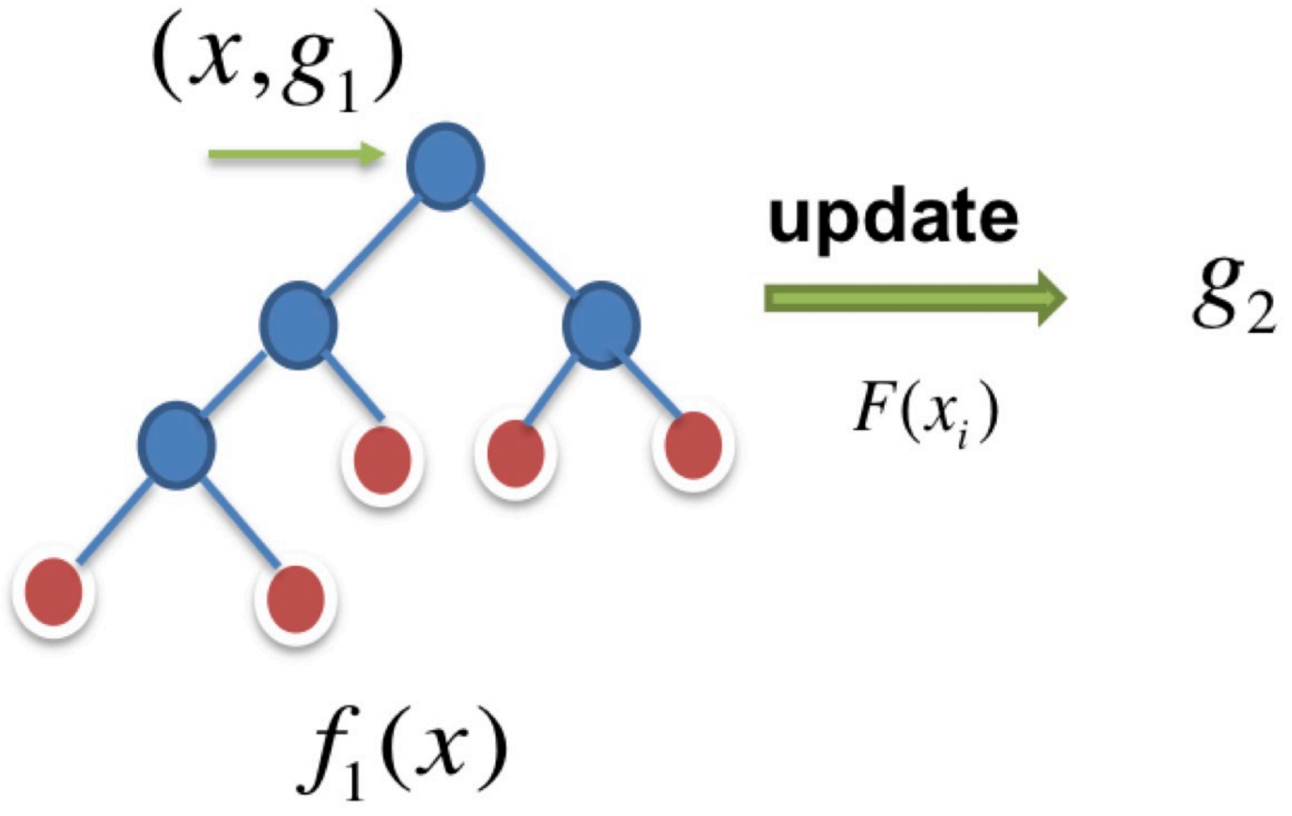

$$F_{m-1}(x_i) = \sum_{j=1}^{m-1} f_j(x_i) \qquad g_m(x_i) = \left.\frac{\partial \ell(y_i, F(x_i))}{\partial F(x_i)}\right|_{F(x_i)=F_{m-1}(x_i)}$$

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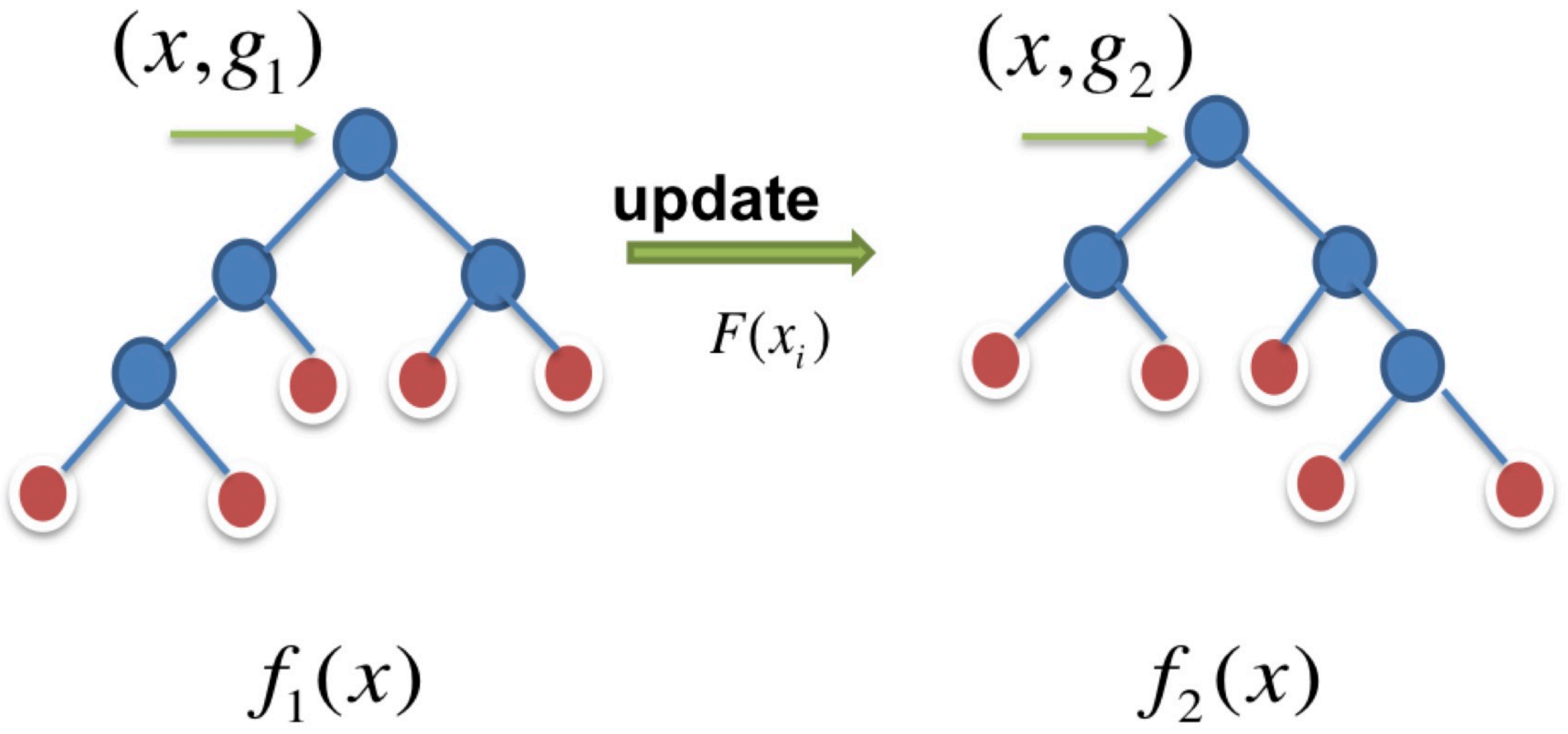

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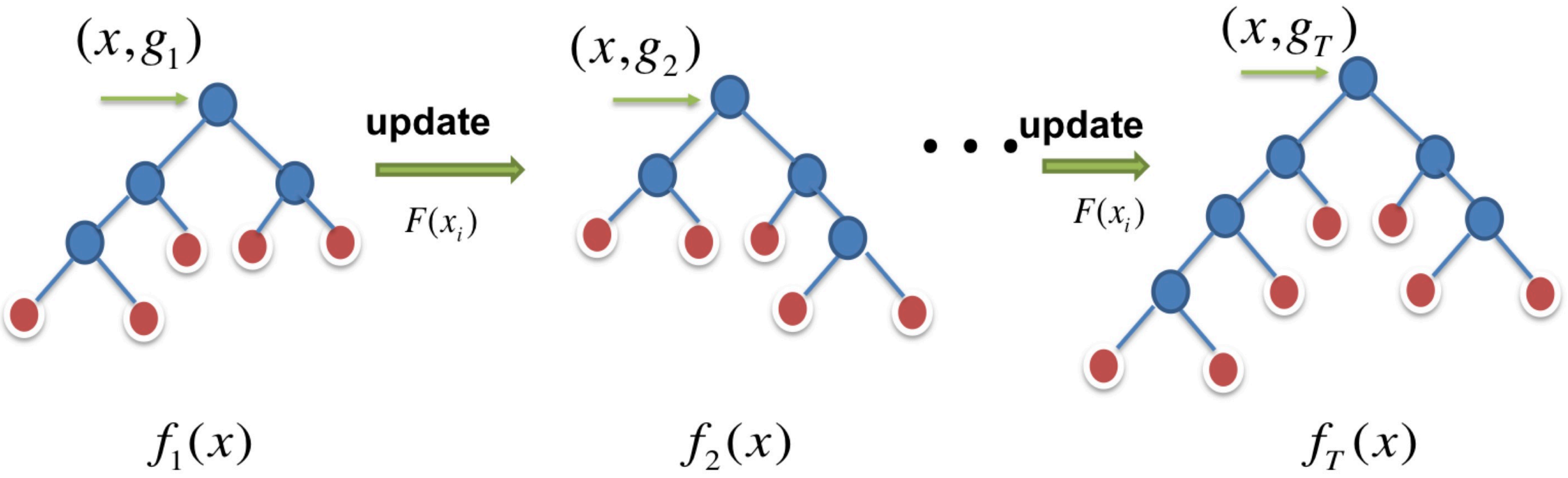

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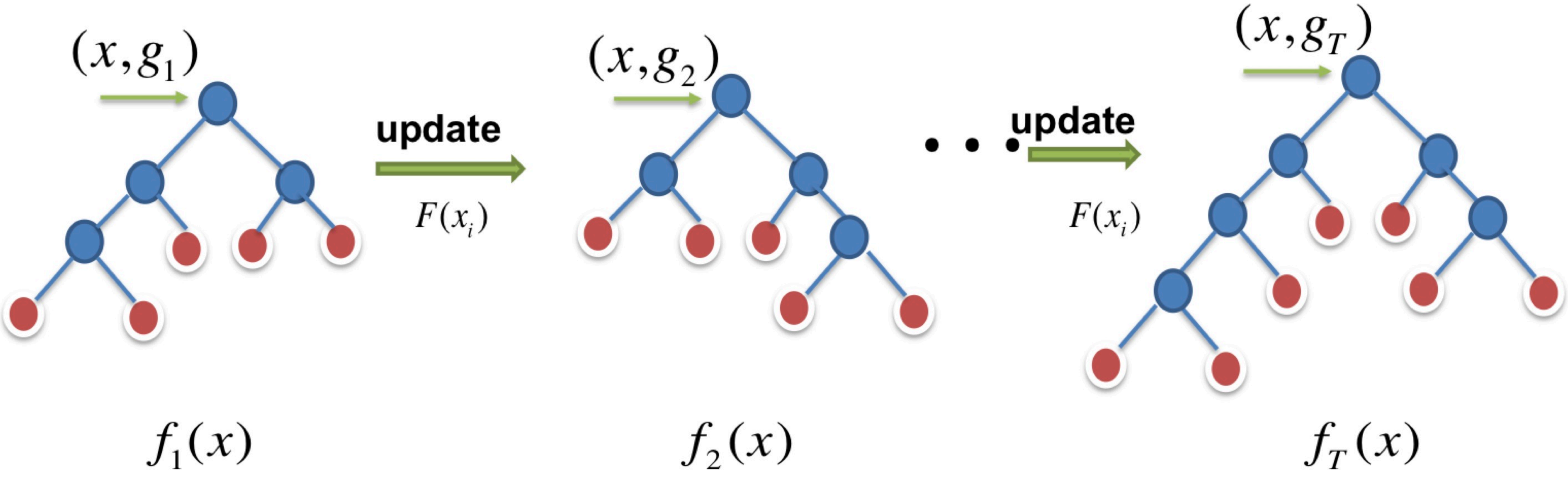

Final prediction $F(x_i) = \sum_{j=1}^{T} f_j(x_i)$

Gradient Boosted Decision Tree

Open source packages

- XGBoost: the first widely used tree-boosting software
- LightGBM: released by Microsoft
    - Histogram-based training approach — much faster than finding the best split
    - Good GPU support