ECS289: Scalable Machine Learning

Cho-Jui Hsieh
UC Davis

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Project Proposal

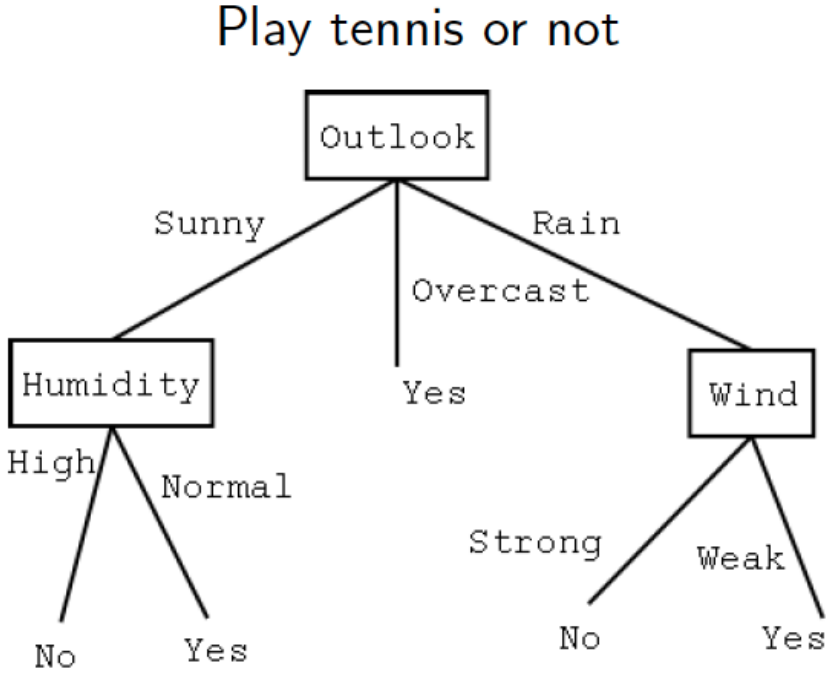
- Deadline: Oct 30 (Sunday), 11:59pm PST.
- Page limit: 2 pages (single column).
- Overview
- Related work (describe what has been done in the literature)
- Main idea and Technical approach
- Experiments (how to conduct experiments, what's the evaluation plan)
- Expect Result

Outline

- Decision Tree
- Random Forest
- Gradient Boosted Decision Tree

Decision Tree

- Decision trees are among the most widely used non-linear methods.



- Fast prediction: $O(p)$ (the average depth of the tree, usually less than 10)
- Small model size $O(2^p)$ (each node only needs two variables).

Splitting the node

- ID3, CART, ...

  Split the node to maximize the entropy

- Let S be the set of data points in a node and $c = 1, \cdots, C$ are the 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 $p(1) = \cdots = p(C)$

- The "information gain" of the split $S = S_1 \cup \cdots \cup S_T$:

$$H(S) - \sum_t \frac{|S_t|}{|S|} H(S_t)$$

Regression Tree

- Commonly used in Gradient Boosted Decision Tree (will see later)
- 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 $y^{(1)} = \frac{1}{|S_1|}\sum_{i\in S_1} y_i$, $y^{(2)} = \frac{1}{|S_2|}\sum_{i\in S_2} y_i$

Splitting the node

- Test all the features $\{1, \cdots, d\}$ and all the potential cutting values, and find the $(feature, value)$ pair that maximize information gain
- Assume the samples are sorted with respect to feature i:

$$(x_{\pi(1),d}, y_{\pi(1)}), (x_{\pi(2),d}, y_{\pi(2)}), \cdots, (x_{\pi(n),d}, y_{\pi(n)})$$

- Search through cut values according to the sorted list:

$$\frac{x_{\pi(1),d} + x_{\pi(2),d}}{2}, \frac{x_{\pi(2),d} + x_{\pi(3),d}}{2}, \cdots, \frac{x_{\pi(n-1),d} + x_{\pi(n),d}}{2}$$

- Maintain the "count" when scanning from left to right:

$$\text{number of class } i \text{ on left/right for all } i$$

  Can be maintained in constant time
- $O(\bar{n}d)$ for splitting each node ($\bar{n}$: $numberofsamplesinthecurrentnode$)

Parameters

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

Parallel Decision Tree

- Naive approach: each thread (machine) computes the split of a node

  Poor performance due to imbalance work load
- Better approach: splitting all the nodes in the same level together

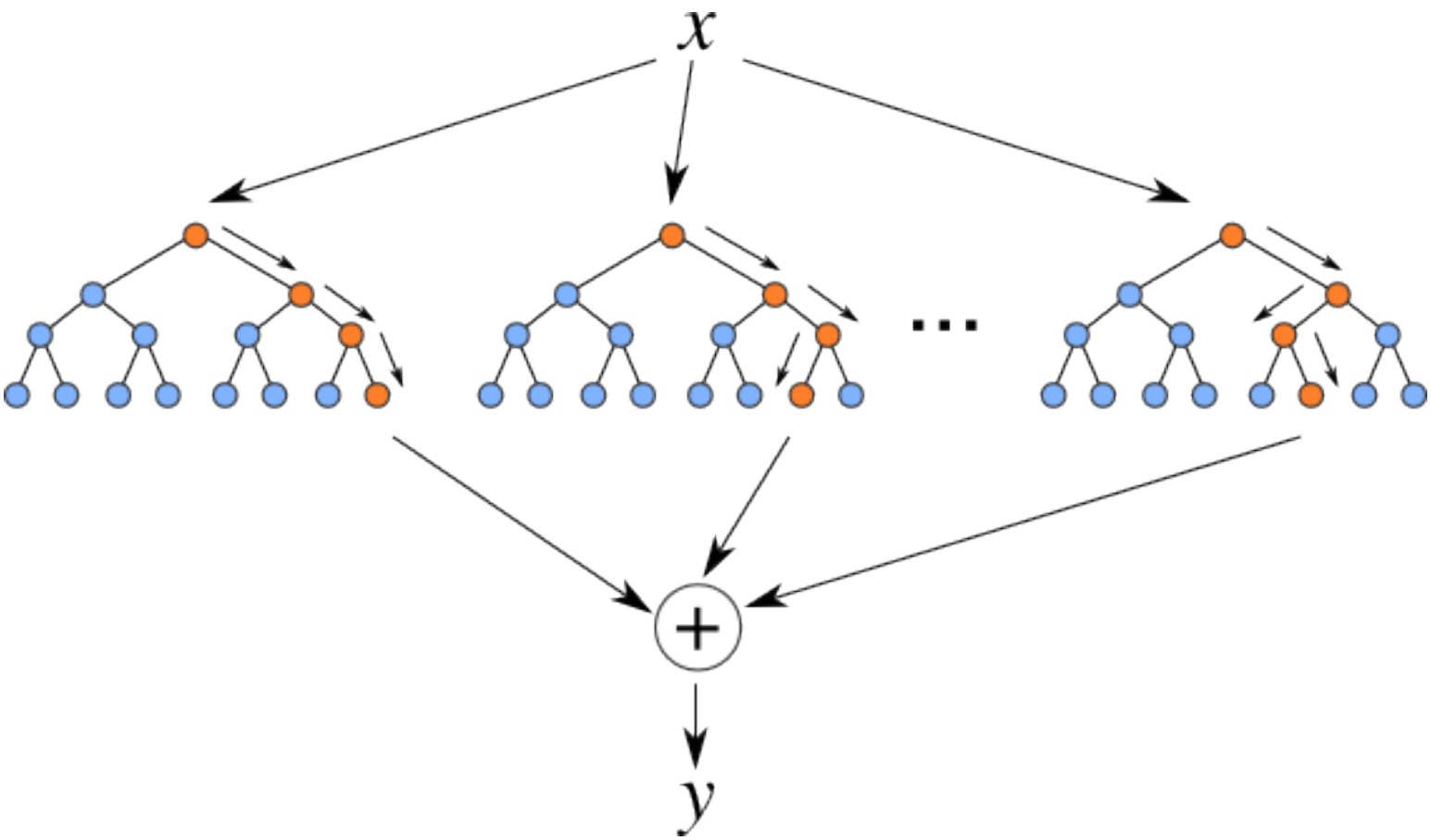
  Feature parallelism

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: Scikit Learn

Random Forest



Embarrassingly parallel

Gradient Boosted Decision Tree

Boosted Decision Tree

- Goal: minimizing a loss function $\ell(y, F(x))$ using boosting method.
- Gradient boosting considers estimating F in an additive form:

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

- Direct loss minimization: at each stage m, find the best function to minimize objective function:
  - solve $\theta_m = \operatorname{argmin}_\theta \sum_{i=1}^{N} \ell(y_i, F_{m-1}(\boldsymbol{x}_i) + f_m(\boldsymbol{x}_i, \theta))$
  - update $F_m(\boldsymbol{x}) \leftarrow F_{m-1}(\boldsymbol{x}) + f_m(\boldsymbol{x}, \theta_m)$
- $F_m(\boldsymbol{x}) = \sum_{j=1}^{m} f_j(\boldsymbol{x}, \theta_j)$ 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:

$$\sum_{i=1}^{n} \ell_i(\hat{y}_i + f_m(\boldsymbol{x}_i)) \approx \sum_{i=1}^{n} \left(\ell_i(\hat{y}_i) + g_i f_m(\boldsymbol{x}_i) + \frac{1}{2} h_i f_m(\boldsymbol{x}_i)^2\right)$$

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

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:

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

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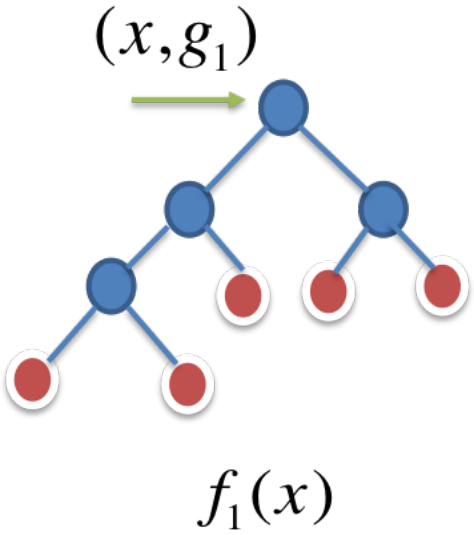
  - XGboost shows computing second order derivative yields better performance
- Algorithm:
  - Computing the current gradient for each $\hat{y}_i$.
  - Building a base learner (decision tree) to fit the gradient.
  - Updating current prediction $\hat{y}_i = F_m(\boldsymbol{x}_i)$ for all i.

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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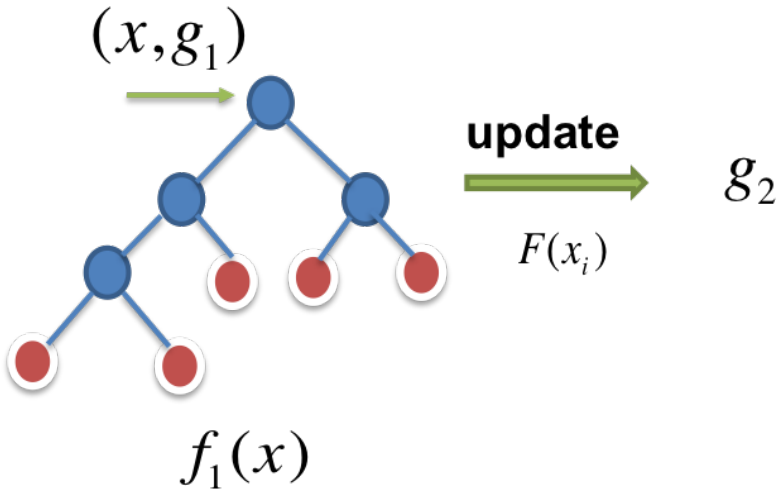

$$F_{m-1}(x_i) = \sum_{j=1}^{m-1} f_j(x_i) \qquad g_m(x_i) = \left. \frac{\partial \ell(y_i, F(x_i))}{\partial F(x_i)} \right|_{F(x_i)=F_{m-1}(x_i)}$$

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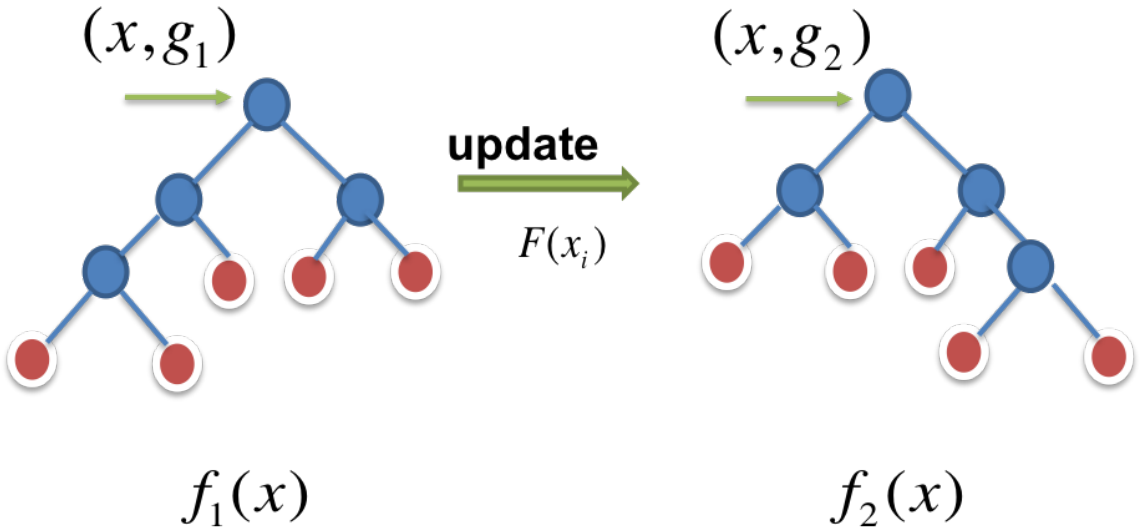

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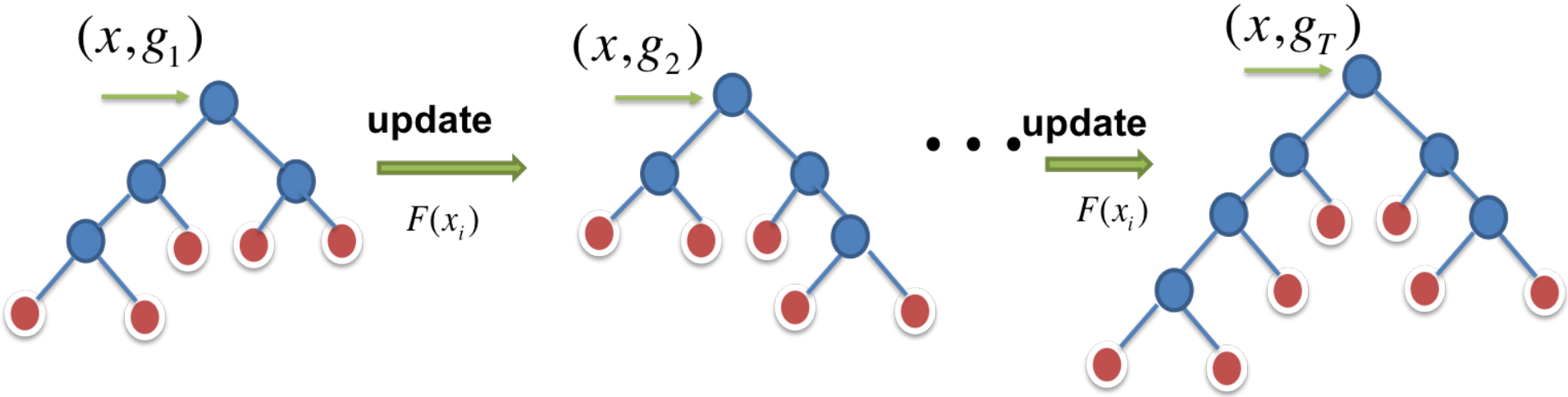

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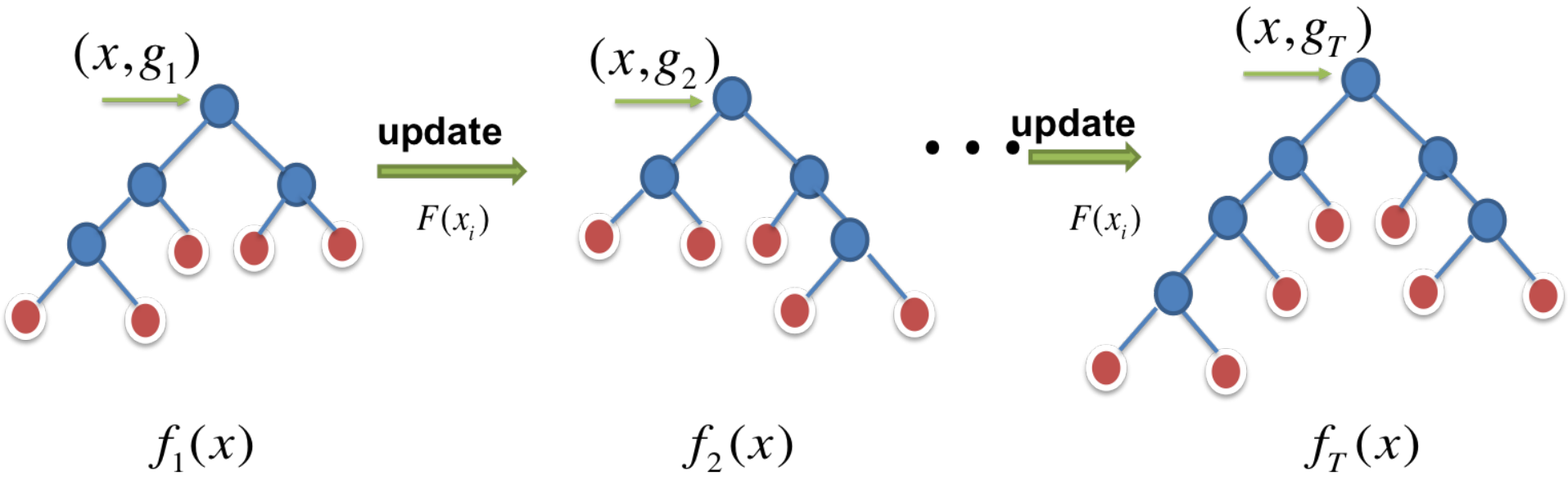

Final prediction $F(x_i) = \sum_{j=1}^{T} f_j(x_i)$

Example

- Learning to rank: given samples $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ and a set of pairwise comparisons $\Omega = (i, j, y_{ij})$, minimize the ranking loss

$$\min_f \sum_{(i,j)\in\Omega} \max(1 - y_{ij}(f(\boldsymbol{x}_i) - f(\boldsymbol{x}_j)), 0).$$

  $y_{ij} = \{+1, -1\}$ is the pairwise comparison results.
- Hard to directly construct a tree to minimize ranking loss
- Easy to compute the gradient of the objective function given the current f

  $\Rightarrow$ GBDT becomes the best algorthm for learning to rank

Parallelism

- Parallelize the construction of decision tree.
- Feature-parallelism: each machine/core computes the best splits for a subset of features.

Coming up

Questions?