# Dive into XGBoost

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# 目录


- 数学理论
- 系统设计
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# 数学理论

$$f(x_{k+1}) = f(x_k + x_{k+1} - x_k) \approx f(x_k) + \nabla f(x_k)(x_{k+1} - x_k)$$

$$f(x_{k+1}) < f(x_k) \Rightarrow \nabla f(x_k)(x_{k+1} - x_k) < 0$$

$$x_{k+1} = x_k - \gamma \nabla f(x_k)$$

$$\nabla f(x_k) = 0, x_{k+1} = x_k$$

# 数学理论

$$f(x) = l(h(x, D), Y) \qquad h(x, d) = \frac{1}{1 + e^{-xd}}$$

$$l(h(x, D), Y) = \prod_{d \in D, y \in Y} (h(x, d)^y (1 - h(x, d)^{1-y}))$$

$$\begin{aligned} l(H(x_{k+1})) &= l(H(x_t) + h(x_{t+1})) \\ &\approx l(H(x_t)) + \nabla l(H(x_t)) h(x_{t+1}) \end{aligned} \qquad H(x_t) = \sum_{i=1}^{t} h(x_i)$$

# 数学理论

$$H(x_{t+1}) = H(x_t) - \gamma \nabla l(H(x_t)) \quad H(x_t) = \sum_{i=1}^{t} h(x_i)$$

$$h(x_{t+1}) = -\gamma \nabla l(H(x_t))$$

$$h : D \xrightarrow{x} \nabla l(H(x_t, D))$$

# 数学理论

**Model Formalization:**

$$\hat{y}_i = \phi(x_i) = \sum_{k=1}^{K} f_k(x_i), f_k \in F$$

**Training Objective:**

$$L(\phi) = \sum_i l(y_i, \hat{y}_i) + \sum_k \Omega(f_k)$$

# 数学理论

$$L^{(t)} = \sum_{i=1}^{n} l(y_i, \hat{y}_i{}^{(t)}) + \sum_{i=1}^{t} \Omega(f_i)$$

$$= \sum_{i=1}^{n} l(y_i, \hat{y}_i{}^{(t-1)} + \boxed{f_t(x_i)}) + \sum_{i=1}^{t} \Omega(f_i)$$

# 数学理论

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

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

**remove constant terms!**

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

# 数学理论

$$q : \mathbb{R}^d \rightarrow \{1, 2, ..., T\}$$

$$f_t(x) = w_{q(x)} \longrightarrow \Omega(f_t) = \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} w_j^2$$

$$\widetilde{L}^{(t)} = \sum_{i=1}^{n} [g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i)] + \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} w_j^2$$

$$= \sum_{j=1}^{T} [(\sum_{i \in I_j} g_i) w_j + \frac{1}{2}(\sum_{i \in I_j} h_i + \lambda) w_j^2] + \gamma T$$

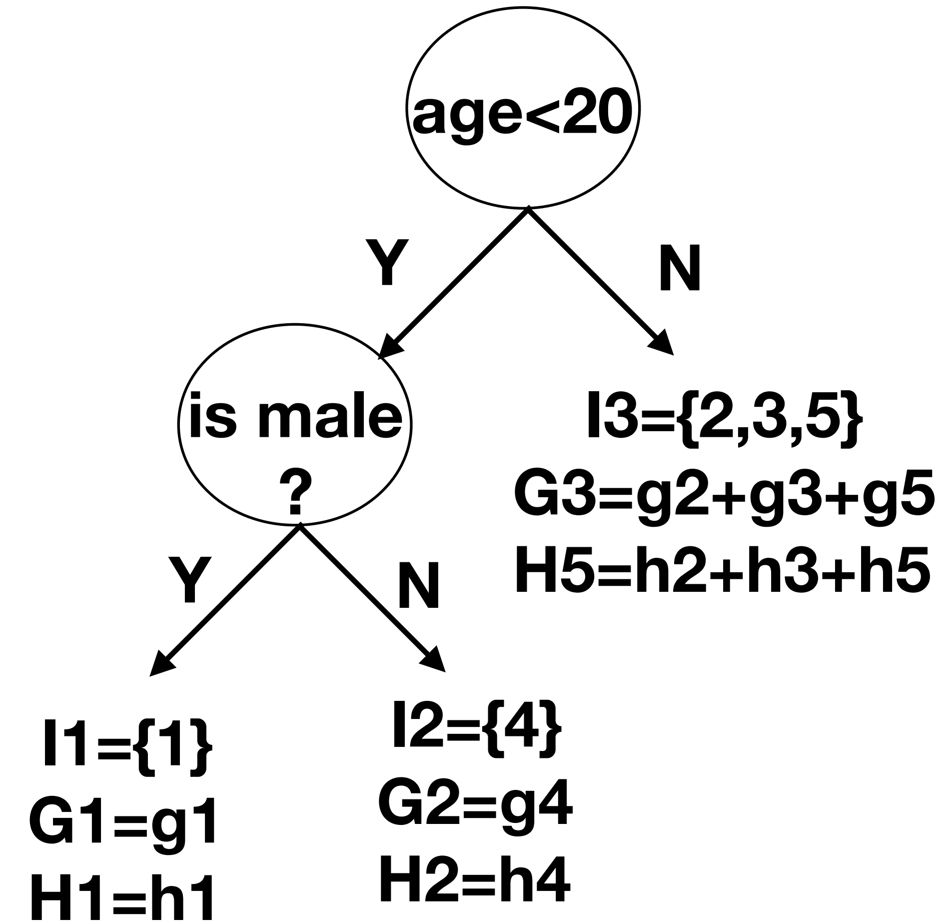
# 数学理论

$$w_j^* = -\frac{\sum_{i \in I_j} g_i}{\sum_{i \in I_j} h_i + \lambda}$$

$$\widetilde{L}^{(t)}(q) = -\frac{1}{2} \sum_{j=1}^{T} \frac{\left(\sum_{i \in I_j} g_i\right)^2}{\sum_{i \in I_j} h_i + \lambda} + \gamma T$$

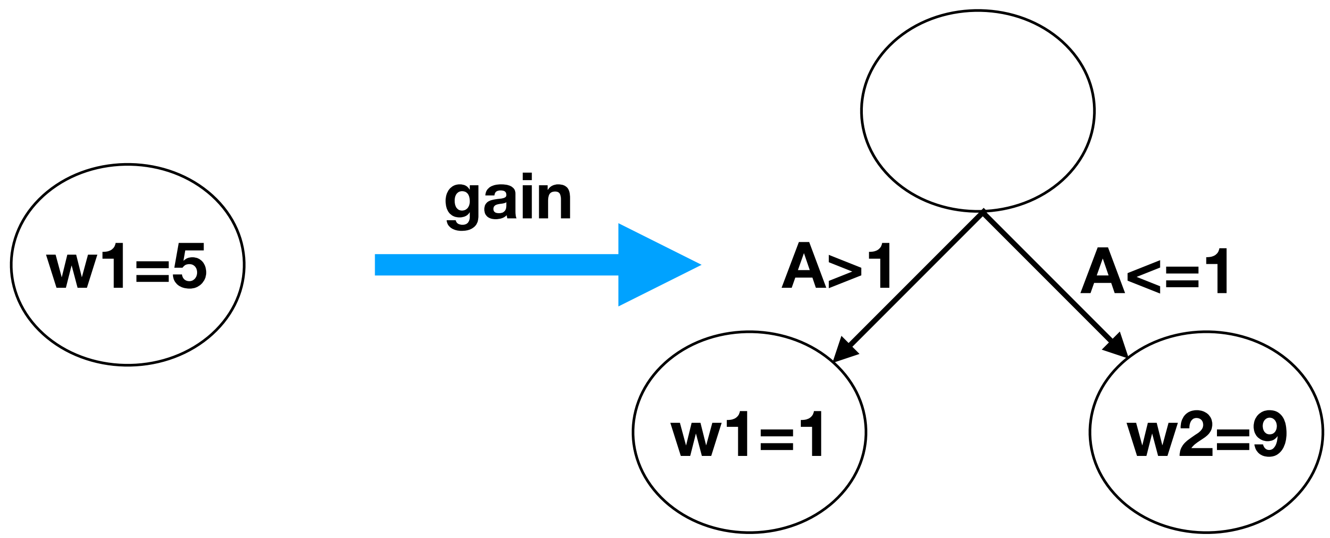
# Example

| Index | G | H |
|---|---|---|
| 1 | g1 | h1 |
| 2 | g2 | h2 |
| 3 | g3 | h3 |
| 4 | g4 | h4 |
| 5 | g5 | h5 |




$$Obj = -\sum_j \frac{G_j^2}{H_j + \lambda} + 3\gamma$$

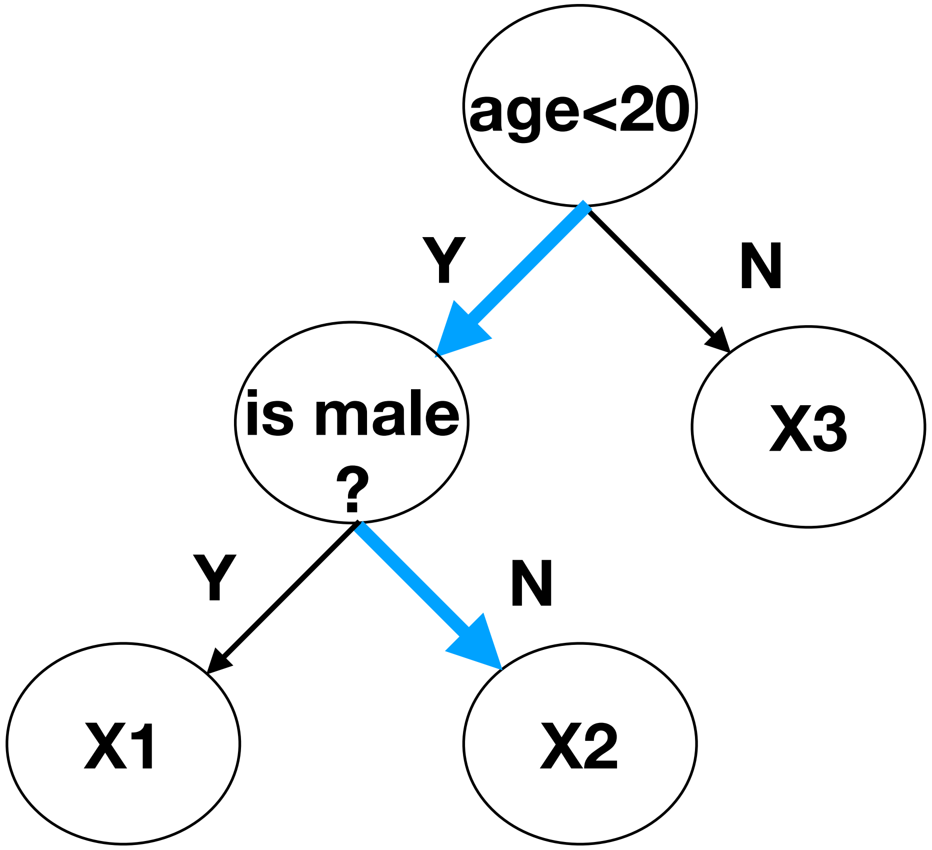
# Tree Growing Algorithm




$$gain = \frac{1}{2}\left[\frac{(\sum_{i\in I_L} g_i)^2}{\sum_{i\in I_L} h_i + \lambda} + \frac{(\sum_{i\in I_R} g_i)^2}{\sum_{i\in I_R} h_i + \lambda} - \frac{(\sum_{i\in I} g_i)^2}{\sum_{i\in I} h_i + \lambda}\right] - \gamma$$

# Missing Values Handling

| example | Age | Gender |
|---|---|---|
| X1 | ? | male |
| X2 | 15 | ? |
| X3 | 25 | female |




**Time Complexity:**

$$O(ndKlogn) \xrightarrow{\text{pre-sorted features}} O(ndK)$$

# Alg-1

**Algorithm 1:** Exact Greedy Algorithm for Split Finding

**Input**: $I$, instance set of current node
**Input**: $d$, feature dimension
$gain \leftarrow 0$
$G \leftarrow \sum_{i \in I} g_i$, $H \leftarrow \sum_{i \in I} h_i$
**for** $k = 1$ ***to*** $m$ **do**
  $G_L \leftarrow 0, \ H_L \leftarrow 0$
  **for** $j$ *in sorted*$(I$, *by* $\mathbf{x}_{jk})$ **do**
    $G_L \leftarrow G_L + g_j, \ H_L \leftarrow H_L + h_j$
    $G_R \leftarrow G - G_L, \ H_R \leftarrow H - H_L$
    $score \leftarrow \max(score, \frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{G^2}{H+\lambda})$
  **end**
**end**
**Output**: Split with max score

# Alg-2

**Algorithm 2:** Approximate Algorithm for Split Finding

**for** $k = 1$ ***to*** $m$ **do**

  Propose $S_k = \{s_{k1}, s_{k2}, \cdots s_{kl}\}$ by percentiles on feature $k$.

  Proposal can be done per tree (global), or per split(local).

**end**

**for** $k = 1$ ***to*** $m$ **do**

  $G_{kv} \leftarrow= \sum_{j \in \{j | s_{k,v} \geq \mathbf{x}_{jk} > s_{k,v-1}\}} g_j$

  $H_{kv} \leftarrow= \sum_{j \in \{j | s_{k,v} \geq \mathbf{x}_{jk} > s_{k,v-1}\}} h_j$

**end**

Follow same step as in previous section to find max score only among proposed splits.

# Alg-3

**Algorithm 3:** Sparsity-aware Split Finding

**Input:** $I$, instance set of current node
**Input:** $I_k = \{i \in I | x_{ik} \neq \text{missing}\}$
**Input:** $d$, feature dimension
*Also applies to the approximate setting, only collect statistics of non-missing entries into buckets*
$gain \leftarrow 0$
$G \leftarrow \sum_{i \in I} g_i, H \leftarrow \sum_{i \in I} h_i$
**for** $k = 1$ *to* $m$ **do**
    *// enumerate missing value goto right*
    $G_L \leftarrow 0, \ H_L \leftarrow 0$
    **for** $j$ *in sorted(*$I_k$*, ascent order by* $\mathbf{x}_{jk}$*)* **do**
        $G_L \leftarrow G_L + g_j, \ H_L \leftarrow H_L + h_j$
        $G_R \leftarrow G - G_L, \ H_R \leftarrow H - H_L$
        $score \leftarrow \max(score, \frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{G^2}{H+\lambda})$
    **end**
    *// enumerate missing value goto left*
    $G_R \leftarrow 0, \ H_R \leftarrow 0$
    **for** $j$ *in sorted(*$I_k$*, descent order by* $\mathbf{x}_{jk}$*)* **do**
        $G_R \leftarrow G_R + g_j, \ H_R \leftarrow H_R + h_j$
        $G_L \leftarrow G - G_R, \ H_L \leftarrow H - H_R$
        $score \leftarrow \max(score, \frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{G^2}{H+\lambda})$
    **end**
**end**
**Output:** Split and default directions with max gain

# 训练过程

初始化模型参数；

设置training sample默认预测值为相同类别，计算grad和hess；

**从第一棵树直到设定的树的数目：**

grad’, hess’=(grad, hess)*sample_weight；

原始数据集行列采样得到采样后数据集D；

对D进行划分，X=(属性集合)，Y=(真实值，预测值，grad’，hess’)；

建树，返回树模型curTree；

更新预测值(学习率*新的预测值)，grad，hess；

子树添加到根树；打印训练信息；

# 建树过程

初始化参数，获取训练数据X,Y；

**判断当前训练样本是否构成叶子节点**，如果是，计算叶子节点score并返回当前TreeNode，内含信息：叶子标志，叶子得分；否则，执行下一步；

对X列采样，得到X_selected;

找到X_selected的最佳属性，最佳属性分割阈值，最佳gain，空值默认分割方向；

如果**最佳gain为负**，构成叶子节点，返回当前TreeNode；

分割X；分别对X的左右子树建树；

属性重要性计数；

返回TreeNode，内含信息：左右子树，分割属性，分割阈值，分割方向；

# 预测过程

初始化预测值pred为0；

对根树中的每一棵子树：//RandomForest的区别

//并行加速

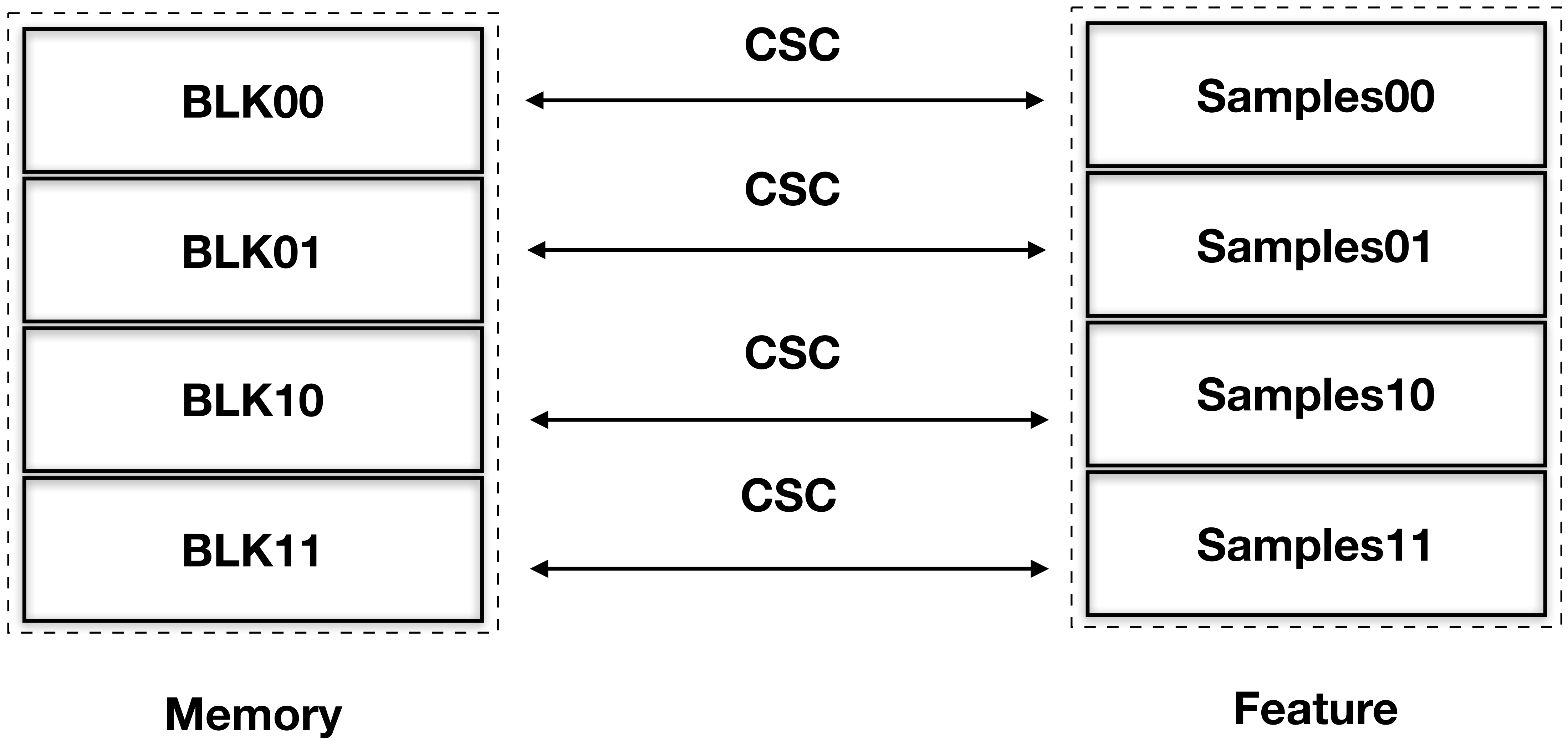
pred += 学习率*每棵树的预测结果；

返回预测结果pred；

# 系统设计

- ☐ Column Block for Parallel Learning
  - ☑ exact greedy, approximate
- ☐ Cache-aware Access
  - ☑ exact greedy: cache-aware prefetching
  - ☑ approximate:  choose better block size to balance cache property  and parallelization
- ☐ Blocks for Out-of-core Computation
  - ☑ block compression, block sharding

# Column-Block



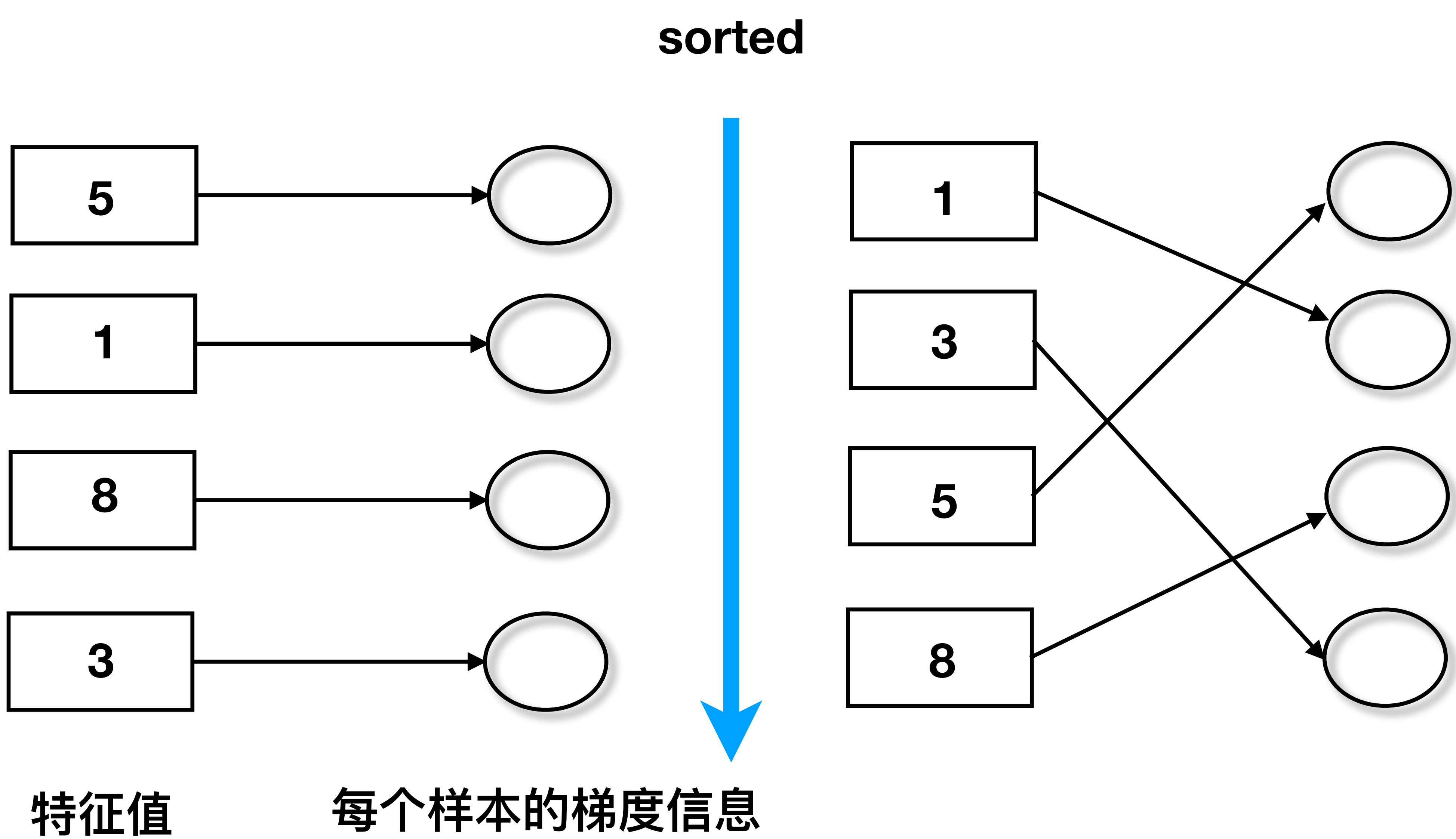
# Compressed Row Storage

$$A = \begin{pmatrix} 10 & 0 & 0 & 0 & -2 & 0 \\ 3 & 9 & 0 & 0 & 0 & 3 \\ 0 & 7 & 8 & 7 & 0 & 0 \\ 3 & 0 & 8 & 7 & 5 & 0 \\ 0 & 8 & 0 & 9 & 9 & 13 \\ 0 & 4 & 0 & 0 & 2 & -1 \end{pmatrix}$$

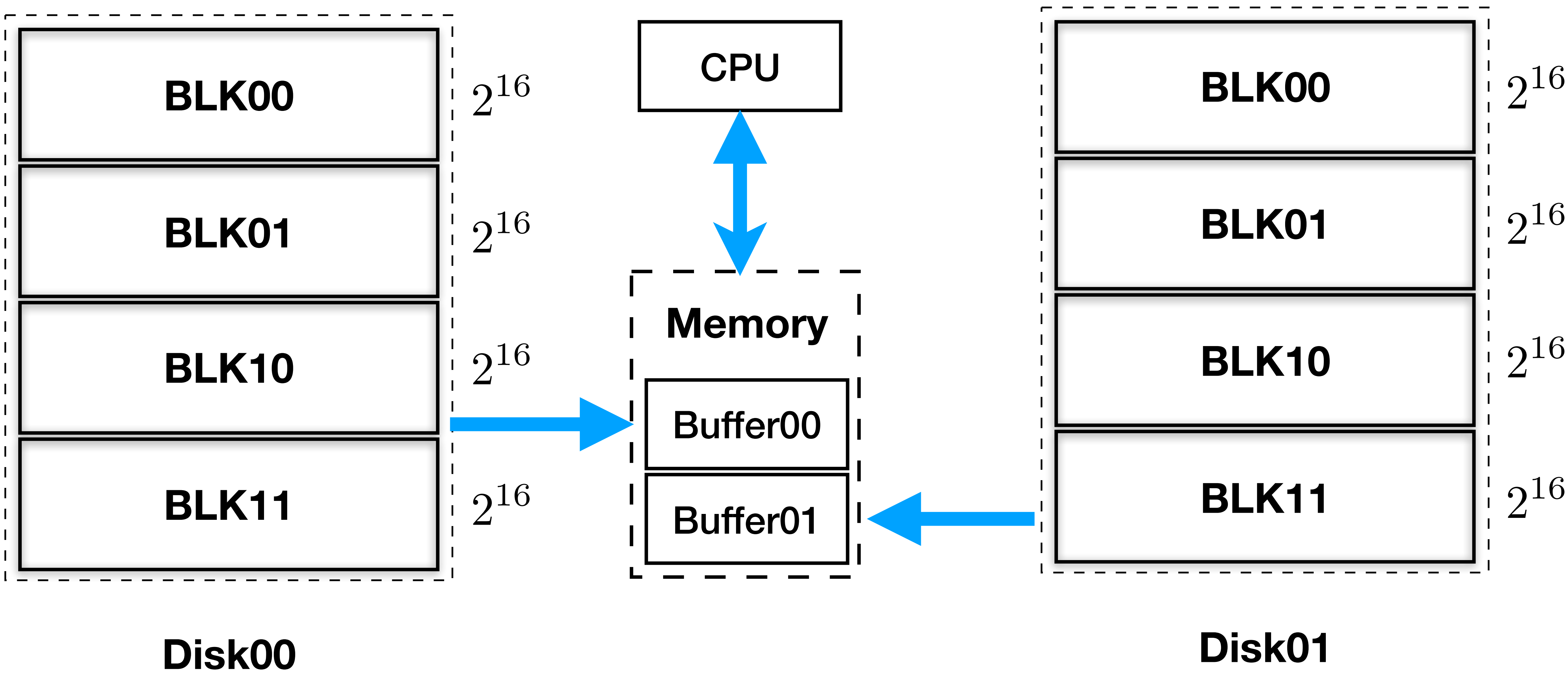
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| row_ptr | 1 | 3 | 6 | 9 | 13 | 17 | 20 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| val | 10 | -2 | 3 | 9 | 3 | 7 | 8 | 7 | 3 ⋯ 9 | 13 | 4 | 2 | -1 |
| col_ind | 1 | 5 | 1 | 2 | 6 | 2 | 3 | 4 | 1 ⋯ 5 | 6 | 2 | 5 | 6 |

# Cache-Aware



# Out-of-core Computation



# 模型应用

- ☑ Feature Importance
- ☑ Customized Metric/Loss Function
- ☑ Combination Features(stacking)

# 参考文献


1.XGBoost的Github地址: https://github.com/dmlc/xgboost

2.XGBoost的tiny实现：https://github.com/zhpmatrix/groot

3.GBDT的实现：https://github.com/liuzhiqiangruc/dml/tree/master/gbdt

4.《Higgs Boson Discovery with Boosted Trees》, JMLR Workshop，Tianqi Chen, Tong He, 2015

5.《XGBoost: A Scalable Tree Boosting System》, KDD, Tianqi Chen, Carlos Guestrin, 2016

6.《Practical Lessons from Predicting Clicks on Ads at Facebook》, Xinran He

7.XGBoost源码阅读：https://zhpmatrix.github.io/2017/03/15/xgboost-src-reading-2

# TKS

有啥问题需要探讨的吗?