# Statistical Machine Learning

7주차

담당: 15기 박지우

1. XgBoost

2. LightGBM

3. CatBoost

# 1. XgBoost

# XgBoost

- XgBoost는 기존 Gradient Tree Boosting 알고리즘에 과적합 방지를 위한 기법이 추가된 지도 학습 알고리즘

정의

1) XgBoost는 Gradient Tree Boosting
2) XgBoost는 과적합 방지를 위한 기법이 추가된 알고리즘

# XgBoost

$$F_0(x) = \arg\min_c \sum_{i=1}^{n} L(y_i, c)$$

$$g_i = \left[ \frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} \right]_{F(x)=F_{m-1}(x)}$$

$$h_i = \left[ \frac{\partial^2 L(y_i, F(x_i))}{\partial F(x_i)^2} \right]_{F(x)=F_{m-1}(x)}$$

$$\phi_m = \arg\min_\phi \sum_{i=1}^{n} \frac{1}{2} h_i \left[ -\frac{g_i}{h_i} - \phi(x_i) \right]^2 + \gamma T + \frac{1}{2} \lambda \|\phi\|^2$$

$$F_m(x) = F_{m-1}(x) + l \cdot \phi_m(x)$$

$$F_M(x) = \sum_{m=0}^{M} F_m(x)$$

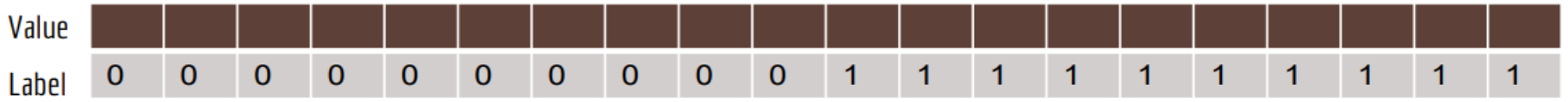
# XgBoost

$$l = \sum_{i=1}^{n} L(y_i, F_{m-1}(x_i) + \phi(x_i)) + \gamma T + \frac{1}{2}\lambda \|\phi\|^2$$

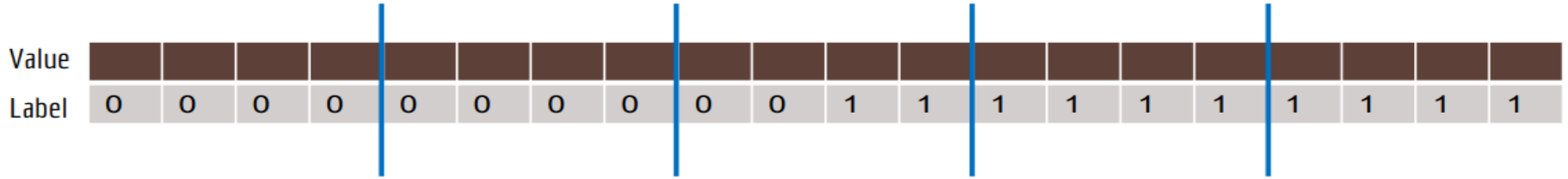
$$\begin{aligned}\tilde{l} &= \sum_{i=1}^{n} \left[ g_i \phi(x_i) + \frac{1}{2} h_i \phi(x_i)^2 \right] + \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} w_j^2 \\ &= \sum_{j=1}^{T} \left[ \left( \sum_{x_i \in R_j} g_i \right) w_j + \frac{1}{2} \left( \sum_{x_i \in R_j} h_i + \lambda \right) w_j^2 + \gamma \right]\end{aligned}$$

# XgBoost

**Previous Tree Models - Basic exact greedy algorithm**

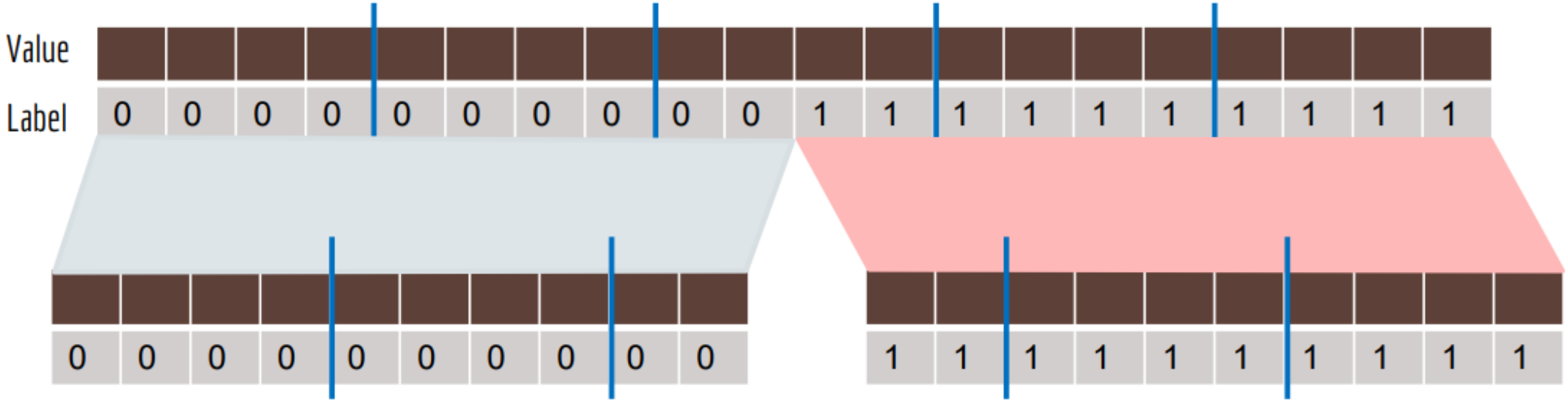



**Split Finding Algorithm**



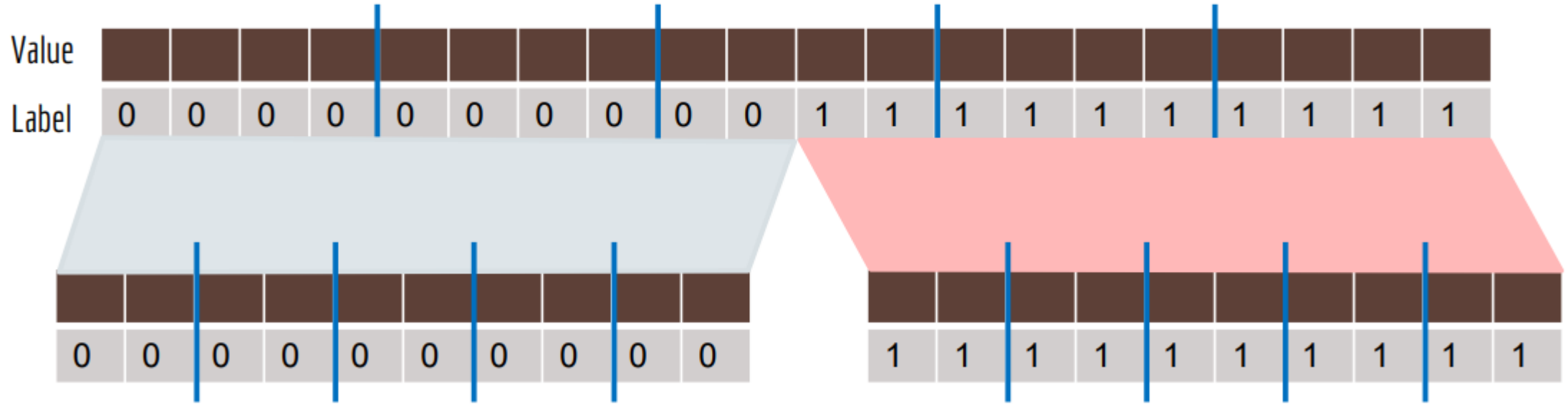
# XgBoost

## Global Variant

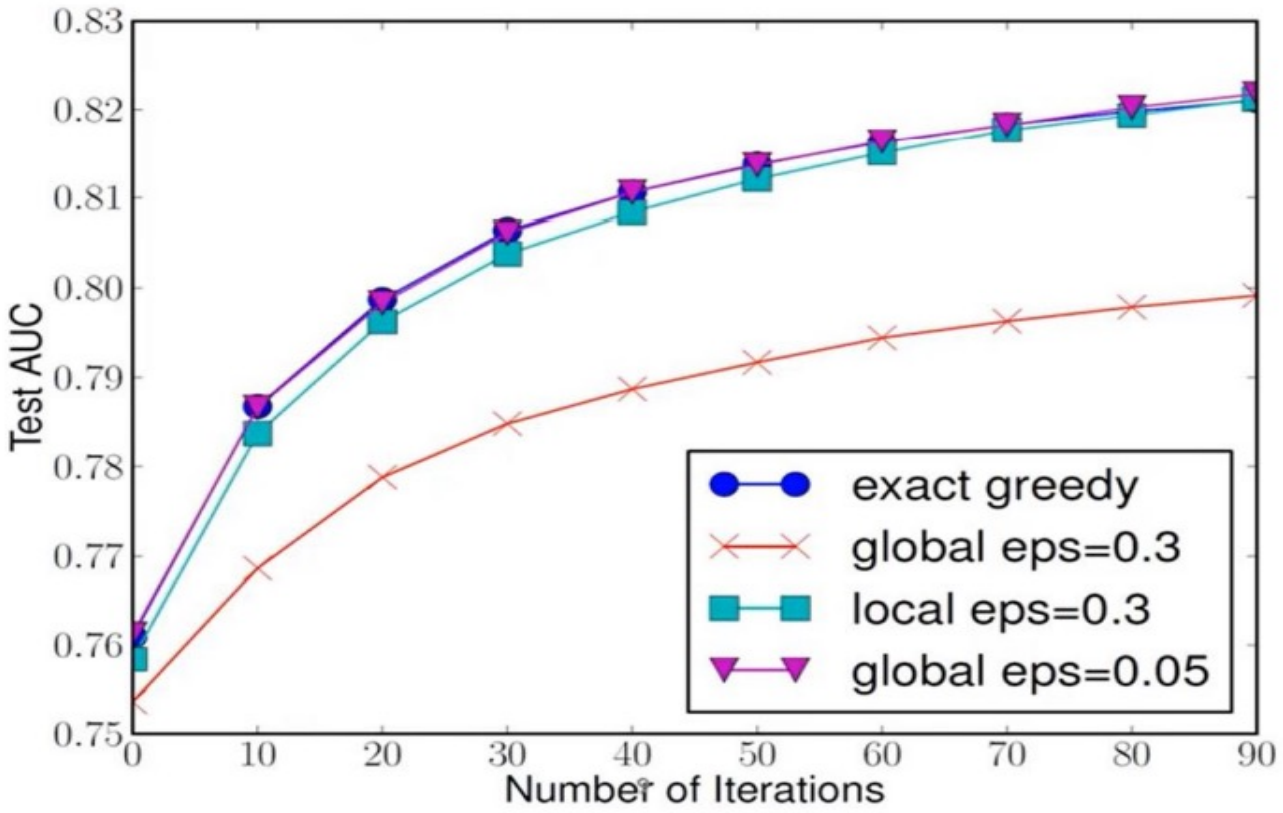


# XgBoost

## Local Variant

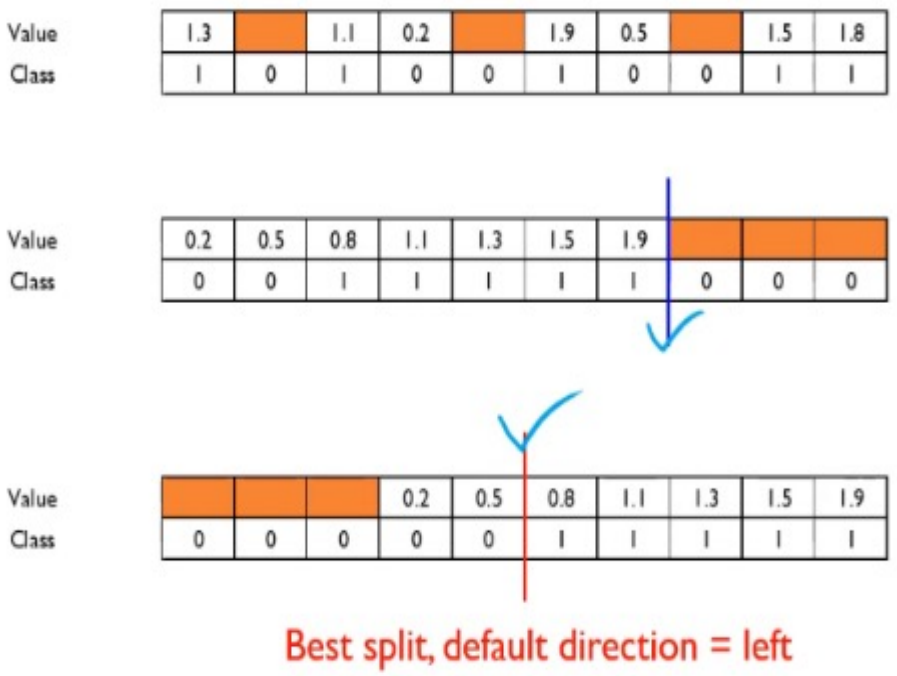


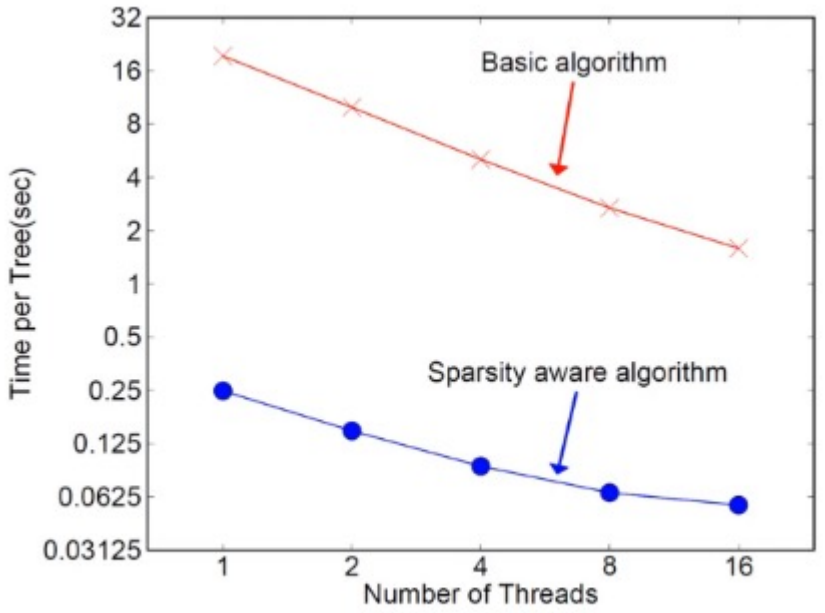
# XgBoost




Number of Buckets: $1/\xi$

# XgBoost


Value
Class
1.3 1.1 0.2 1.9 0.5 1.5 1.8
1 0 1 0 0 1 0 0 1 1
Value
Class
0.2 0.5 0.8 1.1 1.3 1.5 1.9
0 0 1 1 1 1 1 0 0 0
Value
Class
0.2 0.5 0.8 1.1 1.3 1.5 1.9
0 0 0 0 0 1 1 1 1 1
Best split, default direction = left

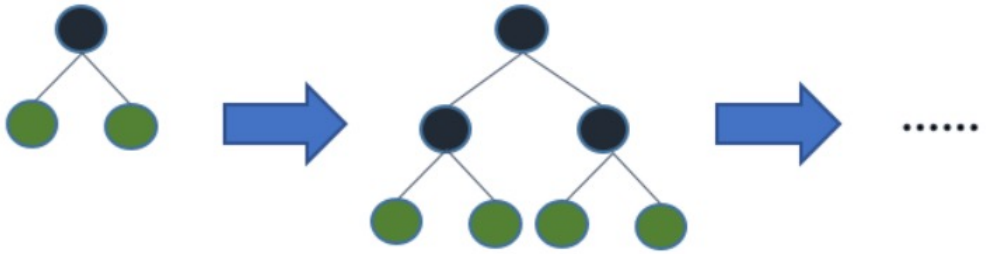

Time per Tree(sec)
32
16
8
4
2
1
0.5
0.25
0.125
0.0625
0.03125
Basic algorithm
Sparsity aware algorithm
1
2
4
8
16
Number of Threads

# XgBoost

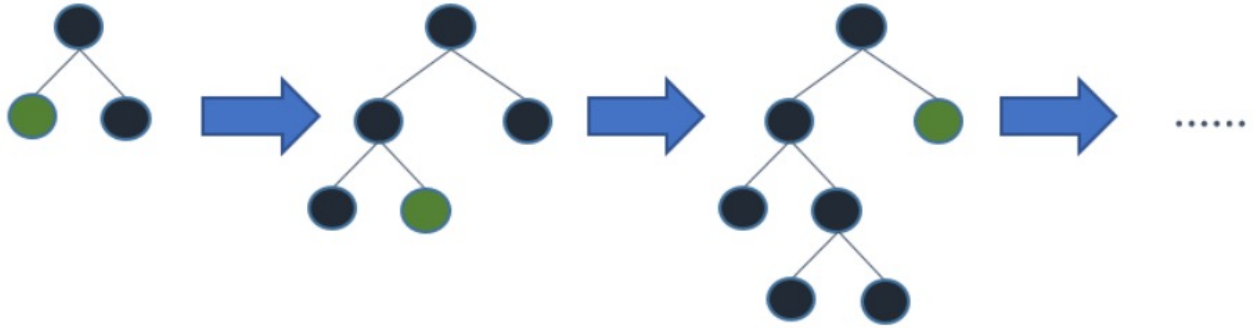
- XGBoost의 파라미터는 크게 일반, 부스터, 학습과정으로 나뉩니다
- 일반 파라미터
  booster : 어떤 부스터 구조를 쓸지 결정 - gbtree, gblinear, dart
  nthread : 몇 개의 쓰레드를 동시에 처리할지 - 디폴트 : 가능한 많이
  num_feature : feature 차원의 숫자를 정하는 옵션 - 디폴트 : 가능한 많이
- 부스팅 파라미터
  eta : learning rate
  gamma : 트리 복잡도 파라미터. 커지면 트리 깊이가 줄어들어서 보수적인 모델이 된다.  - 디폴트 : 0
  max_depth : 한 트리당 깊이 - 디폴트 : 6, 키울수록 과적합 위험 ↑
  lambda : L2 Regularization Form에 달리는 weights이다. 숫자가 클 수록 보수적인 모델이 된다.
  alpha : L1 Regularization Form weights. 숫자가 클수록 보수적인 모델이 된다.
- 학습 과정 파라미터
  object : 목적함수. reg-linear(linear-regression), binary-logistic(binary-logistic classification),
  count-poission(count data poison regression) 등 다양하다.
  eval_metric : 모델의 평가 함수를 조정하는 함수다. Rmse(root mean square error), log loss(log-likelihood),
  MAP(mean average precision) 등, 해당 데이터의 특성에 맞게 평가 함수를 조정한다.
- 커맨드 라인 파라미터
  num_rounds : boosting 라운드를 결정. 적당히 큰 것이 좋고 epoch 옵션과 동일하다.

# 2. LightGBM

# LightGBM



Level-wise tree growth



Leaf-wise tree growth

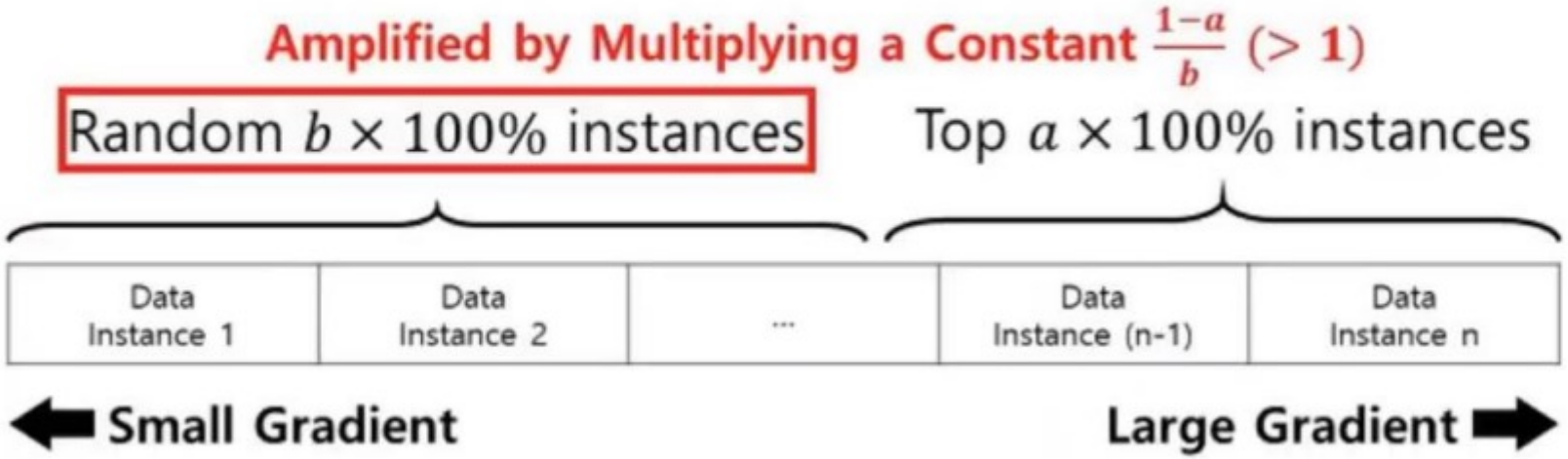
# LightGBM

Gradient based One-Side Sampling (GOSS)

Exclusive Feature Bundling (EFB)

# LightGBM

## Gradient based One-Side Sampling (GOSS)



# LightGBM

## Exclusive Feature Bundling (EFB)

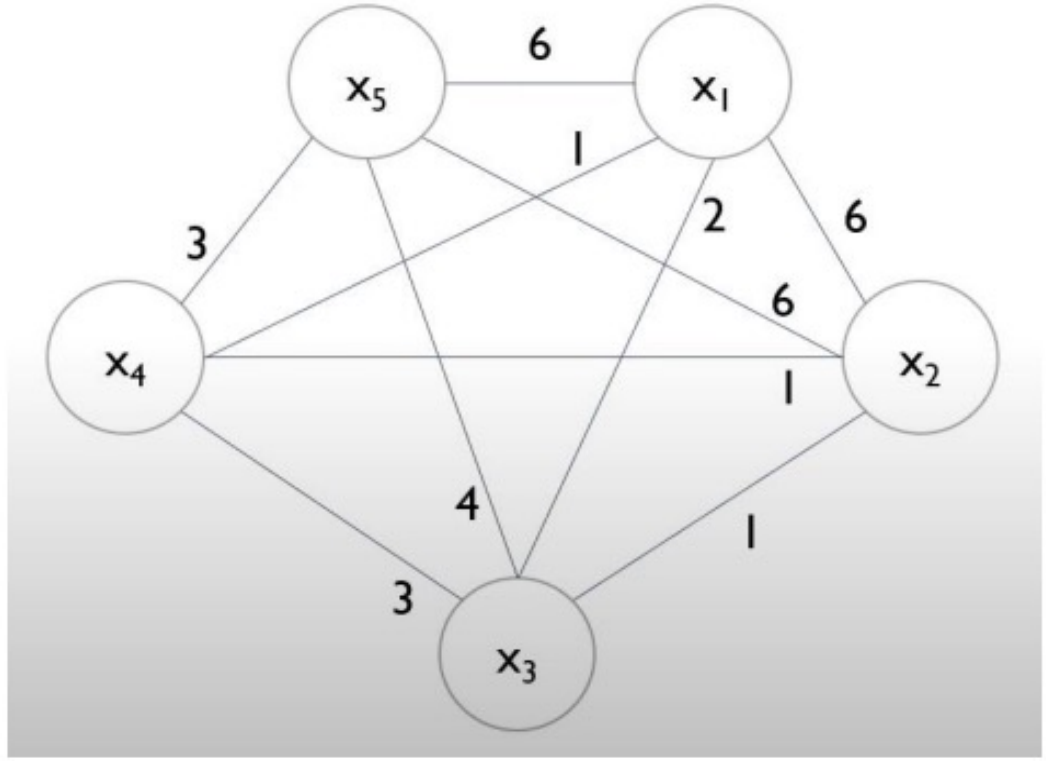
# LightGBM

| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ |
|---|---|---|---|---|---|
| $I_1$ | 1 | 1 | 0 | 0 | 1 |
| $I_2$ | 0 | 0 | 1 | 1 | 1 |
| $I_3$ | 1 | 2 | 0 | 0 | 2 |
| $I_4$ | 0 | 0 | 2 | 3 | 1 |
| $I_5$ | 2 | 1 | 0 | 0 | 3 |
| $I_6$ | 3 | 3 | 0 | 0 | 1 |
| $I_7$ | 0 | 0 | 3 | 0 | 2 |
| $I_8$ | 1 | 2 | 3 | 4 | 3 |
| $I_9$ | 1 | 0 | 1 | 0 | 0 |
| $I_{10}$ | 2 | 3 | 0 | 0 | 2 |

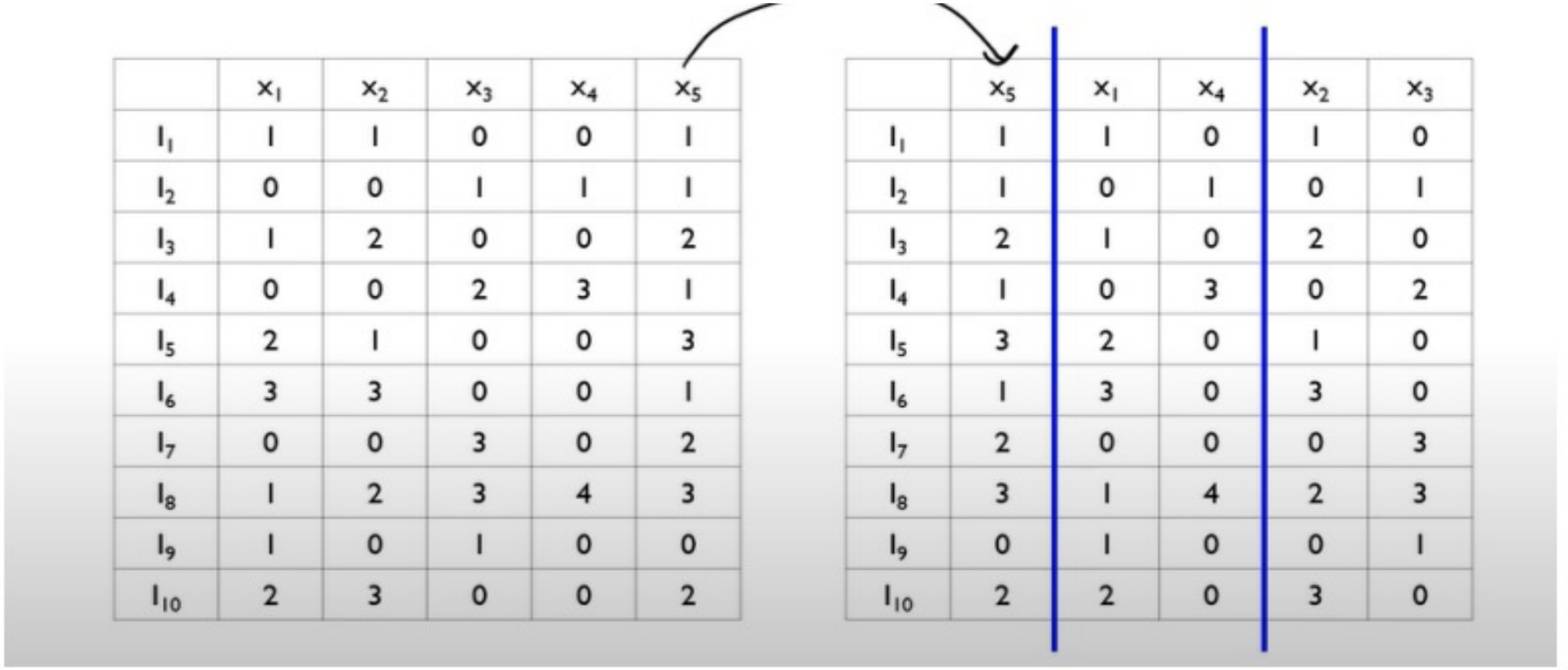
| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ |
|---|---|---|---|---|---|
| $x_1$ | - | 6 | 2 | 1 | 6 |
| $x_2$ | 6 | - | 1 | 1 | 6 |
| $x_3$ | 2 | 1 | - | 3 | 4 |
| $x_4$ | 1 | 1 | 3 | - | 3 |
| $x_5$ | 6 | 6 | 4 | 3 | - |

| | $x_5$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
|---|---|---|---|---|---|
| d | 19 | 15 | 14 | 10 | 8 |

# LightGBM



# LightGBM



| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ |
|---|---|---|---|---|---|
| $I_1$ | 1 | 1 | 0 | 0 | 1 |
| $I_2$ | 0 | 0 | 1 | 1 | 1 |
| $I_3$ | 1 | 2 | 0 | 0 | 2 |
| $I_4$ | 0 | 0 | 2 | 3 | 1 |
| $I_5$ | 2 | 1 | 0 | 0 | 3 |
| $I_6$ | 3 | 3 | 0 | 0 | 1 |
| $I_7$ | 0 | 0 | 3 | 0 | 2 |
| $I_8$ | 1 | 2 | 3 | 4 | 3 |
| $I_9$ | 1 | 0 | 1 | 0 | 0 |
| $I_{10}$ | 2 | 3 | 0 | 0 | 2 |

| | $x_5$ | $x_1$ | $x_4$ | $x_2$ | $x_3$ |
|---|---|---|---|---|---|
| $I_1$ | 1 | 1 | 0 | 1 | 0 |
| $I_2$ | 1 | 0 | 1 | 0 | 1 |
| $I_3$ | 2 | 1 | 0 | 2 | 0 |
| $I_4$ | 1 | 0 | 3 | 0 | 2 |
| $I_5$ | 3 | 2 | 0 | 1 | 0 |
| $I_6$ | 1 | 3 | 0 | 3 | 0 |
| $I_7$ | 2 | 0 | 0 | 0 | 3 |
| $I_8$ | 3 | 1 | 4 | 2 | 3 |
| $I_9$ | 0 | 1 | 0 | 0 | 1 |
| $I_{10}$ | 2 | 2 | 0 | 3 | 0 |

# LightGBM

| | $x_5$ | $x_1$ | $x_4$ | $x_2$ | $x_3$ |
|---|---|---|---|---|---|
| $l_1$ | 1 | 1 | 0 | 1 | 0 |
| $l_2$ | 1 | 0 | 1 | 0 | 1 |
| $l_3$ | 2 | 1 | 0 | 2 | 0 |
| $l_4$ | 1 | 0 | 3 | 0 | 2 |
| $l_5$ | 3 | 2 | 0 | 1 | 0 |
| $l_6$ | 1 | 3 | 0 | 3 | 0 |
| $l_7$ | 2 | 0 | 0 | 0 | 3 |
| $l_8$ | 3 | 1 | 4 | 2 | 3 |
| $l_9$ | 0 | 1 | 0 | 0 | 1 |
| $l_{10}$ | 2 | 2 | 0 | 3 | 0 |

| | $x_5$ | $x_{14}$ | $x_{23}$ |
|---|---|---|---|
| $l_1$ | 1 | 1 | 1 |
| $l_2$ | 1 | 4 | 4 |
| $l_3$ | 2 | 1 | 2 |
| $l_4$ | 1 | 6 | 5 |
| $l_5$ | 3 | 2 | 1 |
| $l_6$ | 1 | 3 | 3 |
| $l_7$ | 2 | 0 | 6 |
| $l_8$ | 3 | 1 | 2 |
| $l_9$ | 0 | 1 | 4 |
| $l_{10}$ | 2 | 2 | 3 |

# 3. CatBoost

# CatBoost

**Distinction**

Target Leakage

→ Ordered TS(Target Statistics)

Prediction Shift

→ Ordered Boosting

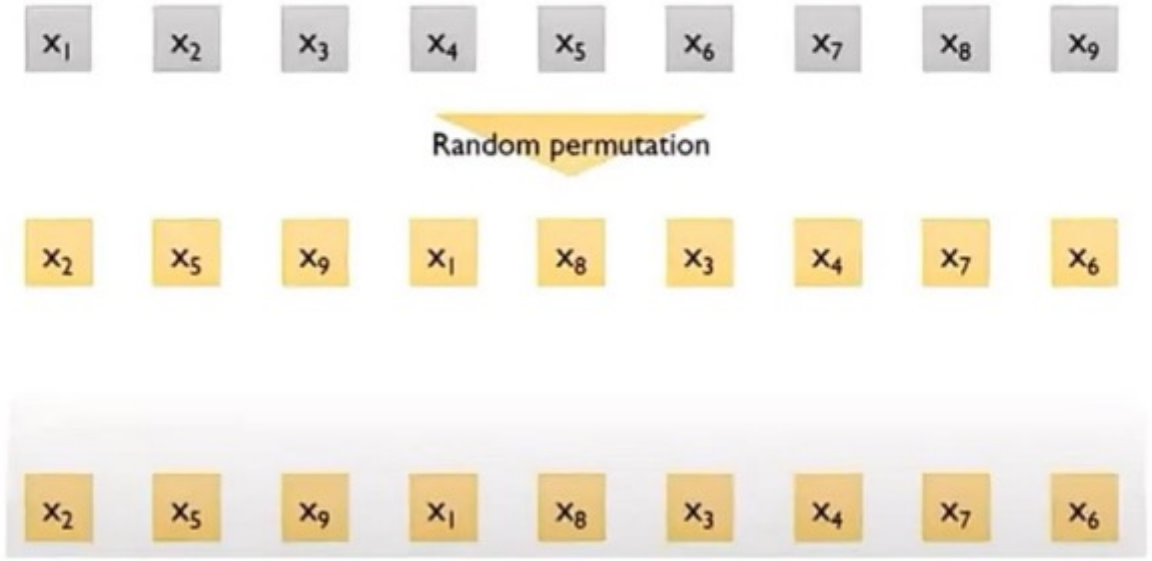
# CatBoost

Ordered Target encoding

# CatBoost

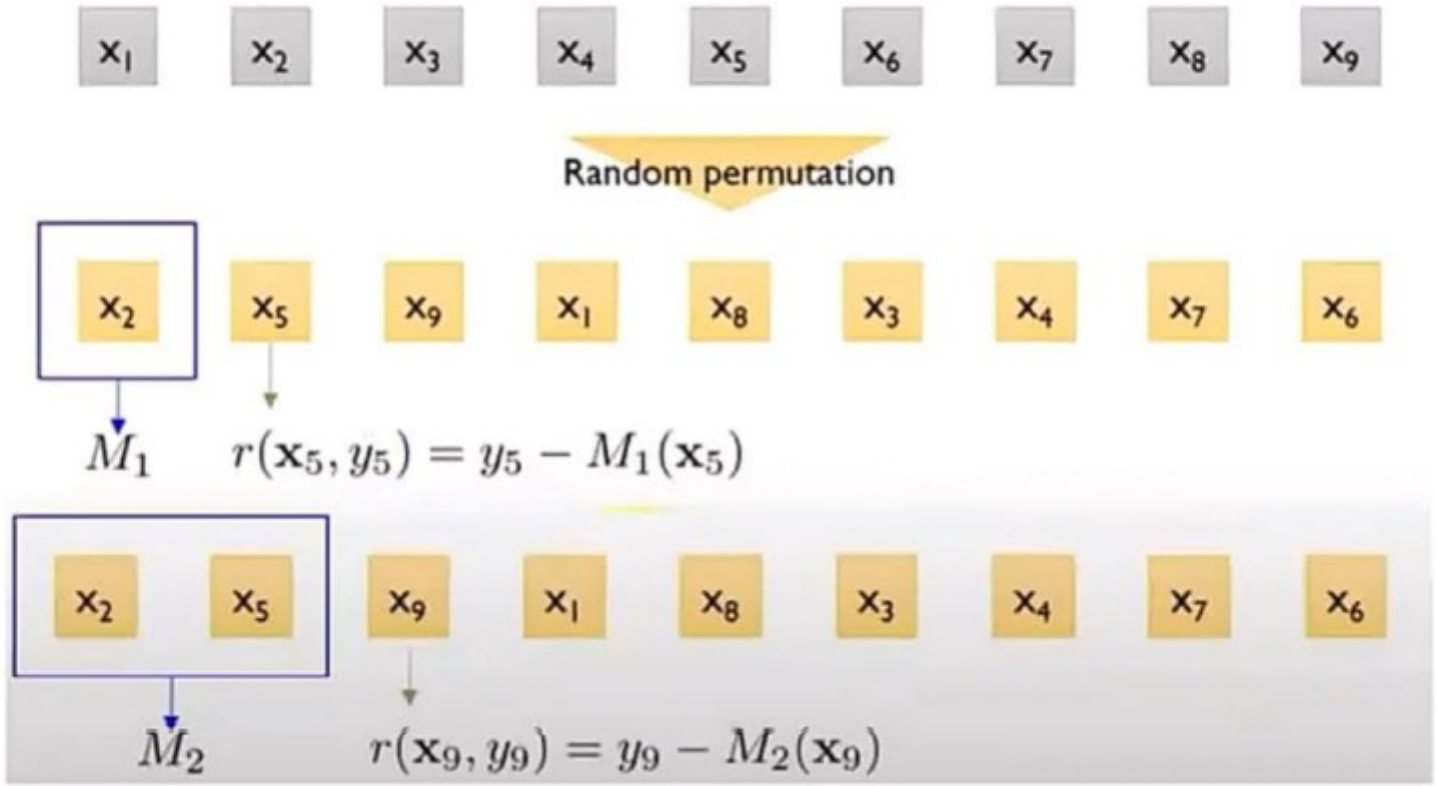
## Ordered Boosting

- Ordered Boosting
  - ✓ A boosting algorithm not suffering from the prediction shift problem



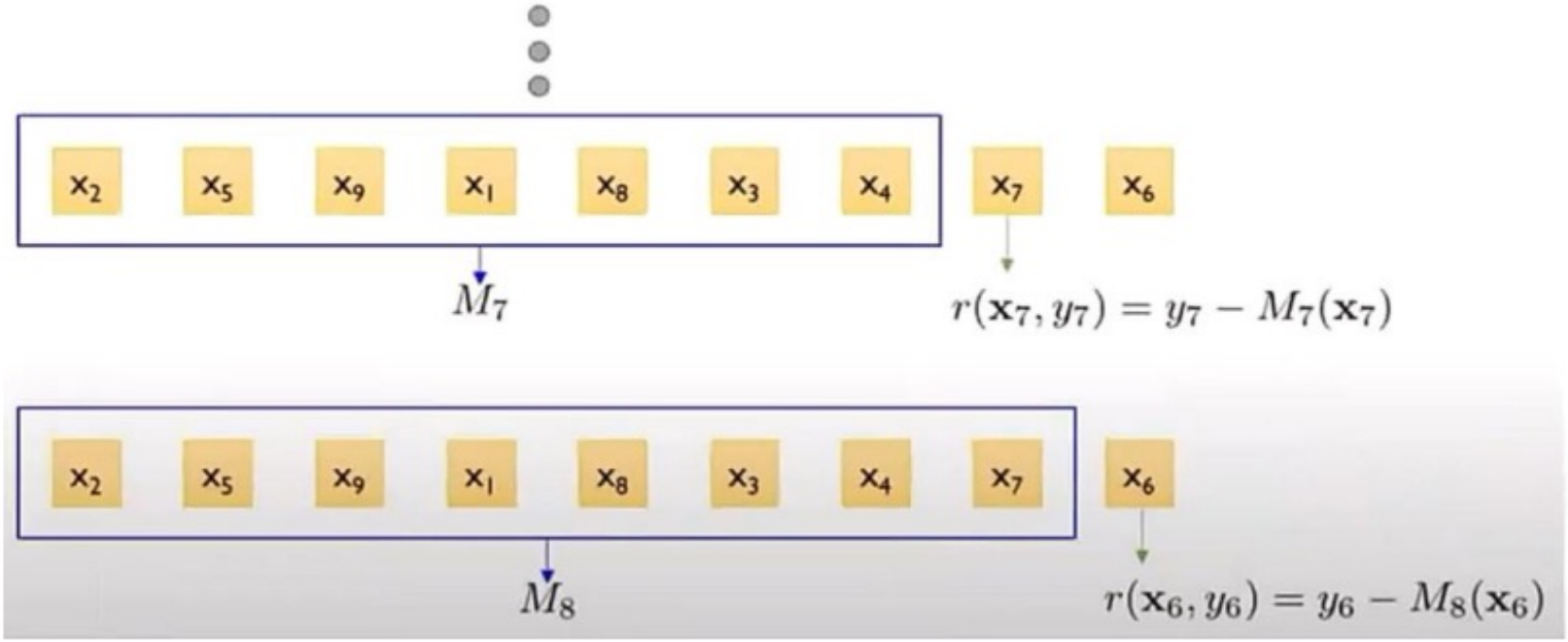
# CatBoost

## Ordered Boosting



# CatBoost

## Ordered Boosting



# Coding Session

1. CatBoost

https://catboost.ai/en/docs/concepts/python-reference_catboostclassifier

2. LightGBM

https://lightgbm.readthedocs.io/en/latest/pythonapi/lightgbm.LGBMClassifier.html

3. XgBoost

https://xgboost.readthedocs.io/en/stable/python/python_api.html#xgboost.XGBRFClassifier
https://xgboost.readthedocs.io/en/stable/python/python_api.html#xgboost.XGBRFRegressor