Ensemble Learning: CatBoost

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CatBoost: Backgrounds

Prokhorenkova et al. (2018)

- Background in brief
  - ✓ Assume we observe a dataset of examples $\mathcal{D} = \{(\mathbf{x}_k, y_k)\}_{k=1,...,n}$
    - where $\mathbf{x}_k = (x_k^1, ..., x_k^m)$ is a random vector of m features and $y_k \in \mathbb{R}$ is a target
  - ✓ Gradient boosting builds iteratively a sequence of approximations $F^t : \mathbb{R}^m \rightarrow \mathbb{R}$ in a greedy fashion
    - $F^t : F^{t-1} + \alpha h^t$ (alpha is a step size and h is a base predictor)
    - h^t is chosen from a family of functions *H* in order to minimize the expected loss

$$h^t = \arg\min_{h \in H} \mathcal{L}(F^{t-1} + h) = \arg\min_{h \in H} \mathbb{E}L(y, F^{t-1}(\mathbf{x}) + h(\mathbf{x}))$$

    - The gradient step h^t is chosen in such a way that $h^t(\mathbf{x})$ approximates $-g^t(\mathbf{x}, y)$, where

$$g^t(\mathbf{x}, y) := \left. \frac{\partial L(y, s)}{\partial s} \right|_{s = F^{t-1}(\mathbf{x})}$$

    - Usually the least squares approximation is used

$$h^t = \arg\min_{h \in H} \ \mathbb{E}\big(-g^t(\mathbf{x}, y) - h(\mathbf{x})\big)^2$$

CatBoost: Backgrounds

March, 2014 — XGBoost initially started as research project by Tianqi Chen but it actually became famous in 2016

Jan, 2017 — Microsoft released first stable version of LightGBM

April, 2017 — Yandex, one of Russia's leading tech companies open sources CatBoost

https://towardsdatascience.com/lightgbm-vs-xgboost-which-algorithm-win-the-race-1ff7dd4917d

Features

1  **Great quality without parameter tuning**

Reduce time spent on parameter tuning, because CatBoost provides great results with default parameters

2 

Categorical features support

Improve your training results with CatBoost that allows you to use non-numeric factors, instead of having to pre-process your data or spend time and effort turning it to numbers.

3  **Fast and scalable GPU version**

Train your model on a fast implementation of gradient-boosting algorithm for GPU. Use a multi-card configuration for large datasets.

4  **Improved accuracy**

Reduce overfitting when constructing your models with a novel gradient-boosting scheme.

5  **Fast prediction**

Apply your trained model quickly and efficiently even to latency-critical tasks using CatBoost's model applier

https://catboost.ai/

CatBoost: Backgrounds

- Gradient Boosting
  - ✓ Statistical Issue 1: Prediction Shift

$$\arg\min_{h \in H} \mathbb{E}\big(-g^t(\mathbf{x}, y) - h(\mathbf{x})\big)^2 \approx \arg\min_{h \in H} \frac{1}{n}\sum_{k=1}^{n}\big(-g^t(\mathbf{x}_k, y_k) - h(\mathbf{x}_k)\big)^2$$

$$\text{Training Dataset}: \; \mathcal{D} = (\mathbf{x}_k, y_k)_{k=1,\ldots,n}$$

$$\text{where} \;\; \mathbf{x}_k = (x_k^1, \ldots, x_k^m), \quad y_k \in \mathbb{R}$$

Conditional distribution

$$F^{t-1}(\mathbf{x}_k)|\mathbf{x}_k$$

for training example $\mathbf{x}_k$

is SHFTED from

$$\neq$$

Conditional distribution

$$F^{t-1}(\mathbf{x})|\mathbf{x}$$

for test example $\mathbf{x}$

CatBoost: Backgrounds

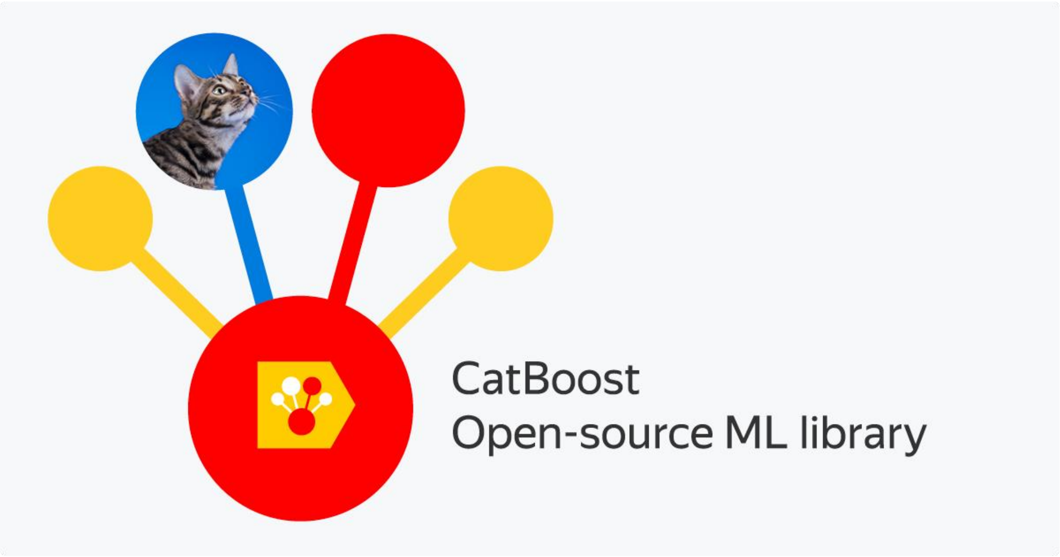
- Gradient Boosting
  - ✓ Statistical Issue 2: Target Leakage
    - Target Statistic (TS): Replace the categorical feature with it mean target value in the training dataset
    - (Problem) Target value of an instance is used to compute its feature value (target information is leaked)

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	B	…	1
I_3	…	C	…	1
I_4	…	A	…	0
I_5	…	B	…	1
I_6	…	C	…	1
I_7	…	B	…	0
I_8	…	C	…	1
I_9	…	C	…	1
I_{10}	…	C	…	0

	…	x^i(TS)	…	y
I_1	…	0.50	…	1
I_2	…	0.67	…	1
I_3	…	0.80	…	1
I_4	…	0.50	…	0
I_5	…	0.67	…	1
I_6	…	0.80	…	1
I_7	…	0.67	…	0
I_8	…	0.80	…	1
I_9	…	0.80	…	1
I_{10}	…	0.80	…	0

CatBoost: Backgrounds

- Solution



Target Leakage → Ordered Target Statistics

Prediction Shift → Ordered Boosting

CatBoost: Ordered TS

- Categorical features in boosted tree
  - ✓ Basic approach: one-hot encoding

	…	x^i	…
I_1	…	A	…
I_2	…	B	…
I_3	…	C	…
I_4	…	A	…
I_5	…	B	…
I_6	…	C	…
I_7	…	B	…
I_8	…	C	…
I_9	…	C	…
I_{10}	…	C	…

	…	$x^i(A)$	$x^i(B)$	$x^i(C)$	…
I_1	…	1	0	0	…
I_2	…	0	1	0	…
I_3	…	0	0	1	…
I_4	…	1	0	0	…
I_5	…	0	1	0	…
I_6	…	0	0	1	…
I_7	…	0	1	0	…
I_8	…	0	0	1	…
I_9	…	0	0	1	…
I_{10}	…	0	0	1	…

CatBoost: Ordered TS

- Categorical features in boosted tree
  - ✓ Another popular method: to group categories by target statistics (TS)
    - an estimate expected target value in each category
    - Greedy TS without smoothing $\hat{x}_k^i \approx \mathbb{E}(y \mid x^i = x_k^i)$
    - i is a categorical feature while k is training example index

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	B	…	1
I_3	…	C	…	1
I_4	…	A	…	0
I_5	…	B	…	1
I_6	…	C	…	1
I_7	…	B	…	0
I_8	…	C	…	1
I_9	…	C	…	1
I_{10}	…	C	…	0

	…	x^i(TS)	…	y
I_1	…	0.50	…	1
I_2	…	0.67	…	1
I_3	…	0.80	…	1
I_4	…	0.50	…	0
I_5	…	0.67	…	1
I_6	…	0.80	…	1
I_7	…	0.67	…	0
I_8	…	0.80	…	1
I_9	…	0.80	…	1
I_{10}	…	0.80	…	0

CatBoost: Ordered TS

- Categorical features in boosted tree
  - ✓ Another popular method: to group categories by target statistics (TS)
    - ▪ Greedy TS with smoothing

$$\hat{x}_k^i = \frac{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

- $a > 0$ is a parameter
- A common setting for p is the average target value in the dataset
- Used to remove the negative effect of low-frequency noisy categories

CatBoost: Ordered TS

- Greedy TS with smoothing example
  - ✓ a = 0.1 (parameter) , p = 0.7 (computed from the training dataset)
  - ✓ For category A

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	B	…	1
I_3	…	C	…	1
I_4	…	A	…	0
I_5	…	B	…	1
I_6	…	C	…	1
I_7	…	B	…	0
I_8	…	C	…	1
I_9	…	C	…	0
I_{10}	…	C	…	1

$$\hat{x}_k^A = \frac{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^A = x_k^A\}} \cdot y_j + ap}{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^A = x_k^A\}} + a}$$

$$= \frac{1 + 0.1 \times 0.7}{2 + 0.1} = 0.5095$$

CatBoost: Ordered TS

- Greedy TS with smoothing example
  - ✓ a = 0.1 (parameter) , p = 0.7 (computed from the training dataset)
  - ✓ For category B

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	B	…	1
I_3	…	C	…	1
I_4	…	A	…	0
I_5	…	B	…	1
I_6	…	C	…	1
I_7	…	B	…	0
I_8	…	C	…	1
I_9	…	C	…	0
I_{10}	…	C	…	1

$$\hat{x}_k^B = \frac{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^B = x_k^B\}} \cdot y_j + ap}{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^B = x_k^B\}} + a}$$

$$= \frac{2 + 0.1 \times 0.7}{3 + 0.1} = 0.6677$$

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CatBoost: Ordered TS

- Greedy TS with smoothing example
  - ✓ a = 0.1 (parameter) , p = 0.7 (computed from the training dataset)
  - ✓ For category C

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	B	…	1
I_3	…	C	…	1
I_4	…	A	…	0
I_5	…	B	…	1
I_6	…	C	…	1
I_7	…	B	…	0
I_8	…	C	…	1
I_9	…	C	…	0
I_{10}	…	C	…	1

$$\hat{x}_k^C = \frac{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^C = x_k^C\}} \cdot y_j + ap}{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^C = x_k^C\}} + a}$$

$$= \frac{4 + 0.1 \times 0.7}{5 + 0.1} = 0.7980$$

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CatBoost: Ordered TS

- Greedy TS with smoothing example
  - ✓ a = 0.1 (parameter) , p = 0.7 (computed from the training dataset)

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	B	…	1
I_3	…	C	…	1
I_4	…	A	…	0
I_5	…	B	…	1
I_6	…	C	…	1
I_7	…	B	…	0
I_8	…	C	…	1
I_9	…	C	…	0
I_{10}	…	C	…	1

	…	x^i(TS)	…	y
I_1	…	0.5095	…	1
I_2	…	0.6677	…	1
I_3	…	0.7980	…	1
I_4	…	0.5095	…	0
I_5	…	0.6677	…	1
I_6	…	0.7980	…	1
I_7	…	0.6677	…	0
I_8	…	0.7980	…	1
I_9	…	0.7980	…	0
I_{10}	…	0.7980	…	1

CatBoost: Ordered TS

- Target leakage
  - ✓ feature $\hat{x}_k^i$ is computed using y_k , the target of $\mathbf{x}_k$
  - ✓ leads to a conditional shift: the distribution of $\hat{x}^i|y$ differs for training and test examples

We should not use this information when we predict the target of current example

$$\hat{x}_k^i = \frac{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{j=1}^{n} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

CatBoost: Ordered TS

- Target leakage
  - ✓ feature $\hat{x}^i_k$ is computed using y_k , the target of $\mathbf{x}_k$
  - ✓ leads to a conditional shift: the distribution of $\hat{x}^i|y$ differs for training and test examples
    - Assume that ith feature is categorical, all its values are unique, $P(y=1|x^i)=0.5, x^i \in \{A,B,C,D,E,F,...\}$

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	B	…	1
I_3	…	C	…	1
I_4	…	D	…	0
I_5	…	E	…	0
I_6	…	F	…	0

	…	x^i	…	y
I_1	…	$\frac{1+ap}{1+a}$	…	1
I_2	…	$\frac{1+ap}{1+a}$	…	1
I_3	…	$\frac{1+ap}{1+a}$	…	1
I_4	…	$\frac{0+ap}{1+a}$	…	0
I_5	…	$\frac{0+ap}{1+a}$	…	0
I_5	…	$\frac{0+ap}{1+a}$	…	0

- Training data can be perfectly classified when the split criterion is set to $x^i = \frac{0.5+ap}{1+a}$

CatBoost: Ordered TS

- Target leakage

Training Set: l_1–l_6; Test Set: l_7–l_{10}

	…	x^i	…	y
l_1	…	A	…	1
l_2	…	B	…	1
l_3	…	C	…	1
l_4	…	D	…	0
l_5	…	E	…	0
l_6	…	F	…	0
l_7	…	G	…	1
l_8	…	H	…	1
l_9	…	I	…	0
l_{10}	…	J	…	0

	…	x^i	…	y
l_1	…	$\frac{1+ap}{1+a}$	…	1
l_2	…	$\frac{1+ap}{1+a}$	…	1
l_3	…	$\frac{1+ap}{1+a}$	…	1
l_4	…	$\frac{0+ap}{1+a}$	…	0
l_5	…	$\frac{0+ap}{1+a}$	…	0
l_6	…	$\frac{0+ap}{1+a}$	…	0
l_7	…	p	…	1
l_8	…	p	…	1
l_9	…	p	…	0
l_{10}	…	p	…	0

Perfect classification by setting the cut off value

$$x^i = \frac{0.5+ap}{1+a}$$

$$\hat{x}^i_k = \frac{\sum_{j=1}^{n} \mathbb{1}_{\{x^i_j = x^i_k\}} \cdot y_j + ap}{\sum_{j=1}^{n} \mathbb{1}_{\{x^i_j = x^i_k\}} + a}$$

All feature values of test instances become p

No discrimination ability

CatBoost: Ordered TS

- Desired property for TS
  - ✓ Property 1:

$$\mathbb{E}(\hat{x}^i \mid y = v) = \mathbb{E}(\hat{x}^i_k \mid y_k = v)$$

$$where\ (\mathbf{x}_k, y_k)\ is\ the\ k-th\ training\ example$$

  - ✓ Property 2:
    - Effective usage of all training data for calculating TS features and for learning a model

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ General idea: compute the TS for $\mathbf{x}_k$ on a subset of examples $\mathcal{D}_k \subset \mathcal{D} \backslash \{\mathbf{x}_k\}$ excluding $\mathbf{x}_k$

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

  - ✓ Holdout TS
    - To partition the training dataset into two part $\mathcal{D} = \hat{\mathcal{D}}_0 \cup \hat{\mathcal{D}}_1$
      - Use the former to compute the TS
      - Use the latter for training
      - Violates the Property 2

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Leave-one-out TS
    - Take $\mathcal{D}_k = \mathcal{D} \backslash \mathbf{x}_k$ for training examples
    - Take $\mathcal{D}_k = \mathcal{D}$ for test ones
    - Does not prevent target leakage

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

	…	x^i	…	y
I_1	…	A	…	1
I_2	…	A	…	0
I_3	…	A	…	1
I_4	…	A	…	0
I_5	…	A	…	1

	…	x^i	…	y
I_1	…	$\frac{2+ap}{4+a}$	…	1
I_2	…	$\frac{3+ap}{4+a}$	…	0
I_3	…	$\frac{2+ap}{4+a}$	…	1
I_4	…	$\frac{3+ap}{4+a}$	…	0
I_5	…	$\frac{2+ap}{4+a}$	…	1

- We can perfectly classify this training dataset by setting the cut-off value $\frac{2.5+ap}{4+a}$

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 0 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…		1
I_3	…	C	…		1
I_4	…	A	…		0
I_5	…	B	…		1
I_6	…	C	…		1
I_7	…	B	…		0
I_8	…	C	…		1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{0 + 0.1 \times 0}{0 + 0.1} = 0$$

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CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 1 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…		1
I_4	…	A	…		0
I_5	…	B	…		1
I_6	…	C	…		1
I_7	…	B	…		0
I_8	…	C	…		1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{0 + 0.1 \times 1.0}{0 + 0.1} = 1.0$$

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    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 1 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…		0
I_5	…	B	…		1
I_6	…	C	…		1
I_7	…	B	…		0
I_8	…	C	…		1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{0 + 0.1 \times 1}{0 + 0.1} = 1.0$$

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 1 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…	1.000	0
I_5	…	B	…		1
I_6	…	C	…		1
I_7	…	B	…		0
I_8	…	C	…		1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{1 + 0.1 \times 1.0}{1 + 0.1} = 1.0$$

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 0.75 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…	1.000	0
I_5	…	B	…	0.977	1
I_6	…	C	…		1
I_7	…	B	…		0
I_8	…	C	…		1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{1 + 0.1 \times 0.75}{1 + 0.1} = 0.977$$

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 0.8 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…	1.000	0
I_5	…	B	…	0.977	1
I_6	…	C	…	0.982	1
I_7	…	B	…		0
I_8	…	C	…		1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{1 + 0.1 \times 0.8}{1 + 0.1} = 0.982$$

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 0.833 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…	1.000	0
I_5	…	B	…	0.977	1
I_6	…	C	…	0.982	1
I_7	…	B	…	0.992	0
I_8	…	C	…		1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{2 + 0.1 \times 0.833}{2 + 0.1} = 0.992$$

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CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 0.714 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…	1.000	0
I_5	…	B	…	0.977	1
I_6	…	C	…	0.982	1
I_7	…	B	…	0.992	0
I_8	…	C	…	0.986	1
I_9	…	C	…		0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{2 + 0.1 \times 0.714}{2 + 0.1} = 0.986$$

CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 0.75 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…	1.000	0
I_5	…	B	…	0.977	1
I_6	…	C	…	0.982	1
I_7	…	B	…	0.992	0
I_8	…	C	…	0.986	1
I_9	…	C	…	0.992	0
I_{10}	…	C	…		1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{3 + 0.1 \times 0.75}{3 + 0.1} = 0.992$$

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CatBoost: Ordered TS

- Ways to avoid conditional shift
  - ✓ Ordered TS: introduce an artificial time
    - a random permutation σ of the training examples

$$\mathcal{D}_k = \{\mathbf{x}_j : \sigma(j) < \sigma(k)\}$$

    - a = 0.1 (parameter) , p = 0.667 (computed from the training dataset)

	…	x^i	…	TS	y
I_1	…	A	…	0.000	1
I_2	…	B	…	1.000	1
I_3	…	C	…	1.000	1
I_4	…	A	…	1.000	0
I_5	…	B	…	0.977	1
I_6	…	C	…	0.982	1
I_7	…	B	…	0.992	0
I_8	…	C	…	0.986	1
I_9	…	C	…	0.992	0
I_{10}	…	C	…	0.748	1

$$\hat{x}_k^i = \frac{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} \cdot y_j + ap}{\sum_{\mathbf{x}_j \in \mathcal{D}_k} \mathbb{1}_{\{x_j^i = x_k^i\}} + a}$$

$$= \frac{3 + 0.1 \times 0.667}{4 + 0.1} = 0.748$$

CatBoost: Ordered Boosting

- Prediction Shift

$$h^t = \arg\min_{h \in H} \ \mathbb{E}\big(-g^t(\mathbf{x}, y) - h(\mathbf{x})\big)^2$$

✓ The expectation is unknown and is usually approximated using the same dataset $\mathcal{D}$

$$h^t = \arg\min_{h \in H} \ \frac{1}{n}\sum_{k=1}^{n}\big(-g^t(\mathbf{x}, y) - h(\mathbf{x})\big)^2$$

- The conditional distribution of the gradient $g^t(\mathbf{x}_k, y_k)|\mathbf{x}_k$ is shifted from that distribution on a test example $g^t(\mathbf{x}, y)|\mathbf{x}$
- In turn, base predictor h^t is biased from the solution
- Finally it affects the generalization ability of the trained model F^t

✓ When we learn a model with I trees, we need to have F^{I-1} trained without the example $\mathbf{x}_k$ to make the residual $r^{I-1}(\mathbf{x}_k, y_k)$ unshifted

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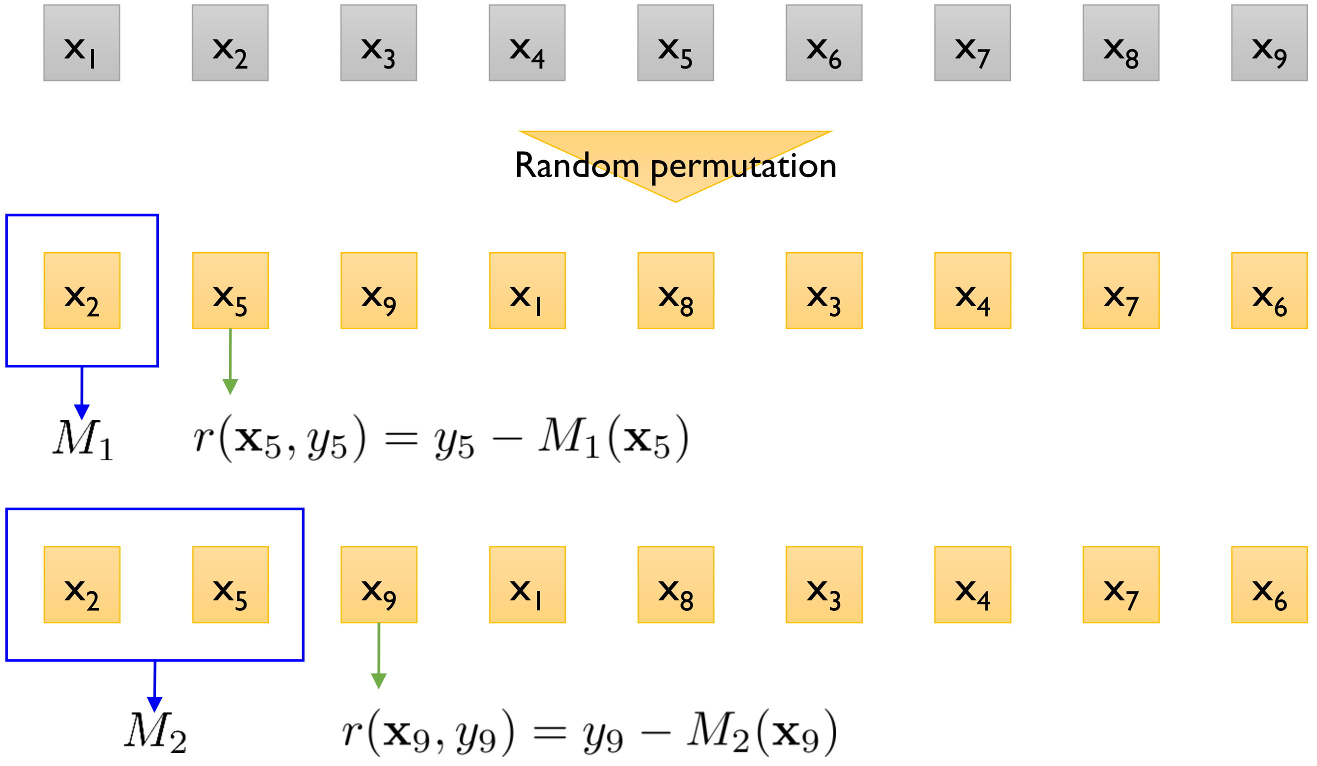
CatBoost: Ordered Boosting

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



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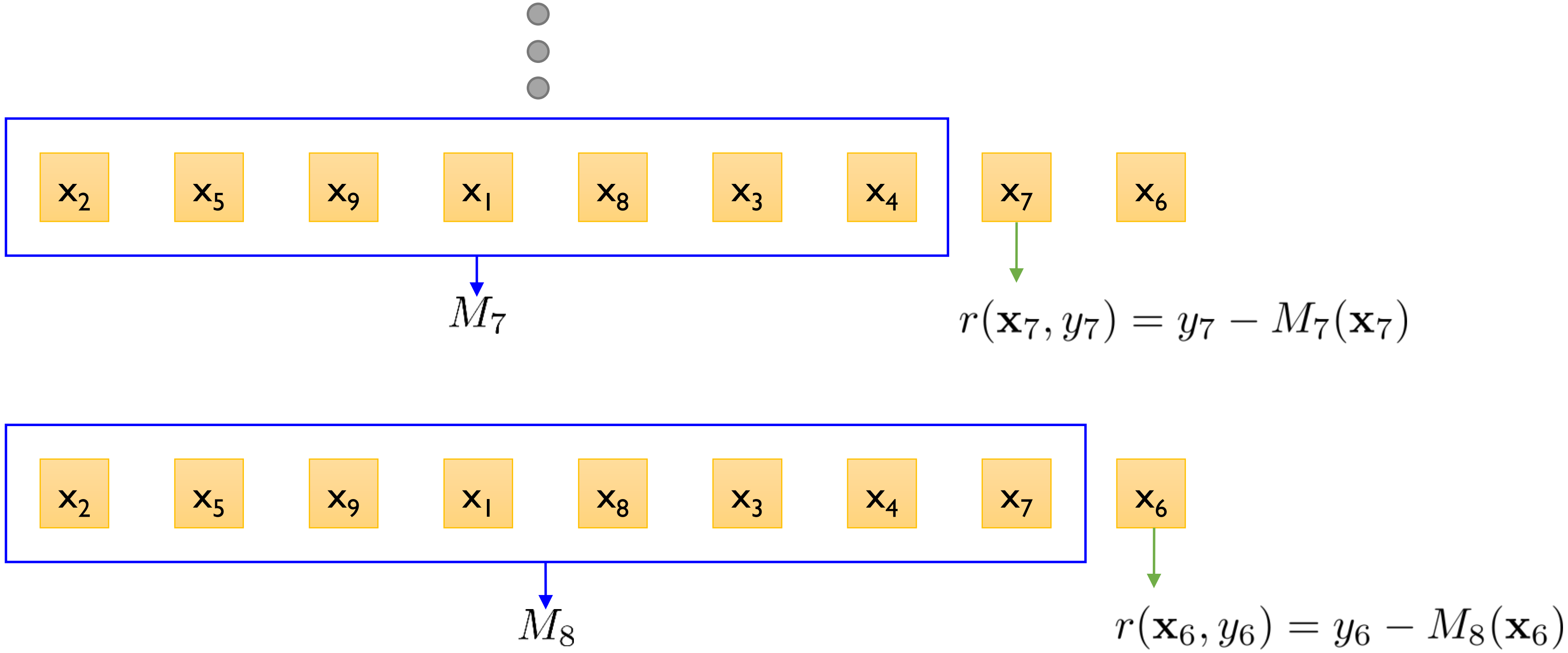
CatBoost: Ordered Boosting

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



  - ✓ The same permutation is used for both TS computing and ordered boosting

CatBoost: Ordered Boosting

- Ordered Boosting and Building a Tree in CatBoost

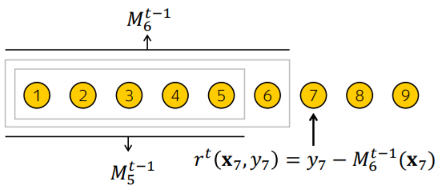


Figure 1: Ordered boosting principle, examples are ordered according to σ.

Algorithm 1: Ordered boosting

input : $\{(\mathbf{x}_k, y_k)\}_{k=1}^n, I$;

$\sigma \leftarrow$ random permutation of $[1, n]$;
$M_i \leftarrow 0$ for $i = 1..n$;
for $t \leftarrow 1$ **to** I **do**
  for $i \leftarrow 1$ **to** n **do**
    $r_i \leftarrow y_i - M_{\sigma(i)-1}(\mathbf{x}_i)$;
  for $i \leftarrow 1$ **to** n **do**
    $\Delta M \leftarrow$
      $LearnModel((\mathbf{x}_j, r_j) : \sigma(j) \leq i)$;
    $M_i \leftarrow M_i + \Delta M$;
return M_n

Algorithm 2: Building a tree in CatBoost

input : $M, \{(\mathbf{x}_i, y_i)\}_{i=1}^n, \alpha, L, \{\sigma_i\}_{i=1}^s, Mode$

$grad \leftarrow CalcGradient(L, M, y)$;
$r \leftarrow random(1, s)$;
if $Mode = Plain$ **then**
  $G \leftarrow (grad_r(i)$ for $i = 1..n)$;
if $Mode = Ordered$ **then**
  $G \leftarrow (grad_{r,\sigma_r(i)-1}(i)$ for $i = 1..n)$;
$T \leftarrow$ empty tree;
foreach *step of top-down procedure* **do**
  foreach *candidate split c* **do**
    $T_c \leftarrow$ add split c to T;
    if $Mode = Plain$ **then**
      $\Delta(i) \leftarrow \text{avg}(grad_r(p)$ for $p : leaf_r(p) = leaf_r(i))$ for $i = 1..n$;
    if $Mode = Ordered$ **then**
      $\Delta(i) \leftarrow \text{avg}(grad_{r,\sigma_r(i)-1}(p)$ for $p : leaf_r(p) = leaf_r(i), \sigma_r(p) < \sigma_r(i))$ for $i = 1..n$;
    $loss(T_c) \leftarrow \cos(\Delta, G)$
  $T \leftarrow \arg\min_{T_c}(loss(T_c))$
if $Mode = Plain$ **then**
  $M_{r'}(i) \leftarrow M_{r'}(i) - \alpha\,\text{avg}(grad_{r'}(p)$ for $p : leaf_{r'}(p) = leaf_{r'}(i))$ for $r' = 1..s, i = 1..n$;
if $Mode = Ordered$ **then**
  $M_{r',j}(i) \leftarrow M_{r',j}(i) - \alpha\,\text{avg}(grad_{r',j}(p)$ for $p : leaf_{r'}(p) = leaf_{r'}(i), \sigma_{r'}(p) \leq j)$ for $r' = 1..s$, $i = 1..n, j \geq \sigma_{r'}(i) - 1$;
return T, M

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CatBoost: Procedure

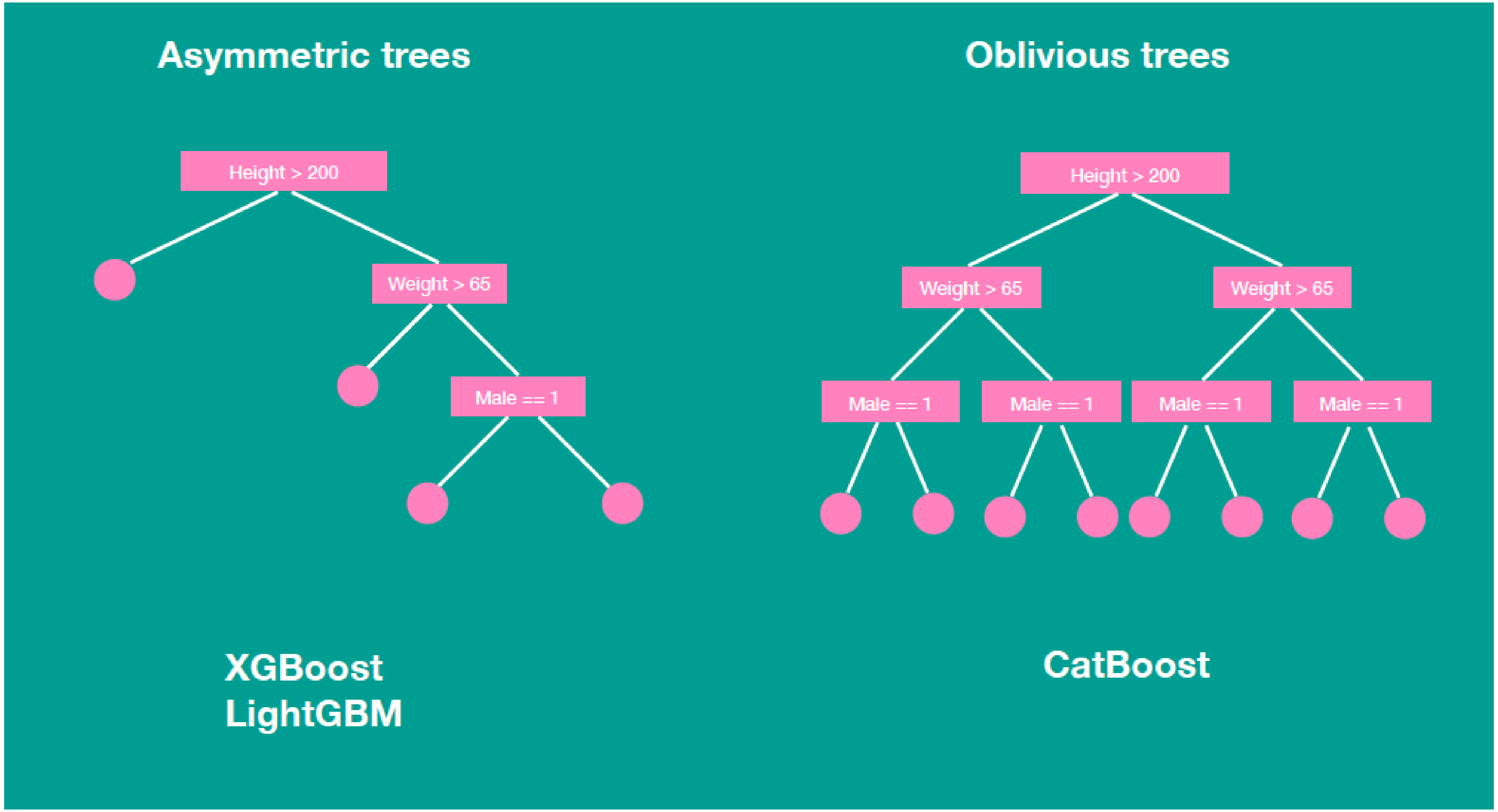
- CatBoost Procedure
  - ✓ Initialization: generate (s+1) independent random permutations of the training dataset
    - s permutations to evaluate the split
    - 1 permutation to compute the leaf value of the obtained trees
  - ✓ Both TS and predictions used by ordered boosting have a high variance
  - ✓ Using only one permutation may increase the variance of the final model predictions, while several permutations can reduce it

CatBoost: Procedure

- CatBoost Procedure
  - ✓ Building an oblivious tree (the same splitting criterion is used across an entire level of the tree) in the ordered boosting mode
    - Maintain the supporting models $M_{r,j}$
    - $M_{r,j}(i)$: the current prediction for the i^{th} example based on the first *j* examples in the permutation r
    - At each iteration t, sample a random permutation σ_r and construct a tree T_t
      - TS are computed according to this permutation σ_r
      - The permutation affects the tree learning procedure
    - For each example i, take the gradient $grad_{r,\sigma_r(i)-1}(i)$
    - While constructing a tree, the loss of the candidate split c is computed by the cosine similarity between the leaf value and the gradient of each example
      - At the candidate splits evaluation step, the leaf value $\Delta(i)$ for example i is obtained individually by averaging the gradients $grad_{r,\sigma_r(i)-1}$ of the preceding example p lying in the same leaf node of i

CatBoost: Procedure

- Oblivious tree

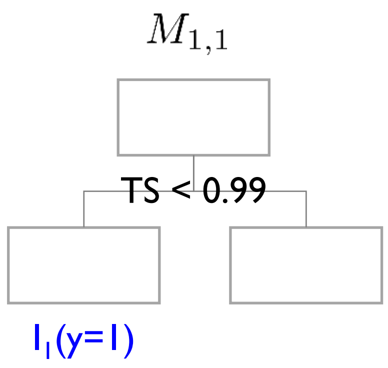


https://towardsdatascience.com/introduction-to-gradient-boosting-on-decision-trees-with-catboost-d511a9ccbd14

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1		
I_3	…	C	…	1.000	1		
I_4	…	A	…	1.000	0		
I_5	…	B	…	0.977	1		
I_6	…	C	…	0.982	1		
I_7	…	B	…	0.992	0		
I_8	…	C	…	0.986	1		
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



$$\boxed{\begin{aligned} G(I_1) &= 0 \\ \Delta(I_1) &= 0 \end{aligned}}$$

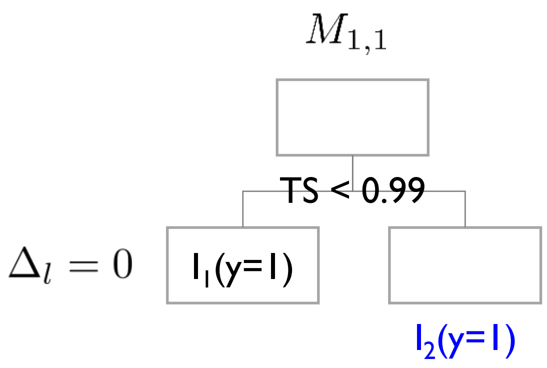
Lecturer's guess

- Initialize both the first gradient and leaf value to 0

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1		
I_4	…	A	…	1.000	0		
I_5	…	B	…	0.977	1		
I_6	…	C	…	0.982	1		
I_7	…	B	…	0.992	0		
I_8	…	C	…	0.986	1		
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



$$\boxed{G(I_2) = 0 \quad \Delta(I_2) = 0}$$

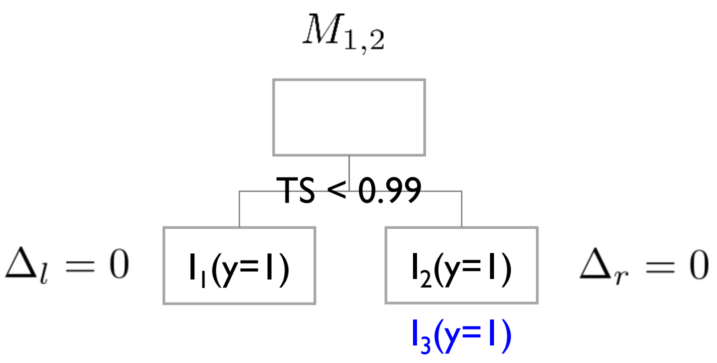
Lecturer's guess

- Initialize both the first gradient and leaf value to 0

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0		
I_5	…	B	…	0.977	1		
I_6	…	C	…	0.982	1		
I_7	…	B	…	0.992	0		
I_8	…	C	…	0.986	1		
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



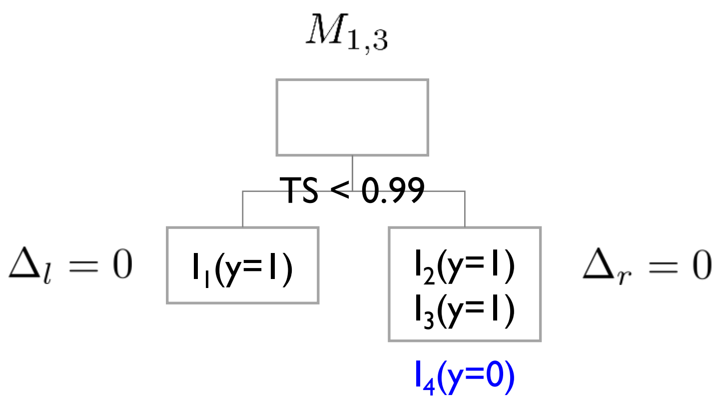
$$G(I_3) = grad_{1,\sigma_1(3)-1}(I_3)$$
$$= \Delta_r - y_3 = 0 - 1 = -1$$

$$\Delta(I_3) = grad_{1,\sigma_1(3)-1}(I_2) = 0$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1		
I_6	…	C	…	0.982	1		
I_7	…	B	…	0.992	0		
I_8	…	C	…	0.986	1		
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



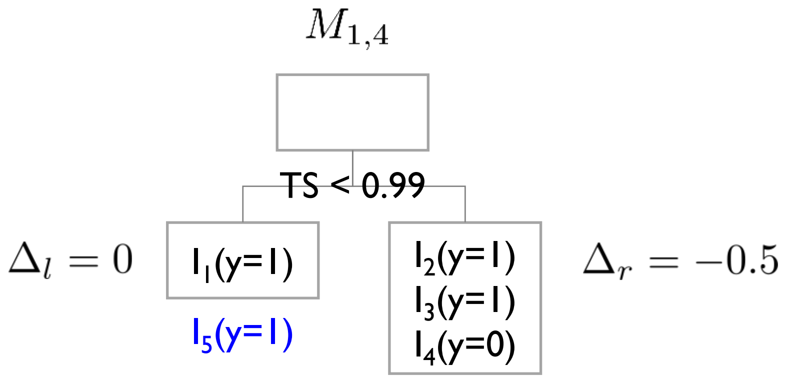
$$G(I_4) = grad_{1,\sigma_1(4)-1}(I_4)$$
$$= \Delta_r - y_4 = 0 - 0 = 0$$

$$\Delta(I_4) = \frac{1}{2}(grad_{1,\sigma_1(5)-1}(I_2) + grad_{1,\sigma_1(5)-1}(I_3))$$
$$= \frac{1}{2}(0 - 1) = -0.5$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1	-1	0
I_6	…	C	…	0.982	1		
I_7	…	B	…	0.992	0		
I_8	…	C	…	0.986	1		
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



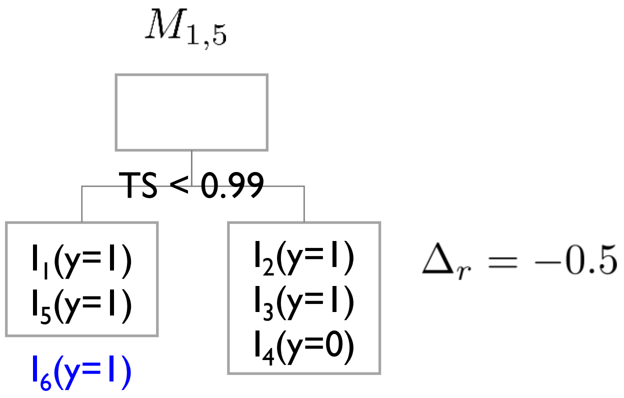
$$G(I_5) = grad_{1,\sigma_1(5)-1}(I_5)$$
$$= \Delta_l - y_5 = 0 - 1 = -1$$

$$\Delta(I_5) = grad_{1,\sigma_1(5)-1}(I_1)$$
$$= 0$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1	-1	0
I_6	…	C	…	0.982	1	-1	-0.5
I_7	…	B	…	0.992	0		
I_8	…	C	…	0.986	1		
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



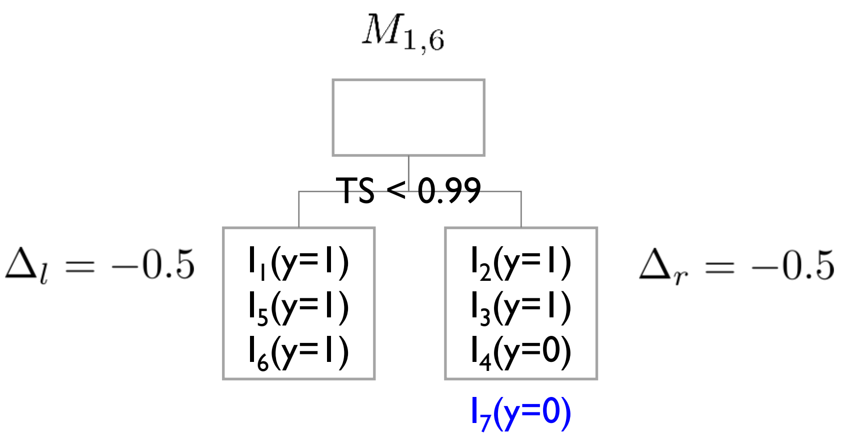
$$G(I_6) = grad_{1,\sigma_1(6)-1}(I_6)$$
$$= \Delta_l - y_6 = 0 - 1 = -1$$

$$\Delta(I_6) = \frac{1}{2}(grad_{1,\sigma_1(6)-1}(I_1) + grad_{1,\sigma_1(6)-1}(I_5))$$
$$= \frac{1}{2}(0 - 1) = -0.5$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1	-1	0
I_6	…	C	…	0.982	1	-1	-0.5
I_7	…	B	…	0.992	0	-0.5	-0.33
I_8	…	C	…	0.986	1		
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



$$G(I_7) = grad_{1,\sigma_1(7)-1}(I_7)$$
$$= \Delta_r - y_7 = -0.5 - 0 = -0.5$$

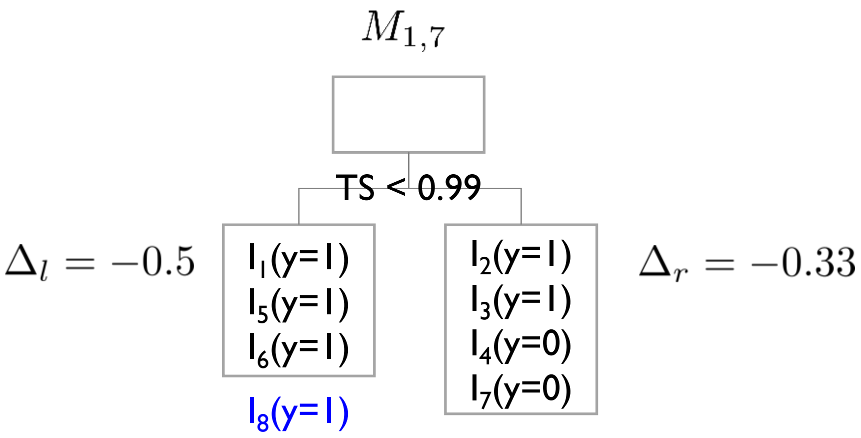
$$\Delta(I_7) = \frac{1}{3}\left(grad_{1,\sigma_1(7)-1}(I_2) + grad_{1,\sigma_1(7)-1}(I_3) + grad_{1,\sigma_1(7)-1}(I_4)\right)$$

$$= \frac{1}{3}(0 - 1 - 0) = -0.33$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1	-1	0
I_6	…	C	…	0.982	1	-1	-0.5
I_7	…	B	…	0.992	0	-0.5	-0.33
I_8	…	C	…	0.986	1	-1.5	-0.67
I_9	…	C	…	0.992	0		
I_{10}	…	C	…	0.748	1		



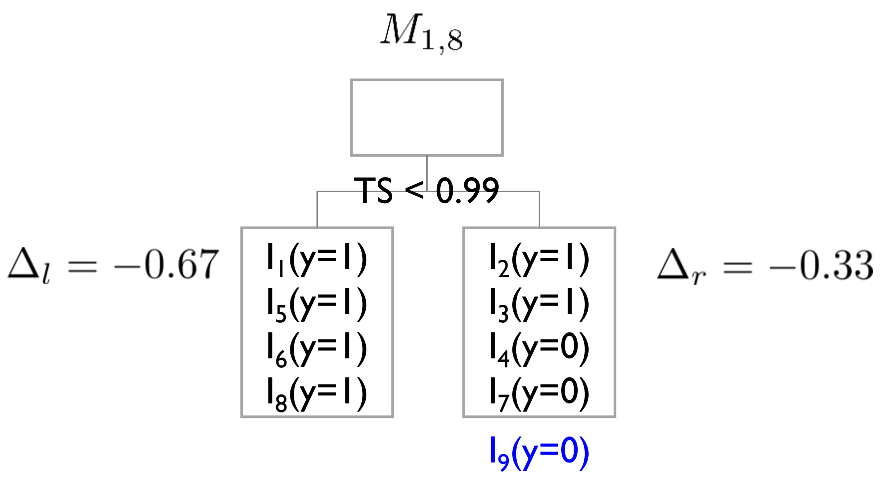
$$G(I_8) = grad_{1,\sigma_1(8)-1}(I_8)$$
$$= \Delta_l - y_8 = -0.5 - 1 = -1.5$$

$$\Delta(I_8) = \frac{1}{3}\left(grad_{1,\sigma_1(8)-1}(I_1) + grad_{1,\sigma_1(8)-1}(I_5) + grad_{1,\sigma_1(8)-1}(I_6)\right)$$
$$= \frac{1}{3}(0 - 1 - 1) = -0.67$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1	-1	0
I_6	…	C	…	0.982	1	-1	-0.5
I_7	…	B	…	0.992	0	-0.5	-0.33
I_8	…	C	…	0.986	1	-1.5	-0.67
I_9	…	C	…	0.992	0	-0.33	-0.38
I_{10}	…	C	…	0.748	1		



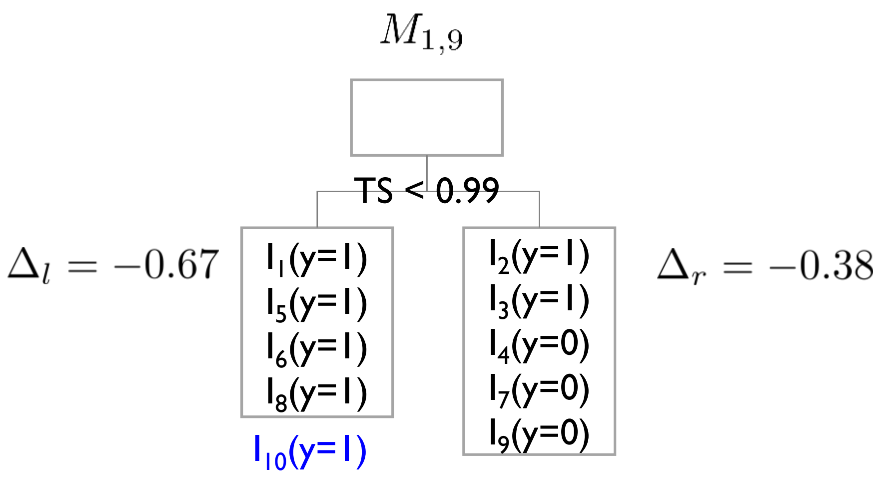
$$G(I_9) = grad_{1,\sigma_1(9)-1}(I_9)$$
$$= \Delta_r - y_9 = -0.33 - 0 = -0.33$$

$$\Delta(I_9) = \frac{1}{4}(grad_{1,\sigma_1(9)-1}(I_2) + grad_{1,\sigma_1(9)-1}(I_3)$$
$$+ grad_{1,\sigma_1(9)-1}(I_4) + grad_{1,\sigma_1(9)-1}(I_7))$$
$$= \frac{1}{4}(0 - 1 - 0 - 0.5) = -0.38$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1	-1	0
I_6	…	C	…	0.982	1	-1	-0.5
I_7	…	B	…	0.992	0	-0.5	-0.33
I_8	…	C	…	0.986	1	-1.5	-0.67
I_9	…	C	…	0.992	0	-0.33	-0.38
I_{10}	…	C	…	0.748	1	-1.67	-0.58



$$G(I_{10}) = grad_{1,\sigma_1(10)-1}(I_{10})$$
$$= \Delta_l - y_{10} = -0.67 - 1 = -1.67$$

$$\Delta(I_9) = \frac{1}{4}\left(grad_{1,\sigma_1(10)-1}(I_1) + grad_{1,\sigma_1(10)-1}(I_5) + grad_{1,\sigma_1(10)-1}(I_6) + grad_{1,\sigma_1(10)-1}(I_8)\right)$$
$$= \frac{1}{4}(0 - 1 - 1 - 0.33) = -0.58$$

CatBoost: Procedure

- Ordered Boosting Example
  - ✓ Assumption: squared loss (gradient: $f(x) - y$)
  - ✓ random permutation is conducted

	…	x^i	…	TS	y	G	Δ
I_1	…	A	…	0.000	1	0	0
I_2	…	B	…	1.000	1	0	0
I_3	…	C	…	1.000	1	-1	0
I_4	…	A	…	1.000	0	0	-0.5
I_5	…	B	…	0.977	1	-1	0
I_6	…	C	…	0.982	1	-1	-0.5
I_7	…	B	…	0.992	0	-0.5	-0.33
I_8	…	C	…	0.986	1	-1.5	-0.67
I_9	…	C	…	0.992	0	-0.33	-0.38
I_{10}	…	C	…	0.748	1	-1.67	-0.58

foreach *step of top-down procedure* **do**
  foreach *candidate split* c **do**
    $T_c \leftarrow$ add split c to T;
    if $Mode = Plain$ **then**
      $\Delta(i) \leftarrow \text{avg}(grad_r(p)$ for $p : leaf_r(p) = leaf_r(i))$ for $i = 1..n$;
    if $Mode = Ordered$ **then**
      $\Delta(i) \leftarrow \text{avg}(grad_{r,\sigma_r(i)-1}(p)$ for $p : leaf_r(p) = leaf_r(i), \sigma_r(p) < \sigma_r(i))$ for $i = 1..n$;
    $loss(T_c) \leftarrow \cos(\Delta, G)$
  $T \leftarrow \arg\min_{T_c}(loss(T_c))$

$$loss(T_c) = cos(\Delta, G) = 0.3575$$

(TS < 0.99)

CatBoost: Procedure

- Choosing leaf values
  - ✓ Given all the trees constructed, the leaf values of the final model F are calculated by the standard gradient boosting procedure
  - ✓ Training examples i are matched to leaves $leaf_0(i)$ using permutation σ_0 to calculate TS
  - ✓ When the final model F is applied to a new example at testing time, TS is calculated on the whole training data

CatBoost: Performance

- Experimental Results

Table 8: Comparison with baselines: logloss / zero-one loss, relative increase is presented in the brackets.

	CatBoost	LightGBM	XGBoost
Adult	**0.2695 / 0.1267**	0.2760 (+2.4%) / 0.1291 (+1.9%)	0.2754 (+2.2%) / 0.1280 (+1.0%)
Amazon	**0.1394 / 0.0442**	0.1636 (+17%) / 0.0533 (+21%)	0.1633 (+17%) / 0.0532 (+21%)
Click	**0.3917 / 0.1561**	0.3963 (+1.2%) / 0.1580 (+1.2%)	0.3962 (+1.2%) / 0.1581 (+1.2%)
Epsilon	**0.2647 / 0.1086**	0.2703 (+1.5%) / 0.114 (+4.1%)	0.2993 (+11%) / 0.1276 (+12%)
Appetency	**0.0715 / 0.01768**	0.0718 (+0.4%) / 0.01772 (+0.2%)	0.0718 (+0.4%) / 0.01780 (+0.7%)
Churn	**0.2319 / 0.0719**	0.2320 (+0.1%) / 0.0723 (+0.6%)	0.2331 (+0.5%) / 0.0730 (+1.6%)
Internet	**0.2089 / 0.0937**	0.2231 (+6.8%) / 0.1017 (+8.6%)	0.2253 (+7.9%) / 0.1012 (+8.0%)
Upselling	**0.1662 / 0.0490**	0.1668 (+0.3%) / 0.0491 (+0.1%)	0.1663 (+0.04%) / 0.0492 (+0.3%)
Kick	**0.2855 / 0.0949**	0.2957 (+3.5%) / 0.0991 (+4.4%)	0.2946 (+3.2%) / 0.0988 (+4.1%)

CatBoost: Performance

- XGBoost vs. LightGBM vs. CatBoost

Function	XGBoost	CatBoost	Light GBM
Important parameters which control overfitting	1. **learning_rate or eta** – optimal values lie between 0.01-0.2 2. **max_depth** 3. **min_child_weight:** similar to min_child leaf; default is 1	1. **Learning_rate** 2. **Depth** - value can be any integer up to 16. Recommended - [1 to 10] 3. No such feature like min_child_weight 4. **l2-leaf-reg**: L2 regularization coefficient. Used for leaf value calculation (any positive integer allowed)	1. **learning_rate** 2. **max_depth**: default is 20. Important to note that tree still grows leaf-wise. Hence it is important to tune **num_leaves** (number of leaves in a tree) which should be smaller than 2^(max_depth). It is a very important parameter for LGBM 3. **min_data_in_leaf**: default=20, alias= min_data, min_child_samples
Parameters for categorical values	Not Available	1. **cat_features**: It denotes the index of categorical features 2. **one_hot_max_size**: Use one-hot encoding for all features with number of different values less than or equal to the given parameter value (max – 255)	1. **categorical_feature:** specify the categorical features we want to use for training our model
Parameters for controlling speed	1. **colsample_bytree**: subsample ratio of columns 2. **subsample**: subsample ratio of the training instance 3. **n_estimators**: maximum number of decision trees; high value can lead to overfitting	1. **rsm:** Random subspace method. The percentage of features to use at each split selection 2. No such parameter to subset data 3. **iterations**: maximum number of trees that can be built; high value can lead to overfitting	1. **feature_fraction:** fraction of features to be taken for each iteration 2. **bagging_fraction:** data to be used for each iteration and is generally used to speed up the training and avoid overfitting 3. **num_iterations:** number of boosting iterations to be performed; default=100

https://towardsdatascience.com/catboost-vs-light-gbm-vs-xgboost-5f93620723db

CatBoost: Performance

Anghel et al. (2019)

- XGBoost vs. LightGBM vs. CatBoost

Table 3: Best test scores across algorithms and datasets.

Dataset	Baseline		XGBoost		LightGBM		Catboost	
	Test	Val	Test	Val	Test	Val	Test	Val
Higgs	0.4996	0.5005	0.8353	0.8512	*0.8573*	0.8577	0.8498	0.8496
Epsilon	0.4976	0.5008	-	-	0.9513	0.9518	*0.9537*	0.9538
Microsoft	0.2251	0.3974	*0.4917*	0.6443	0.4871	0.6473	0.3782	0.5492
Yahoo	0.5802	0.8106	*0.7983*	0.9146	0.7965	0.9142	0.7351	0.8849

CatBoost: Performance

Anghel et al. (2019)

- XGBoost vs. LightGBM vs. CatBoost

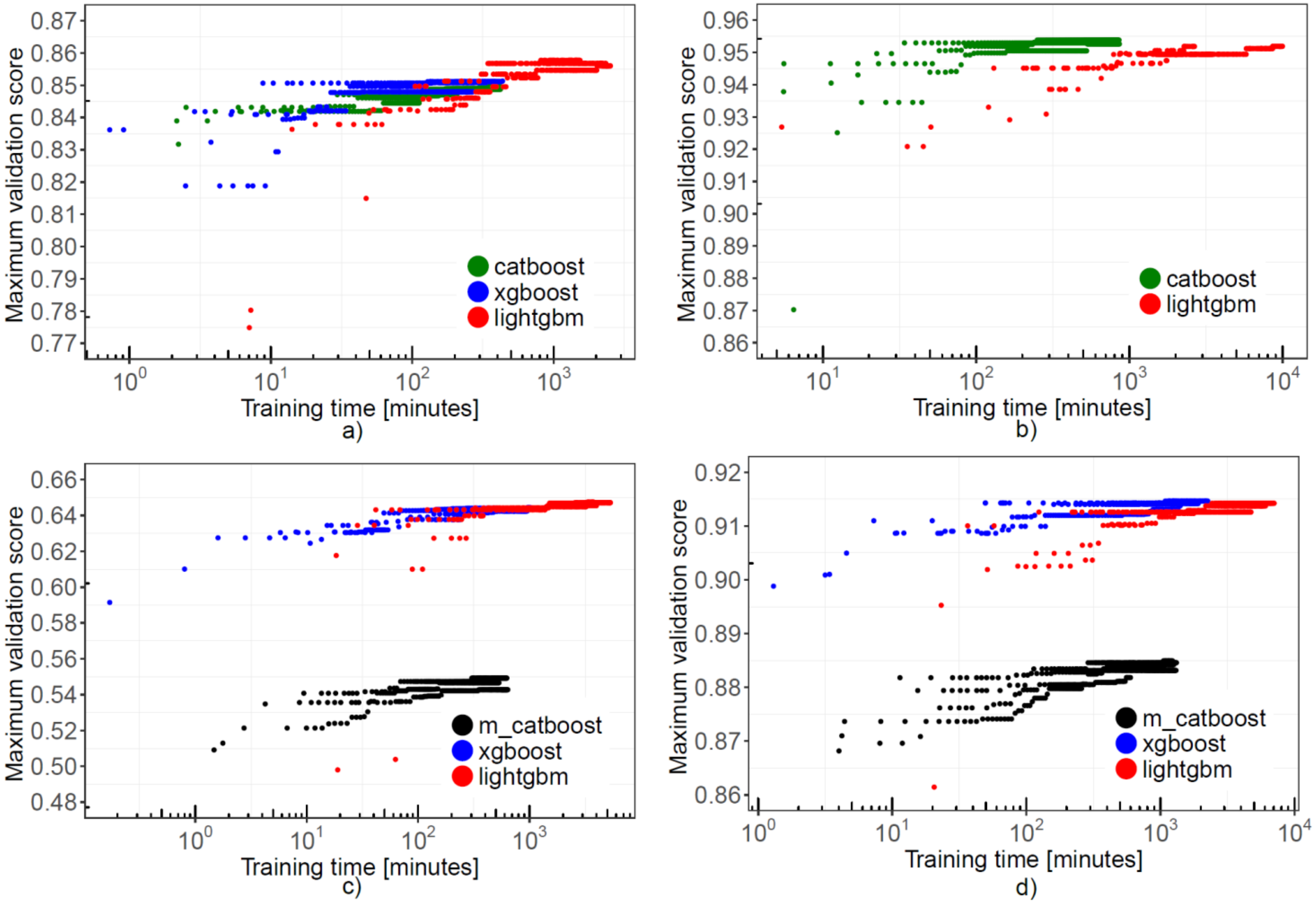


Figure 2: Max. validation score vs. total HPO runtime (a) Higgs (b) Epsilon (c) Microsoft (d) Yahoo.

CatBoost

- Optional resource
  - ✓ Youtube DSBA channel → [Papers You Must Read] playlist → [Paper Review] XGBoost: A Scalable Tree Boosting System (https://youtu.be/-w_6wDJQCZY)


Q & A