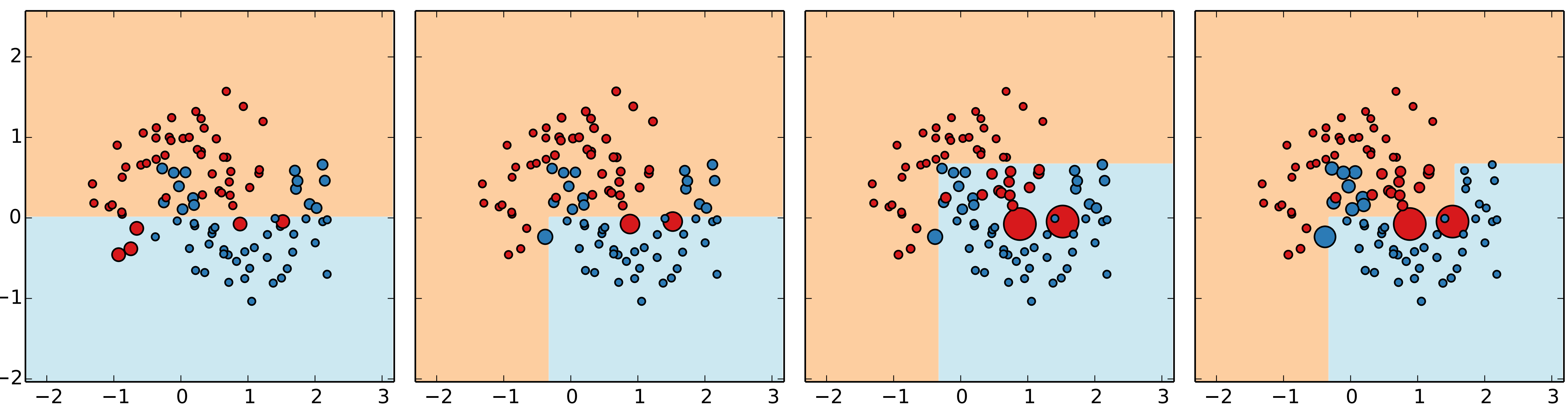
Advanced Data Science
part 2

Alexandre Gramfort
Thomas Moreau

Ensemble of experts: Boosting

- Each model is an expert on the errors of its predecessor
- Iteratively re-weights training examples based on errors
- ERM with weights:

$$\arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_i w_i \ell(f(x_i), y_i)$$



AdaBoost [Y. Freund & R. Schapire, 1995]

For binary classification

$\textsc{AdaBoost}(D_n = \{(\mathbf{x}_i, y_i)\}_{i=1}^n, \textsc{Base}(\cdot,\cdot), T)$

$\mathbf{w}^{(1)} \leftarrow (1/n, \ldots, 1/n)$ $\quad\triangleright$ *initial weights*

for $t \leftarrow 1$ **to** T

$\quad h^{(t)} \leftarrow \textsc{Base}\big(D_n, \mathbf{w}^{(t)}\big)$ $\quad\triangleright$ *calling the base learner*

$\quad \gamma^{(t)} \leftarrow \sum_{i=1}^{n} w_i^{(t)} h^{(t)}(\mathbf{x}_i) y_i$ $\quad\triangleright$ $\textit{edge} = 1 - 2 \times \textit{error}$

$\quad \alpha^{(t)} \leftarrow \frac{1}{2} \ln\left(\frac{1+\gamma^{(t)}}{1-\gamma^{(t)}}\right)$ $\quad\triangleright$ *coefficient of* $h^{(t)}$

$\quad$ **for** $i \leftarrow 1$ **to** n $\quad\triangleright$ *re-weighting the points*

$\quad\quad$ **if** $h^{(t)}(\mathbf{x}_i) \neq y_i$ **then**

$\quad\quad\quad w_i^{(t+1)} \leftarrow w_i^{(t)} \frac{1}{1-\gamma^{(t)}}$

$\quad\quad$ **else**

$\quad\quad\quad w_i^{(t+1)} \leftarrow w_i^{(t)} \frac{1}{1+\gamma^{(t)}}$

return $f^{(T)}(\cdot) = \sum_{t=1}^{T} \alpha^{(t)} h^{(t)}(\cdot)$

Remark: Freund & Schapire won the Gödel prize 2003

Gradient Boosting

- Gradient Boosting generalizes adaboost to any arbitrary loss
- a.k.a. GB(R)T, Gradient boosting (regression) trees
- It was originally proposed by [J. Friedman, 1999]
- Variants of the original GBT algorithm are now state-of-the-art models.
- Numerous successes in Kaggle competitions
- State-of-the-art implementations:
    - XGBoost [Chen & Guestrin, Arxiv 2016] (w. Apple, NVidia)
    - LightGBM [Ke et al., Proc. NIPS 2017] (by Microsoft)
    - CatBoost [Prokhorenkova et al. Arxiv 2017] (by Yandex)
    - sklearn.ensemble.HistGradientBoostingClassifier (v0.21)

Gradient Boosting vs. Deep Learning

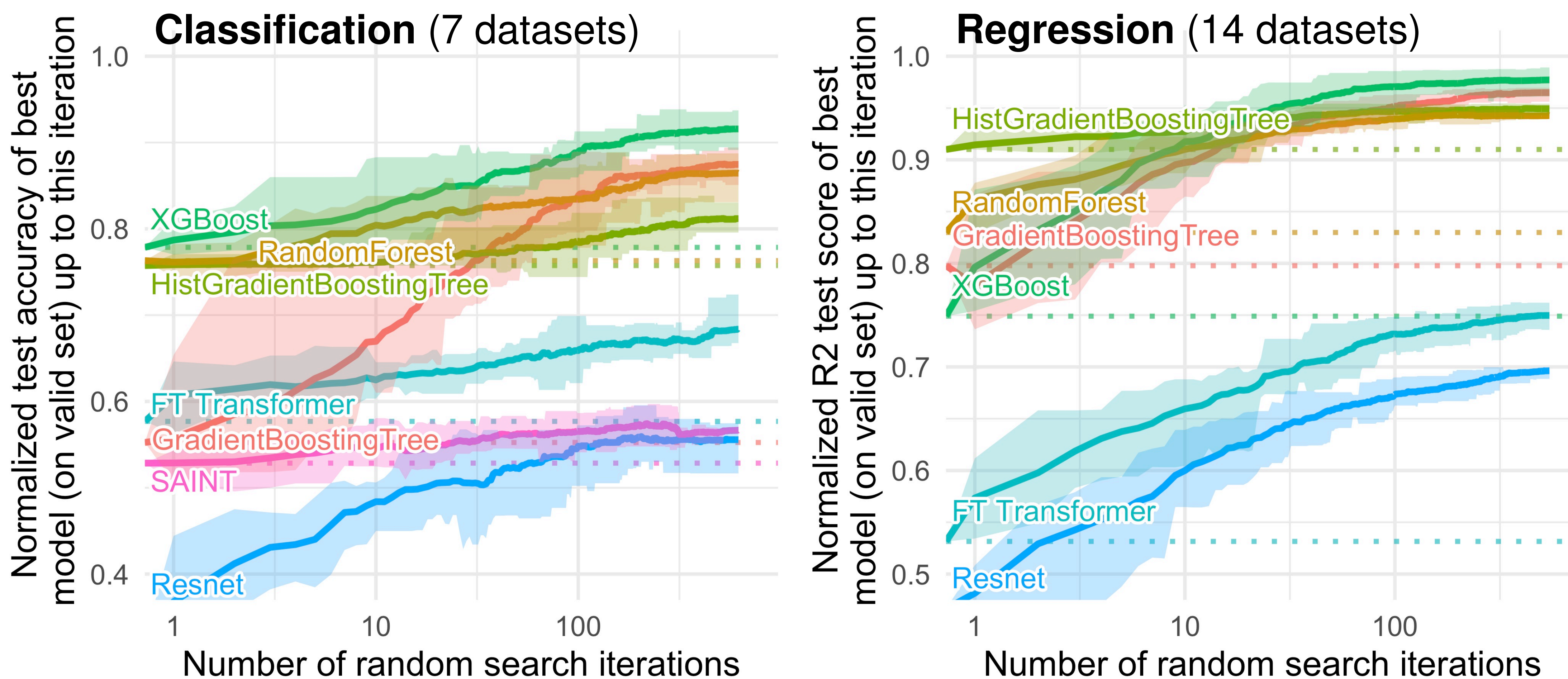


Figure 2: **Benchmark on medium-sized datasets, with both numerical and categorical features**. Dotted lines correspond to the score of the default hyperparameters, which is also the first random search iteration. Each value corresponds to the test score of the best model (on the validation set) after a specific number of random search iterations, averaged on 15 shuffles of the random search order. The ribbon corresponds to the minimum and maximum scores on these 15 shuffles.

Benchmark on 45 tabular datasets from OpenML

Why do tree-based models still outperform deep learning on tabular data?

Léo Grinsztajn (SODA), Edouard Oyallon (ISIR, CNRS), Gaël Varoquaux (SODA, https://arxiv.org/abs/2207.08815

Tree Boosting in a Nutshell

$$\hat{y}_i = \sum_{t=1}^{T} f_t(x_i),\ f_t \in \mathcal{F}$$ (additive ensemble model)

where $\mathcal{F} = \{f(x) = z^f_{q(x)}\}$ (set of trees with K leafs)

with $q : \mathbb{R}^m \rightarrow \{1,\ldots,K\}$ (tree partitioning structure)

and $z^f \in \mathbb{R}^K$ (leaf values)

Each f_t has a different tree structure

Remark: Continuous values even for classification

based on [Chen & Guestrin, Arxiv 2016]

TREE BOOSTING IN A NUTSHELL

(smooth convex loss function)

Objective function:

$$\mathscr{L}(f_1, \ldots, f_T) = \sum_i \ell(y_i, \hat{y}_i) + \sum_t \Omega(f_t)$$

Where: $\Omega(f) = \gamma K + \frac{\lambda}{2} \|z^f\|^2$ (penalize complex trees)

Remark: Original GBT algo. by Friedman had no regularization

Example with MSE / L2 loss:

$$\mathscr{L}(f_1, \ldots, f_T) = \sum_i \|y_i - \hat{y}_i\|^2 + \sum_t \Omega(f_t)$$

TREE BOOSTING IN A NUTSHELL

Model is trained in a sequential / additive manner:

$$\mathcal{L}^{(t)} = \sum_{i=1}^{n} \ell(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)) + \Omega(f_t)$$

Recap:

Taylor approximation (order 2): $\boxed{v(y+\epsilon) \approx v(y) + \epsilon v'(y) + \frac{\epsilon^2}{2} v''(y)}$

$$\mathcal{L}^{(t)} \approx \sum_{i=1}^{n} \left[\ell(y_i, \hat{y}_i^{(t-1)}) + f_t(x_i) g_i + \frac{f_t^2(x_i)}{2} h_i \right] + \Omega(f_t)$$

$$g_i = \partial_{\hat{y}^{(t-1)}} \ell(y_i, \hat{y}^{(t-1)})$$ (gradient)

$$h_i = \partial^2_{\hat{y}^{(t-1)}} \ell(y_i, \hat{y}^{(t-1)})$$ (hessian)

Tree Boosting in a nutshell

$$\mathscr{L}^{(t)} \approx \sum_{i=1}^{n} \left[\ell(y_i, \hat{y}_i^{(t-1)}) + f_t(x_i) g_i + \frac{f_t^2(x_i)}{2} h_i \right] + \Omega(f_t)$$

Example with MSE / L2 loss:

$$\ell(y_i, \hat{y}_i^{(t-1)}) = \|y_i - \hat{y}_i^{(t-1)}\|^2$$

$$g_i = \partial_{\hat{y}_i^{(t-1)}} \ell(y_i, \hat{y}_i^{(t-1)}) = -2(y_i - \hat{y}_i^{(t-1)})$$

$$h_i = \partial^2_{\hat{y}_i^{(t-1)}} \ell(y_i, \hat{y}_i^{(t-1)}) = 2$$

Tree Boosting in a nutshell

$$\mathscr{L}^{(t)} \approx \sum_{i=1}^{n} \left[\ell(y_i, \hat{y}_i^{(t-1)}) + f_t(x_i) g_i + \frac{f_t^2(x_i)}{2} h_i \right] + \Omega(f_t)$$

Removing constant terms we just need to minimize w.r.t. f_t :

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

Tree Boosting in a Nutshell

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

which can be rewritten:

$$\tilde{\mathscr{L}}^{(t)} = \sum_{i=1}^{n} \left[f_t(x_i) g_i + \frac{f_t^2(x_i)}{2} h_i \right] + \gamma K + \frac{\lambda}{2} \sum_{k=1}^{K} (z_k^{f_t})^2$$

$$= \sum_{k=1}^{K} \left[\left(\sum_{i \in I_k} g_i \right) z_k^{f_t} + \frac{1}{2} \left(\lambda + \sum_{i \in I_k} h_i \right) (z_k^{f_t})^2 \right] + \gamma K$$

where: $I_k = \{ i \mid q(x_i) = k \}$ (samples in leaf j)

Tree Boosting in a nutshell

Minimizing this:

$$\tilde{\mathcal{L}}^{(t)} = \sum_{k=1}^{K} \left[\left(\sum_{i \in I_k} g_i \right) z_k^{f_t} + \frac{1}{2} \left(\lambda + \sum_{i \in I_k} h_i \right) (z_k^{f_t})^2 \right] + \gamma K$$

leads to: $$z_k^* = - \frac{\sum_{i \in I_k} g_i}{\lambda + \sum_{i \in I_k} h_i}$$

and: $$\tilde{\mathcal{L}}^{(t)} = - \frac{1}{2} \sum_{k=1}^{K} \frac{\left(\sum_{i \in I_k} g_i \right)^2}{\lambda + \sum_{i \in I_k} h_i^2} + \gamma K$$

Tree Boosting in a nutshell

Greedy optimization of:

$$\tilde{\mathscr{L}}^{(t)} = -\frac{1}{2}\sum_{k=1}^{K}\frac{\left(\sum_{i\in I_k} g_i\right)^2}{\lambda + \sum_{i\in I_k} h_i^2} + \gamma K$$

For one leaf splitting it leads to the following criteria that should be <u>maximized</u>:

$$\boxed{\mathscr{C}_{\text{split}} = \frac{1}{2}\left[\frac{\left(\sum_{i\in I_L} g_i\right)^2}{\lambda + \sum_{i\in I_L} h_i^2} + \frac{\left(\sum_{i\in I_R} g_i\right)^2}{\lambda + \sum_{i\in I_R} h_i^2} - \frac{\left(\sum_{i\in I} g_i\right)^2}{\lambda + \sum_{i\in I} h_i^2}\right] - \gamma}$$

It corresponds to the loss reduction by splitting: $I = I_L \cup I_R$

Tree Boosting in a nutshell

Criteria that should be <u>maximized</u>:

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

Example with MSE / L2 loss: $\ell_i(y_i, \hat{y}_i) = \|y_i - \hat{y}_i\|^2$

$$\mathscr{C}_{\text{split}} = \frac{1}{2}\left[\frac{(\sum_{i\in I_L} 2(y_i - \hat{y}_i^{(t-1)}))^2}{\lambda + \sum_{i\in I_L} 4} + \frac{(\sum_{i\in I_R} 2(y_i - \hat{y}_i^{(t-1)}))^2}{\lambda + \sum_{i\in I_R} 4} - \frac{(\sum_{i\in I} 2(y_i - \hat{y}_i^{(t-1)}))^2}{\lambda + \sum_{i\in I} 4}\right] - \gamma$$

Remark: It's close to a variance impurity criterion but not equal

Tree Boosting algorithm

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

Going beyond:

- Approximate splitting (feature binning)
- Parallel implementation (multi-thread & multi-machine)
- Sparsity aware split finding (think one-hot encoding)
- Cache-aware access
- Monotonic constraints

APPROXIMATE SPLITTING

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.

Questions?

GBRT Hands on

See: code in `tinygbt.py` folder