# Analytic formulas for marginal feature attributions of oblivious decision trees

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SIAM Conference on Mathematics of Data Science October 2024 1 Overview: why feature attributions?

2 Challenges: how to compute feature attributions?

3 Solution in a special case: oblivious trees

# Explaining outcomes of a complex model

#### Setup

- ▶ the features are random variables  $\mathbf{X} = (X_1, \dots, X_n)$ ;
- ▶ the input-output function of the model  $X \mapsto f(X)$ ;
- ▶ f can be a linear model, a random forest, a neural net etc.

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ECOA/Regulation B require lenders to inform applicants of the primary reasons for decline or other adverse actions.

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#### Three ingredients:

▶ features **X** and model *f*:

- ▶ games  $S \mapsto v(S; \mathbf{X}, f)(\mathbf{x})$  ( $S \subseteq \{1, ..., n\}$ ) assigned to every point  $\mathbf{x}$ ;
- **y** game value *h* quantifying contribution of  $i^{th}$  feature as  $h_i[v]$  at given **x**.

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  Examples) f is a piecewise constant/linear function implemented by a tree ensemble/a ReLU network.
- ▶ games  $S \mapsto v(S; \mathbf{X}, f)(\mathbf{x})$  ( $S \subseteq \{1, \dots, n\}$ ) assigned to every point  $\mathbf{x}$ ; Examples) the conditional game  $S \mapsto \mathbb{E}[f(\mathbf{X}) \mid \mathbf{X}_S = \mathbf{x}_S]$  "true to the data" and the marginal game  $S \mapsto \mathbb{E}[f(\mathbf{x}_S, \mathbf{X}_{-S})]$  "true to the model".
- game value h quantifying contribution of i<sup>th</sup> feature as h<sub>i</sub>[v] at given x. Example) the Shapley value:

$$\varphi_{i}[v] := \sum_{S \subseteq \{1,...,n\} \setminus \{i\}} \frac{|S|!(n-|S|-1)!}{n!} \left( v(S \cup \{i\} - v(S)) \right).$$

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  - Remedy: Grouping features based on dependencies and using coalitional variants of the Shapley value (e.g. the Owen value) unifies the two frameworks and yields more stable explanations [Miroshnikov-Kotsiopoulos-F.-Ravi Kannan 2022].
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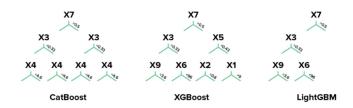
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### Different boosting libraries construct trees differently.



Picture from Medium.

- The CatBoost library utilizes oblivious (symmetric) decision trees as base learners [Dorogush-Ershov-Gulin 2018].
- Despite this constraint, ensembles of symmetric trees demonstrate competitive predictive power [Ferov-Modrý 2016], [Hancock-Khoshgoftaar 2020].

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Let  $\mathcal{T}$  be an ensemble of symmetric decision trees of depth  $\leq d$  trained on a dataset D. (Typically, D is very large and  $d \leq 10$ .)

▶ There is **an explicit formula** for marginal Shapley values of  $\mathcal{T}$  solely in terms of the model's parameters. (In principle, it can be used to compute marginal Shapley values of any decision tree.)

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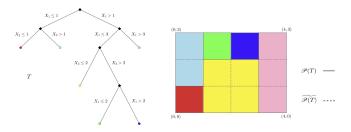
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- ▶ Based on this analytic solution, we designed **an algorithm for estimating marginal feature attributions** of  $\mathcal{T}$  according to certain precomputed look-up tables.
- ▶ The algorithm is **fast** (the computation complexity is  $O(|\mathcal{T}| \cdot d)$ ) and **accurate** (variance of error  $\propto \frac{1}{|D|}$ ).

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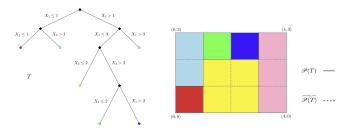
For a tree T, marginal feature attributions based on a linear game value are piecewise constant, but only with respect to a grid partition  $\mathscr{P}(T)$ , which is often finer than the tree's partition  $\mathscr{P}(T)$ . They coincide when T is symmetric.



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Game value computations can be simplified by exploiting the symmetry.