THE UNIVERSITY OF BRITISH COLUMBIA

NEURAL INFORMATION PROCESSING SYSTEMS

Differentiable Decision Tree via "ReLU+Argmin" Reformulation

39th Conference on Neural Information Processing Systems (NeurIPS 2025)

🏴 Spotlight Paper

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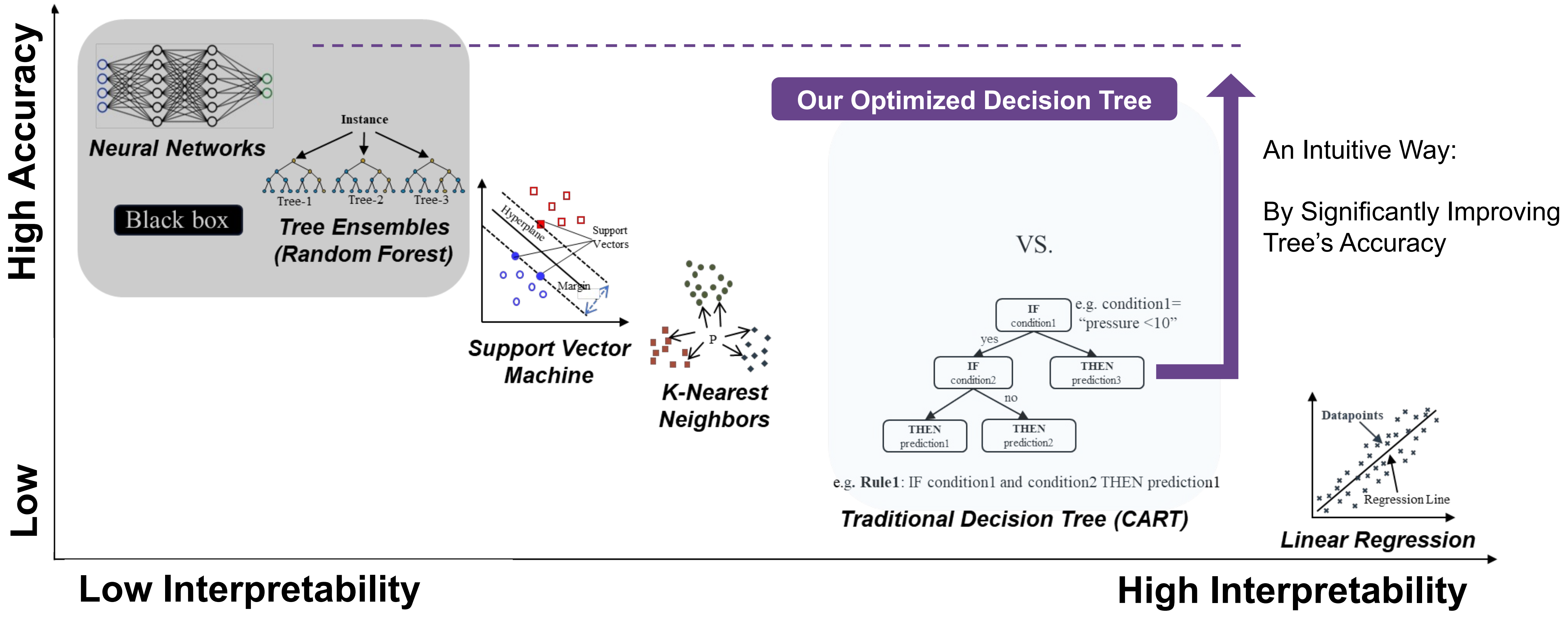
Introduction and Motivation

Decision Tree's Two Key Issues That Limit Its Broader Applicability: Lower testing accuracy and Non-differentiability



First aim: to improve tree's accuracy

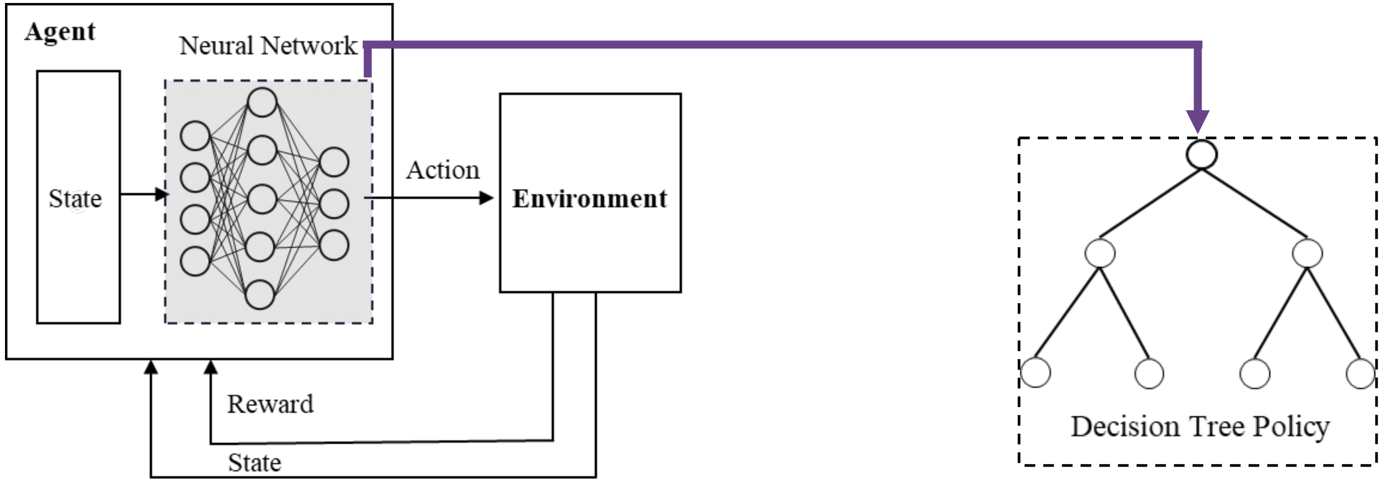
Introduction and Motivation

Decision Tree's Two Issues: Lower test accuracy and Non-differentiability

Non-differentiability: **two sources of hard decisions**

- Hard splits at branch nodes for sample branching.
- Unique decision path at leaf node for sample prediction.

Limitation in gradient-based optimization tasks.



Second aim:
differentiable tree

decision tree policy optimization in reinforcement learning.

Introduction and Motivation

Improve Decision Tree's Accuracy Through Advanced Optimization

- **Greedy Optimization**
  CART (Breiman et al., 1984)
  OC1 (Murthy et al., 1994)
- **Mixed-integer Programming**
  OCT/ORT (Bertsimas and Dunn, 2017)
  Scalability Issue
- **Other optimization**
  Gradient-based
  …
  Solvability Benefit

Concerns on existing gradient-based trees

- Straight-through estimator: suboptimal. ☹
- Approximate hard decisions (0 or 1) with probability (0, 1): soft tree. ☹

➡ How can high accuracy be achieved in a differentiable tree **while** preserving the two sources of hard decisions?

More literature and related work on tree optimization have been thoroughly reviewed and discussed in our paper:
Mao et al., 2025. Differentiable Decision Tree via "ReLU+Argmin" Reformulation. NeurIPS. Spotlight.

Contents

“ReLU+Argmin”-based Differentiable Decision Tree

Unconstrained Oblique Decision Tree Reformulation

Basic mathematical notations

Dataset: $\{\boldsymbol{x}_i, y_i\}_{i=1}^n$ Tree Depth: D Brach node: $\mathbb{T}_B$ Leaf node: $\mathbb{T}_L$

Weight : $\boldsymbol{a}_t \in \mathbb{R}^p \quad t \in \mathbb{T}_B$

Threshold: $b_t \in \mathbb{R} \quad t \in \mathbb{T}_B$

Tree split parameters

Leaf value: $\theta_t = \{\boldsymbol{k}_t \in \mathbb{R}^p, h_t \in \mathbb{R}\} \quad t \in \mathbb{T}_L$ for regression

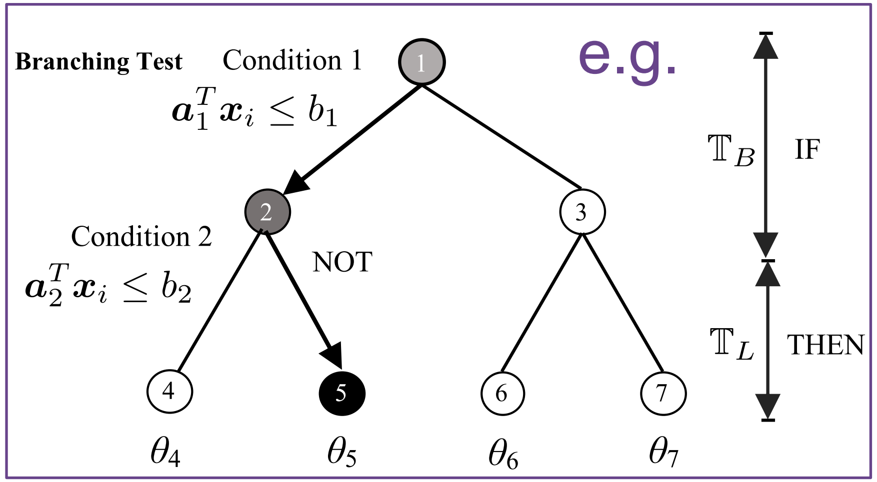
$\theta_t = \{h_t \in \mathbb{R}^c\}$ for classification

Leaf prediction parameter

Final prediction:

$\hat{y}_i = h_t$ for tree with constant predictions

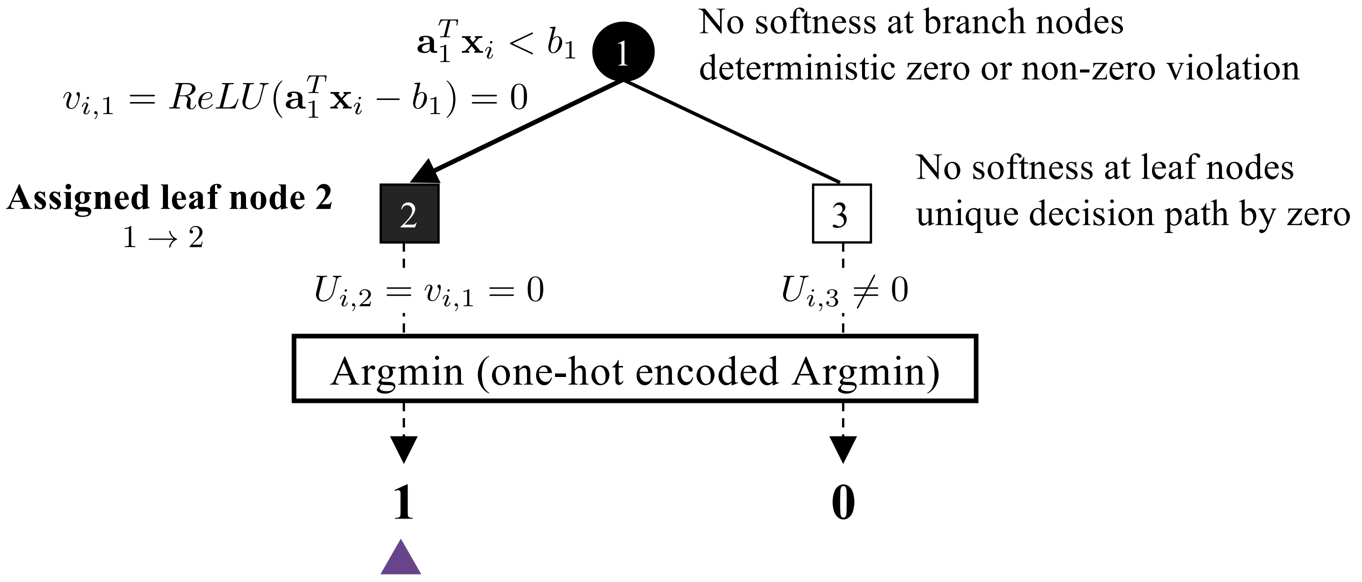
$\hat{y}_i = \boldsymbol{k}_t^T \boldsymbol{x}_i + h_t$ for tree with linear predictions



“ReLU+Argmin”-based Differentiable Decision Tree

Unconstrained Oblique Decision Tree Reformulation

Example of 1-depth tree (correct sample assignment $1 \rightarrow 2$)



- Violations of correctly-directed path

$$v_{i,1} = ReLU(\mathbf{a}_1^T\mathbf{x}_i - b_1) = 0$$

Correct-direction; No violation.

- Cumulative violations: only *one* zero-violation at the *unique* path

Path to node 2: $U_{i,2} = 0$

Path to node 3: $U_{i,3} \neq 0$

- Loss function: $\mathcal{L}_i = (y_i - \theta_2)^2$

$$\mathcal{L}_i = \left[\underline{1} \cdot (y_i - \theta_2)^2 + 0 \cdot (y_i - \theta_3)^2\right]$$

Correctly Assigned

A 2-depth tree example is discussed in the paper.

Unconstrained Oblique Tree Exact Reformulation

ReLU-based hard splits → left-right branching (zero or non-zero violation).

No softness for sample branching

- Correct direction: violation $v_{i,j} = 0$

Cumulative violations across all ancestors $\mathbb{A}_t = \mathbb{A}_t^l \cup \mathbb{A}_t^r$

$$U_{i,t} = \sum_{j \in \mathbb{A}_t^l} v_{i,j} + \sum_{j \in \mathbb{A}_t^r} v_{i,j}$$

- Unique decision path formulation using Argmin (*No* softness for sample prediction)

$$\mathbb{M}\left(U_{i,t}\right) = \mathbb{1}\left(t = \left(\mathrm{Argmin}(\mathbf{U}_i) + \lceil T/2 \rceil\right)\right)$$
$$\mathbf{U}_i = \{U_{i,\lfloor T/2 \rfloor + 1}, \cdots, U_{i,T}\}$$

Only outputting one when $U_{i,t} = 0$; otherwise 0.

Unique tree path (correctly assigned)

- Unconstrained optimization task

$$\mathcal{L} = \sum_{i=1}^{n} \sum_{t \in \mathbb{T}_L} \mathbb{M}\left(U_{i,t}\right) \ell\left(y_i, \hat{y}_i\right)$$

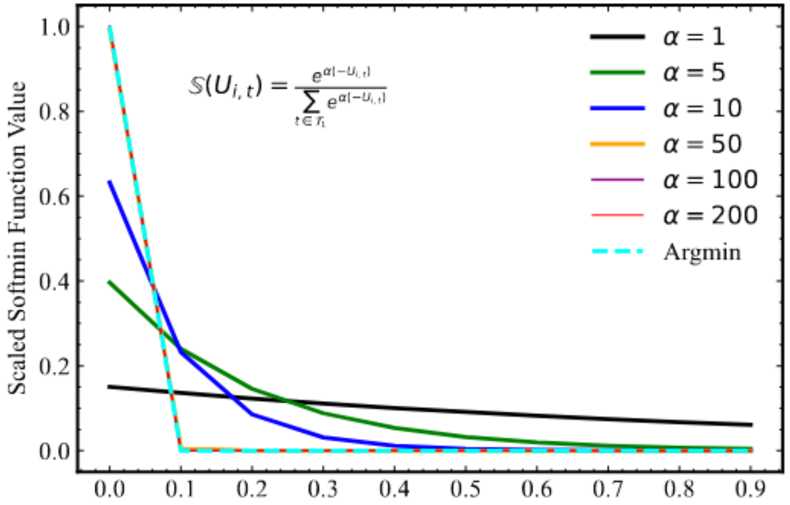
Multi-run Warm Start Annealing Strategy For Scaling Softmin Operations

$$\mathcal{L} = \sum_{i=1}^{n} \sum_{t \in \mathbb{T}_L} \underline{\mathbb{M}\left(U_{i,t}\right)} \ell\left(y_i, \hat{y}_i\right)$$

Involve Argmin operation $\longrightarrow$ undefined gradient

◆ Scaled Softmin to approximate Argmin

$$\mathbb{S}\left(U_{i,t}\right) = \frac{e^{\alpha(-U_{i,t})}}{\sum_{t \in \mathbb{T}_L} e^{\alpha(-U_{i,t})}} \longrightarrow \mathcal{L} = \sum_{i=1}^{n} \sum_{t \in \mathbb{T}_L} \mathbb{S}\left(U_{i,t}\right) \ell\left(y_i, \hat{y}_i\right)$$



By starting with a smaller α and gradually increasing it

The solution from an optimization task with a smaller α is used to warm-start the next task with a larger α.

Trade-off between approximation accuracy and numerical stability

Gradient-based Entire Tree Optimization Framework for RADDT

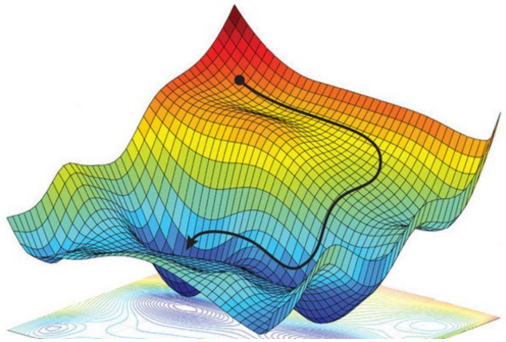
Why to implement optimization within existing frameworks?

TensorFlow
PyTorch

- Efficient gradient calculations
  Mature auto differentiation tools.

- Efficient parameter updates
  Powerful gradient-based **optimizers**, e.g. Adam optimizer.

- High-performance computing
  Distributed multi-GPU parallelization.



Contents

14 compared baselines across 8 groups

- (a) greedy: `CART`, `HHCART` (Wickramarachchi et al., 2015), `RandCART` (Blaser and Fryzlewicz, 2016), `OC1` (Murthy et al., 1994)
- (b) non-greedy tree: `TAO` (Zharmagambetov and Carreira-Perpinan, 2020)
- (c) gradient-based trees using STE: `GradTree` (Marton et al., 2023), `DGT` (Karthikeyan et al., 2022), `DTSemNet` (Panda et al., 2024)
- (d) sigmoid-based soft tree: `SoftDT` (Frosst and Hinton, 2017)
- (e) relaxed MIP-based tree solved via implicit differentiation `LatentTree` (Zantedeschi et al., 2021)
- (f) Local search `ORT-LS` (Dunn, 2018)
- (g) soft tree variant using smooth-step function `TEL` (Hazimeh et al.,2020) (Tree ensemble)
- (h) other ensembles like random forest `RF` and `XGBoost`

Since it remains uncertain whether oblique trees can match tree ensemble's accuracy, we include `RF` and `XGBoost` as a commonly used and strong ensemble baselines, and `TEL` as the oblique ensemble counterpart.

Numerical Experiments and Discussions

Evaluation on 4 groups of datasets

- (i) 17 medium-sized regression datasets (primary focus)
- (ii) 27 classification and 9 regression datasets used in the papers of certain baselines (for a more credible comparison)
- (iii) 4 real-world small datasets, and 3 synthetic datasets (for comparing global optimality)
- (iv) 7 million-scale datasets (for evaluating scalability).

We mainly evaluate regression tasks, but also include the same classification datasets used by certain baselines for a more convincing comparison.

This slide does not cover all experiments; more comprehensive empirical analyses can be found in the paper.

Numerical Experiments and Discussions

Test Accuracy Comparison

Our tree with constant predictions RADDT

	Greedy Methods				Gradient-based[1, 2]		Local Search	Ours
	CART	RandCART	HHCART	OC1	GradTree	SoftDT	ORT-LS	RADDT
Testing Accuracy (R^2, %)	74.85	71.20	76.75	73.31	64.30	72.72	78.67	**82.39**
Tree Depth	10.24	8.12	8.29	8.12	10.29	10.29	6.24	7.29
Friedman Rank	4.65	5.88	3.65	5.06	7.00	4.76	3.24	**1.76**

[1] Other two gradient-based DGT and LatentTree are compared later with fixed depths due to scalability issues at depth 12.
[2] More results on their originally-used dataset are discussed in the paper, include GradTree, SoftDT, DGT, and DTSemNet.

7.54% higher than CART

3.72% higher than ORT-LS

Our tree with linear predictions RADDT-Linear

	RF	XGBoost	TEL	RADDT	RADDT-Linear
Number of Trees	314.71	352.94	10	1	1
Test Accuracy (R^2, %)	82.62	83.51	83.87	82.39	**84.63**
Friedman Rank	2.88	**2.24**	3.29	4.35	**2.24**

- RADDT-Linear outperforms RF by 2.01%

Our aim is NOT to claim superiority over ensembles. Instead, we provide a reference showing that our tree can match ensemble's accuracy with far fewer parameters.

Numerical Experiments and Discussions

Superior Testing Accuracy Analysis: From Training Optimality Perspective

Fixed-depth comparison of training, testing accuracy and training time on Group (i) datasets.

	D	Greedy Methods				Gradient-based Trees				Local Search	Ours
		CART	RankCART	HHCART	OC1	GradTree	SoftDT	DGT	LatenTree	ORT-LS	RADDT
Train (R^2,%)	2	46.95	32.81	46.20	49.59	39.42	50.59	64.48	66.94	66.43	**71.78**
	4	61.16	54.09	62.65	63.21	53.29	56.83	75.83	72.25	79.52	**82.18**
	8	81.45	77.51	82.26	81.43	64.65	66.81	82.01	74.54	90.91	**90.93**
	12	93.45	93.06	94.74	93.02	66.86	73.03	/	/	97.46	96.36
Test (R^2,%)	2	46.14	32.47	45.61	47.95	38.53	49.94	63.81	66.42	64.51	**70.07**
	4	58.92	52.69	61.30	60.22	51.45	56.32	75.16	71.03	75.06	**78.98**
	8	69.77	69.93	74.57	69.08	62.40	66.44	79.99	70.77	74.93	**77.89**
	12	68.28	64.13	68.37	65.57	63.81	72.45	/	/	68.25	**73.11**
Time (s)	2	0.03	0.70	4.43	3,216	31.32	22.24	2,102	1,624	457.21	542.22
	4	0.04	1.56	7.45	4,192	54.74	81.88	2,577	2,194	868.08	478.81
	8	0.07	5.08	12.52	4,803	298.92	1,209	4,049	2,381	9,336	602.69
	12	0.10	12.61	22.01	5,103	10,417	54,829	/	/	210,141	2,643

- Our `RADDT` outperforms the baseline `CART` by 24.83%, 21.02% and 9.48% in training for depths of 2, 4 and 8

⇨ showcase the efficacy of our tree optimization to achieve better training optimality.

High train accuracy → High test accuracy (if no overfitting)

Numerical Experiments and Discussions

GPU Acceleration (Training Time), Model Complexity (Inference Time)

- Our method scales to 12-depth deep tree on **million-scale** datasets, where existing gradient-based trees fail.

- For a similar accuracy, our oblique tree may NOT require more parameters overall than orthogonal tree.

- Interpretability depends on **multiple factors:** tree depth, feature number, and the accuracy-simplicity trade-off.

More detailed empirical results, model parameters calculation and interpretability analysis can be found in the paper.

Limitation and Future Work

- Inadequate regularization.
- A lack of theoretical analysis.
- Fail to consider the corner case where both $\boldsymbol{a}_j = 0$ and $\boldsymbol{b}_j = 0$.

- More tuning on regularization parameters for tree ensembles.
- Apply our proposed optimization strategies to other gradient-based trees.
- Try different alternatives for scaled softmin operations, e.g. entmax function.

Detailed limitation analysis and future work can be found in the paper.

Reference

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[12] Hazimeh, H., Ponomareva, N., Mol, P., Tan, Z., Mazumder, R., 2020. The tree ensemble layer: differentiability meets conditional computation.

Other references can be found in the paper of “Differentiable decision tree via ‘Relu+Argmin’ reformulation”.

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Thank you.

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