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Improving the validity of Decision Trees as Explanations

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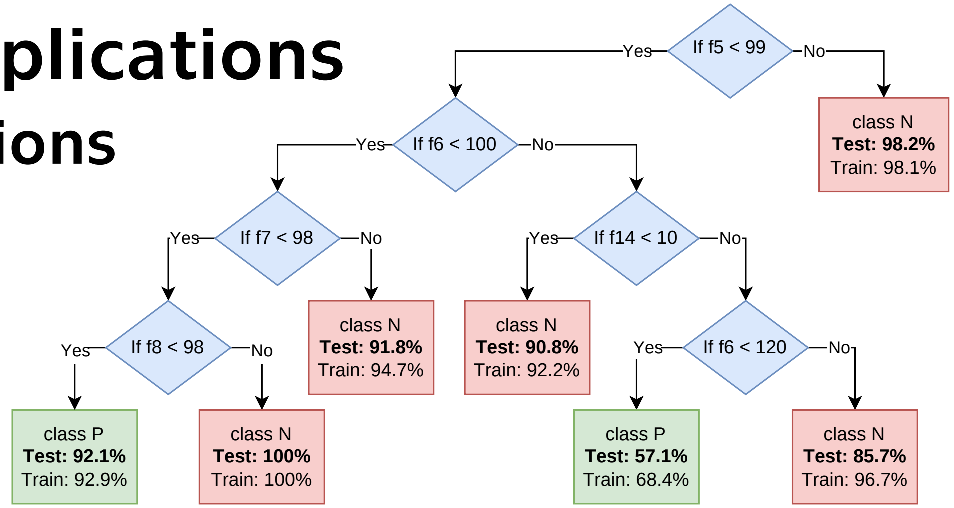
What are we talking about?

- Decision trees
  - Classification
- Explainability applications
  - Univariate decisions
  - Shallow



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Decision Trees

- Global optimality NP-hard
- Heuristic algorithms
  - Good empirically
  - Greedy top-down
    - Information gain
    - Gini impurity

  \+ Pruning

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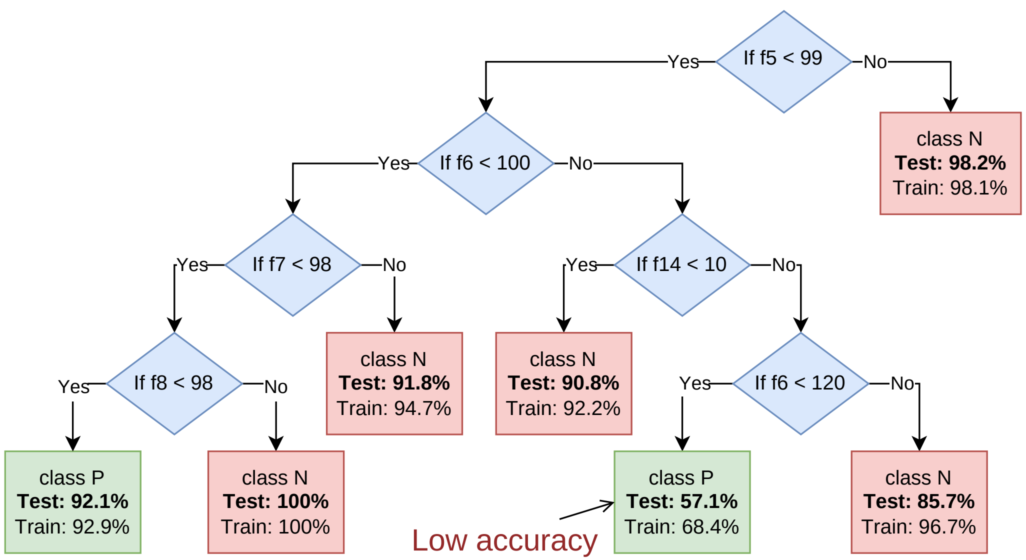
The problem

- CART creates a leaf with low accuracy
  → Misleading (~unfair) explanation



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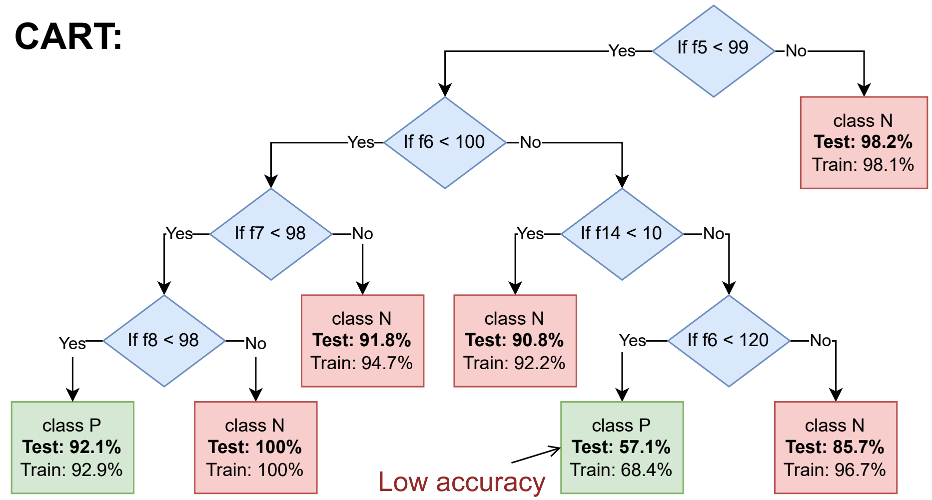
Proposed solution

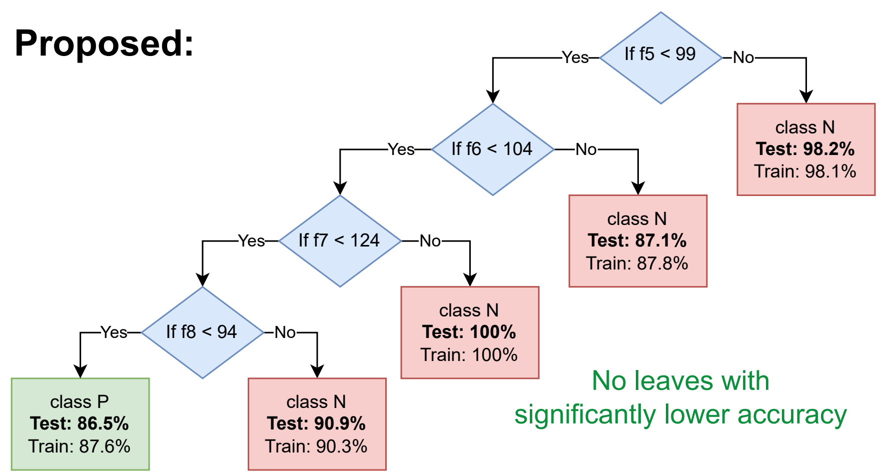
- Maximize leaf accuracy
  - Minimal accuracy across leaves

$$A_L(T) := \min_{l \in \mathcal{L}(T)} \frac{1}{|X_l|} \sum_{(\boldsymbol{x},y) \in X_l} [\![y = C_l]\!]$$

CART:



Proposed:



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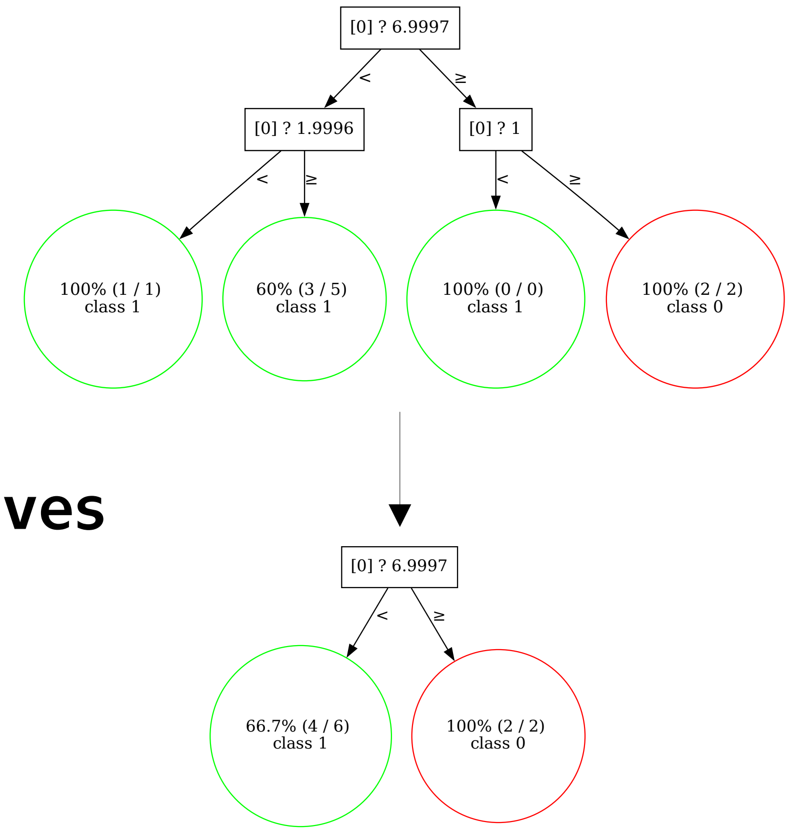
Training Process

- Create a Tree
    - MIP formulation
- Reduce
    - Remove redundant leaves
- Extend leaves
    - Any ML model
    - Improve the total model accuracy



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MIP formulation

- Based on Optimal Classification Tree (OCT) formulation [Bertsimas and Dunn, 2017]
- Change the objective to Leaf Accuracy
  - Details in the paper

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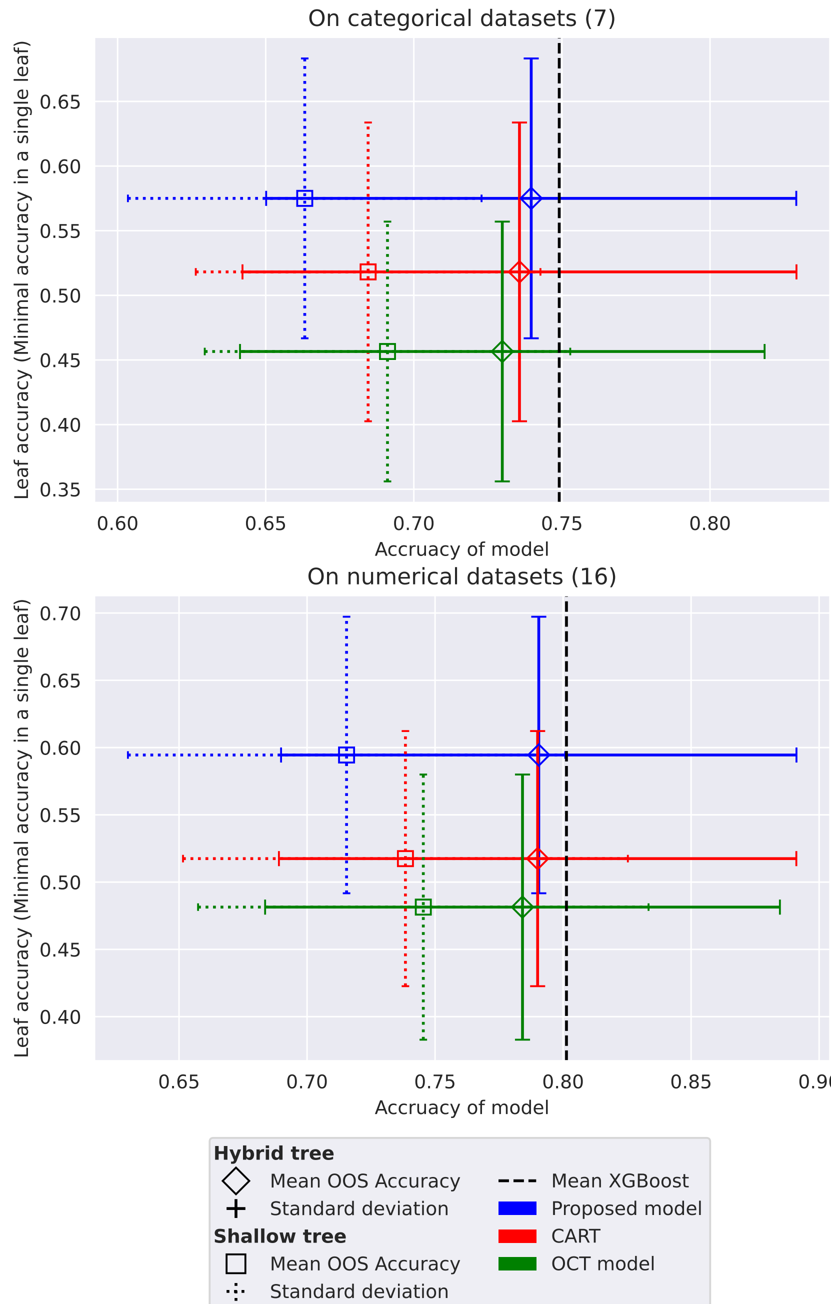
Results

- Categorical and Numerical tabular data [Grinsztajn et al., 2022]
- At least 50 samples in each leaf
- Tree depth = 4
- 10 random runs
- MIP time limited to 8 hours



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Summary

- Top-down algorithms for trees can make unbalanced leaves (in terms of accuracy)
- Maximizing leaf accuracy improves this
- Trade-off between leaf and model accuracy
- When extended, the model has comparable performance + added explainability

- MIP limitations (dataset, tree depth)

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Questions?

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References

- Dimitris Bertsimas and Jack Dunn. **Optimal classification trees.** *Machine Learning*, 106(7):1039–1082, July 2017. ISSN 1573-0565. doi: 10.1007/s10994-017-5633-9.
- Léo Grinsztajn, Edouard Oyallon, and Gael Varoquaux. **Why do tree-based models still outperform deep learning on typical tabular data?** *In Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*, 2022. URL https://openreview.net/forum?id=Fp7 phQszn

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Tabulated results

	Data Type	Min	Mean ($\pm$ std)	Max
Compared to CART				
Leaf Accuracy	categorical	-0.0142	0.0569 ± 0.0533	0.1206
	numerical	-0.0061	0.0770 ± 0.0556	0.1841
Hybrid-tree Acc.	categorical	-0.0078	0.0040 ± 0.0071	0.0147
	numerical	-0.0244	0.0004 ± 0.0082	0.0087
Compared to XGBoost				
Hybrid-tree Acc.	categorical	-0.0228	-0.0095 ± 0.0064	-0.0036
	numerical	-0.0276	-0.0108 ± 0.0076	0.0005

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