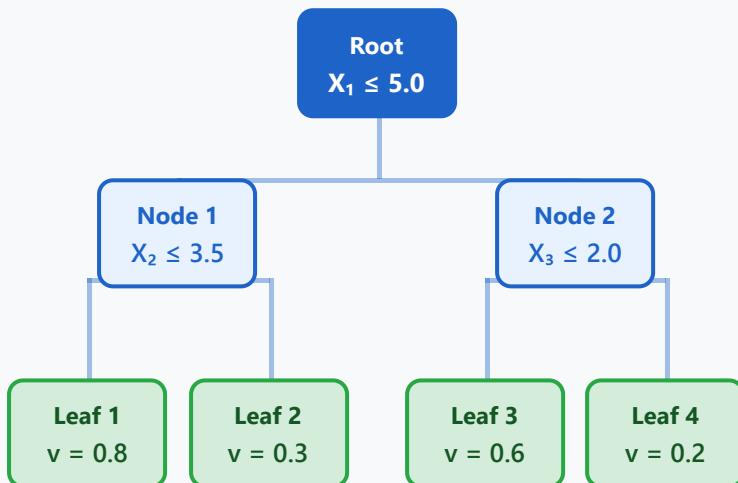


# TreeSHAP: Optimized for Tree-Based Models

Polynomial time algorithm with exact Shapley values

## Tree Traversal Example



## Complexity Analysis

$$O(TLD^2) \text{ vs } O(2^M)$$

T: trees, L: leaves, D: max depth, M: features



## Speed Advantage

10-100x faster than KernelSHAP for tree models



## Exact Values

Computes exact Shapley values using tree structure



## Model Support

Random Forest, XGBoost, LightGBM, CatBoost

## ⌚ Speed Comparison

TreeSHAP

1x

KernelSHAP

100x

## TreeSHAP Computation Principles

## 1 Tree Structure Exploitation

TreeSHAP efficiently computes Shapley values by leveraging the hierarchical structure of tree-based models. It tracks decision paths at each node while reusing computations for feature combinations that share the same subtree.

$$\varphi_i = \sum_{S \subseteq M \setminus \{i\}} |S|! (M - |S| - 1)! / M! \times [f_{S \cup \{i\}}(\mathbf{x}_{S \cup \{i\}}) - f_S(\mathbf{x}_S)]$$

Original Shapley value definition

## 2 Recursive Computation

The algorithm recursively traverses the tree from root to leaves, tracking two pieces of information at each node:

### Tracked Information

- **Coverage:** The proportion of possible feature combinations passing through the current node
- **Contribution:** The impact each feature has on the prediction value

**RECURSE(j, m, p<sub>z</sub>, p<sub>o</sub>, v)**

j: current node, m: unique path, p<sub>z</sub>: zero probability, p<sub>o</sub>: one probability, v: node value

## 3 Path Integration

When the same feature is used across multiple paths, the final Shapley value is calculated by taking a weighted average of each path's contribution. This process obtains exact values without explicitly enumerating all possible paths in the tree.

$$\varphi_i = \sum_{\text{paths}} w_{\text{path}} \times \Delta v_{i,\text{path}}$$

## 4 Ensemble Integration

For ensemble models like Random Forest or Gradient Boosting, the Shapley values are computed independently for each tree and then averaged to generate the final explanation.

$$\varphi_i^{\text{ensemble}} = (1/T) \times \sum_{t=1}^T \varphi_i^{(t)}$$

T: number of trees,  $\varphi_i^{(t)}$ : Shapley value of feature i for the t-th tree



### TreeSHAP vs KernelSHAP

#### TreeSHAP

**Computation:** Direct use of tree structure

**Complexity:** O(TLD<sup>2</sup>)

**Accuracy:** Exact Shapley values

**Speed:** Very fast (polynomial time)

**Application:** Tree-based models only

#### KernelSHAP

**Computation:** Sampling-based approximation

**Complexity:** O(2<sup>M</sup>)

**Accuracy:** Approximate values

**Speed:** Slow (exponential time)

**Application:** Any model

#### Key Insights

- TreeSHAP reduces exponential complexity to polynomial complexity by efficiently computing conditional expectations in trees

- It leverages dynamic programming principles to eliminate redundant computations and maximize memory efficiency
- Unlike model-agnostic KernelSHAP, it enables accurate and fast computation by exploiting the model's internal structure