COMS4995W32
Applied Machine Learning

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Columbia University | Fall 2025

Tree Models & Ensembles

Agenda

- Motivation
- Decision Trees
- Ensembles
- Summary

Motivation

Why do we need Tree Models? 🌲

In previous:

- Linear Regression → assume linear decision boundary
- Naive Bayes → assume feature independence

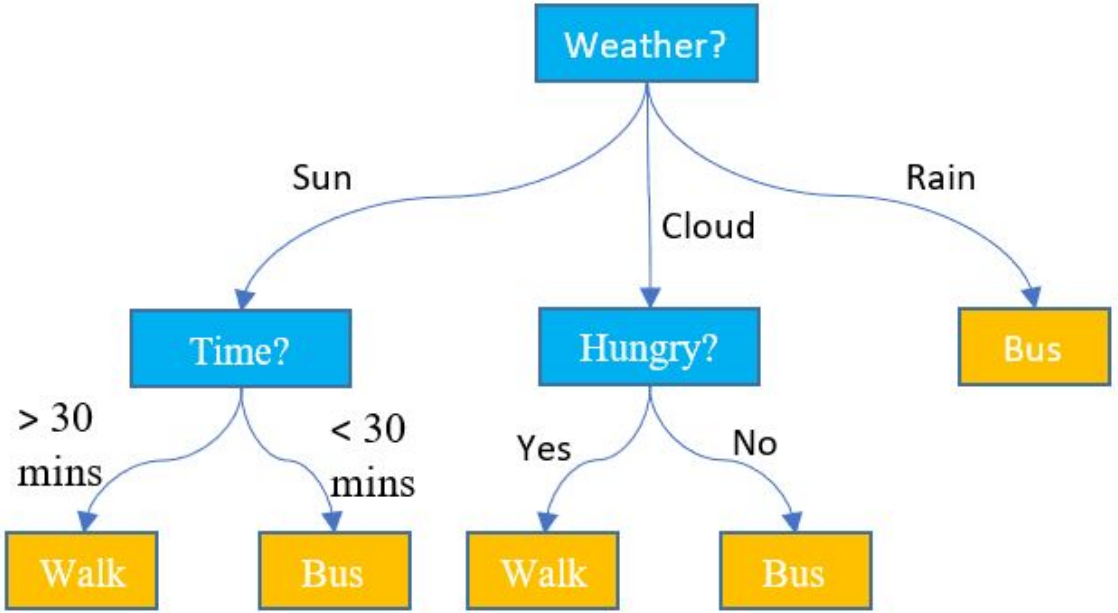
But… real-world data is often non-linear, complex, and mixed

Why do we need Tree Models? 🌲

Decision Trees:

- Flexible → no strict distribution or linearity assumptions
- Versatile → handle both numeric & categorical features
- Non-linear power → capture curved/complex decision boundaries
- Interpretability → rules easy to visualize & explain to non-experts
- Foundation of Ensembles → Random Forests, Boosting, XGBoost 🚀

Why do we need Tree Models? 🌲



Decision Trees

What is a Decision Tree? 🌳

[Inference] A decision tree is like a 20 Questions game 🎲

- At each step → ask a yes/no question about the data
- Each answer leads you further down the tree
- Finally, you reach the final decision / prediction

Example:

Shall we have the mid-term test next week?

→ Yes → take mid-term

→ No → take mid-term :)

Decision Tree in Action

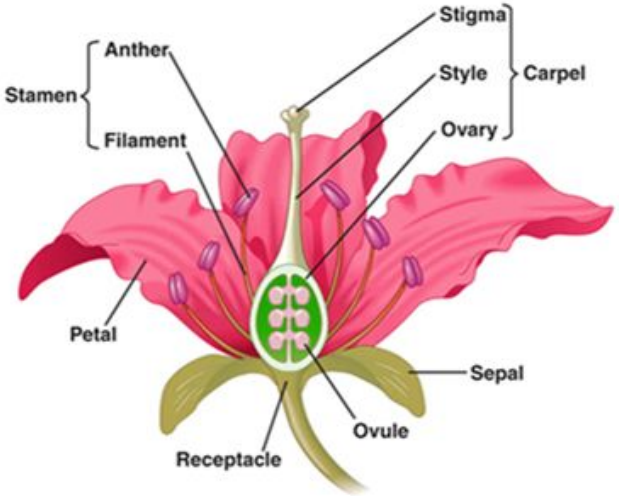
Iris Dataset: 150 flowers → 3 classes

Features:

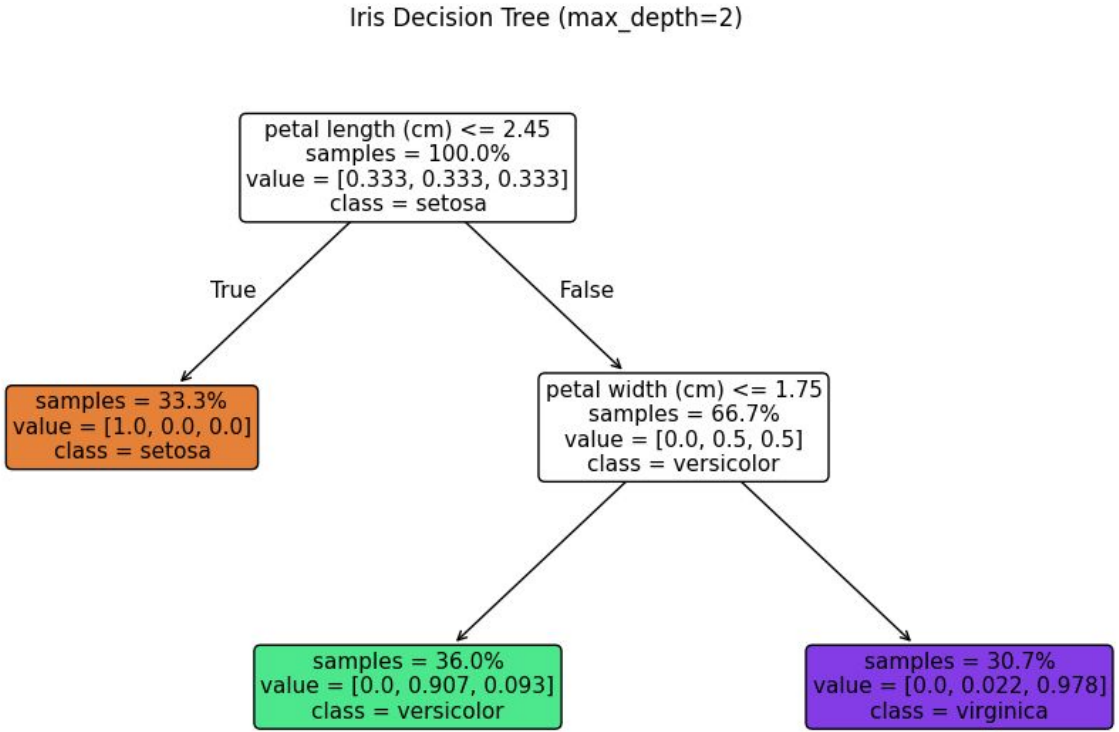
- Sepal length
- Sepal width
- Petal length
- Petal width

Target labels:

- [0] Iris Setosa 🌱
- [1] Iris Versicolor 🌷
- [2] Iris Virginica 🌼


Stigma
Anther
Style
Carpel
Stamen
Ovary
Filament
Petal
Sepal
Ovule
Receptacle

Visualizing a Simple Decision Tree 👀



Components of a Decision Tree 🌳

Root Node → initial state

Internal Nodes → decision points (questions based on features)

Branches → outcomes of questions (Yes / No, > / = / <)

Leaves → final prediction (class label / value)

Decision Path → sequence of rules from root to leaf

- one classification rule

Tree Depth → longest path from root to leaf (tree complexity)

Two Flavors of Trees 🌲

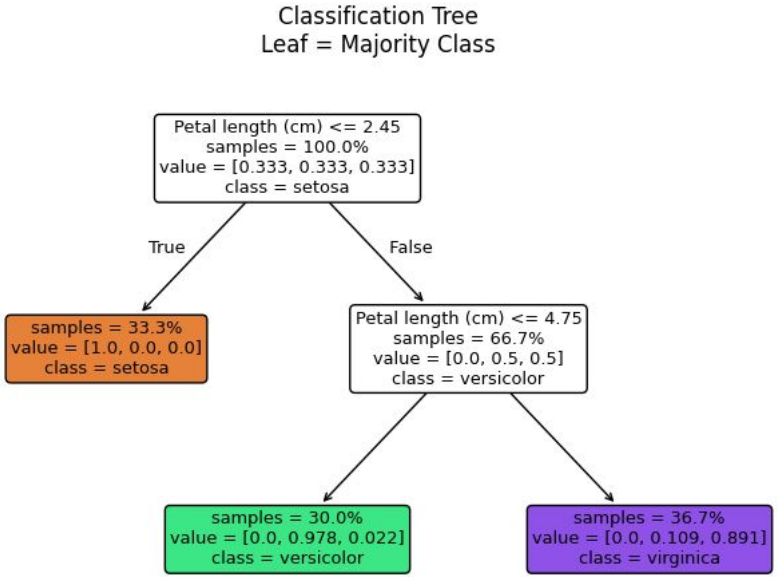
Classification Tree:

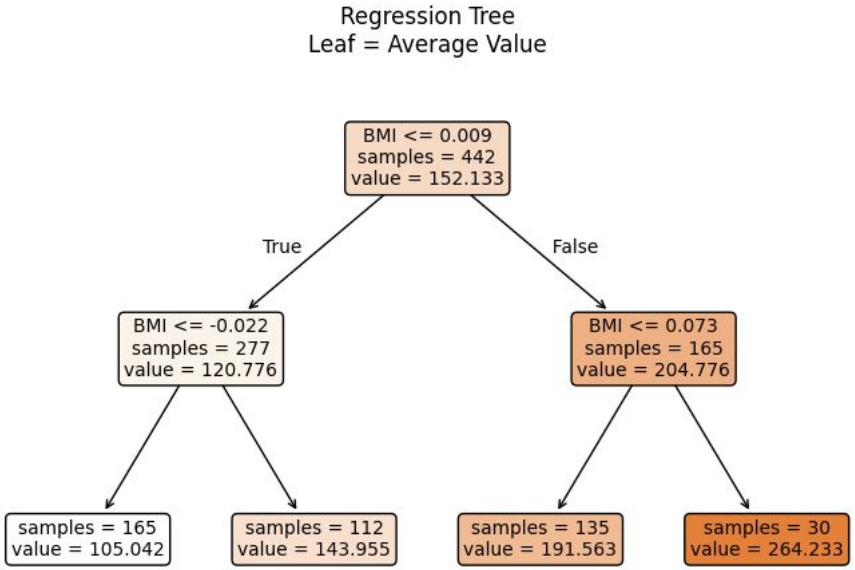
- Output = discrete label
- Leaf prediction = majority class

Regression Tree:

- Output = continuous value
- Leaf prediction = average of samples

Two Flavors of Trees 🌲





How do we train (aka split)? ✂️

💡 Idea: Make children nodes “purer” than the parent

Pure node → samples mostly belong to one class

Example intuition:

- Before split:
  - 50% red 🔴, 50% blue 🔵 (100)
- After split:
  - left node 90% red 🔴 (40)
  - right node 80% blue 🔵 (60)
- Better separation → better classification capability

Mathematical Support 📐

Pure definition:

Gini Impurity $$Gini(S) = 1 - \sum_{i=1}^{C} p_i^2$$

Entropy $$H(S) = -\sum_{i=1}^{C} p_i \log p_i$$

p_i : proportion of samples in node S that belong to class i

Smaller → Better

Entropy vs Gini

Gini Impurity: How mixed the classes are in a node

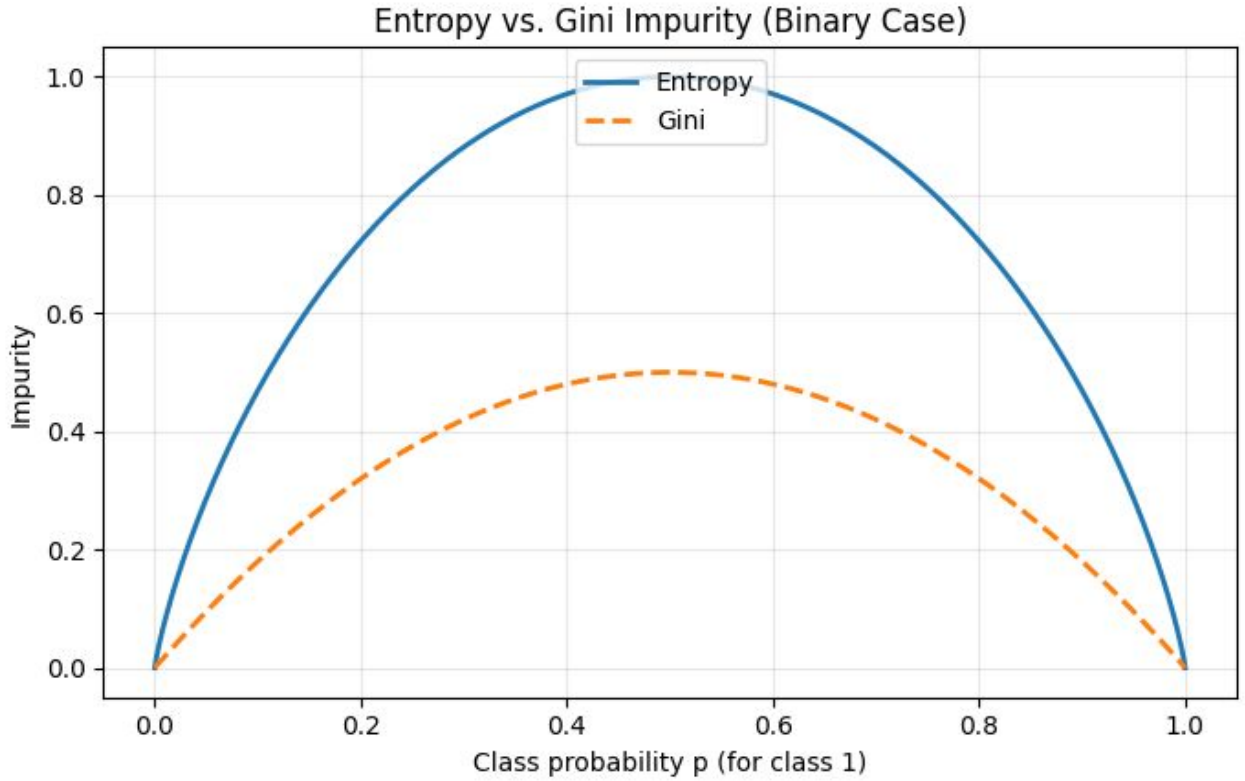
Entropy: What the uncertainty degree is in a node

0 = pure, higher = more mixed

Both are similar in shape

Used interchangeably in practice

Entropy vs Gini



Decision Tree Algorithm


```
func build_tree(data) → current node:
    if stopping_condition(data):
        return Leaf(prediction=data.label_majority)
    best_feature, threshold = choose_best_split(data)
    left_data, right_data = split(data, best_feature, threshold)
    node = Node(feature=best_feature, threshold=threshold)
    node.left  = build_tree(left_data)
    node.right = build_tree(right_data)
    return node
```

How to Split?


```
func choose_best_split(data) → (feature, threshold):
    best_split = None; best_gain  = -inf
    for feature in features:
        for threshold in possible_thresholds(feature):
            left, right = split(data, feature, threshold)
            if left or right is empty: continue
            gain = impurity(parent) - weighted_impurity(left, right)
            if gain > best_gain:
                best_gain = gain;  best_split = (feature, threshold)
    return best_split
```

When to Stop?


```
func stopping_condition(data, depth):
    if all_same_label(data):
        return True
    if depth >= MAX_DEPTH:
        return True
    if split_gain(data) < MIN_GAIN:
        return True
    # Otherwise, continue splitting
    return False
```

Deep Trees = Overfitting ⚠️

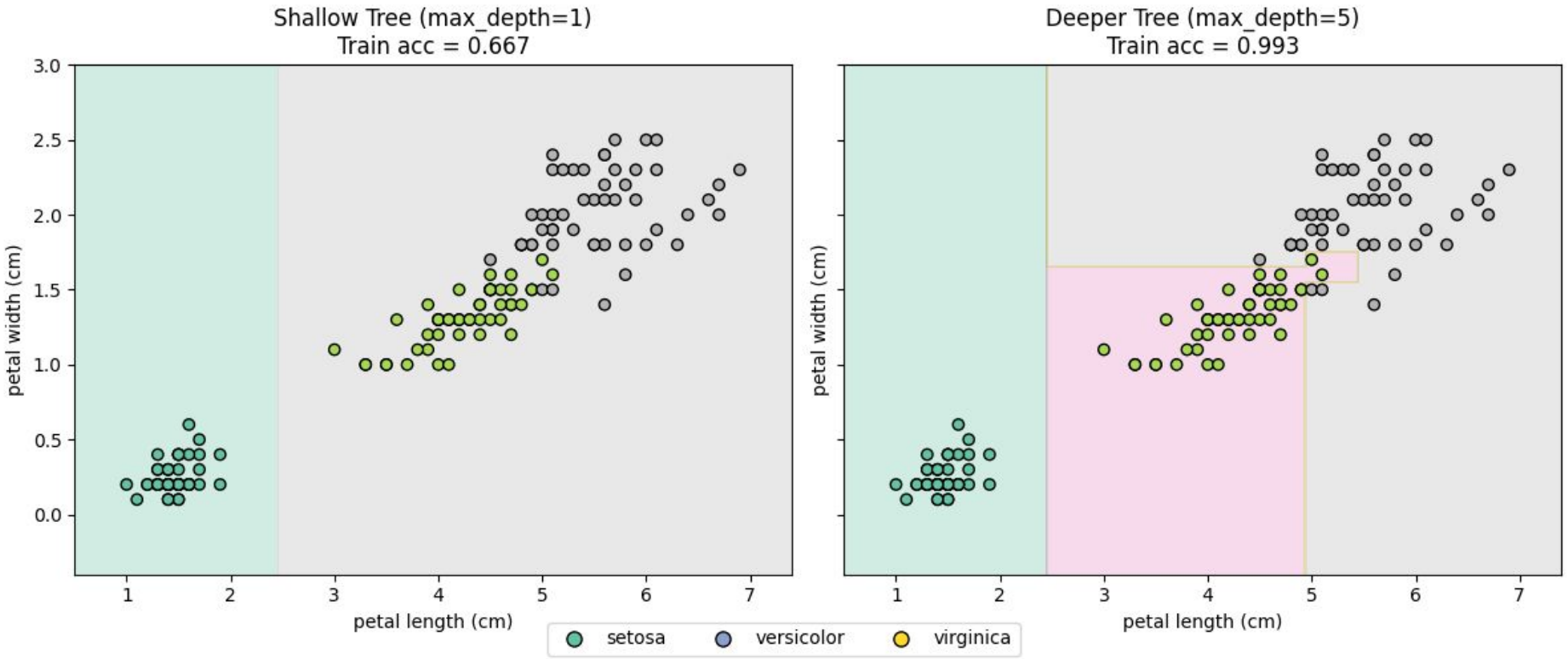
Deep tree memorizes training data → high variance

Small perturbation in data → different splits

Example: depth=1 vs depth=5

Need control: `max_depth`, `min_samples_split`

Deep Trees = Overfitting ⚠️



Why Pruning? 🌳✂️

Without limits, trees grow very deep → low training error, overfitting 😵

Pruning = controlling tree growth to improve generalization

2 perspectives:

- When to prune (Pre vs Post)
- How much to prune (Moderate vs Strong)

Pre-pruning (Early Stopping) ⏸️ When

Put pruning rules **inside** `stopping_condition()`:

- Max depth, min samples, min gain…

Stops growth before overfitting appears

✅ Fast, simple

❌ Risk of underfitting if too strict

Post-pruning (Cost-Complexity) 🔄 When

Steps:

- First grow a big tree 🌳
- Then cut back unnecessary branches
- Use cross-validation to decide how much to prune

CART (Classification and Regression Trees)

- balance accuracy vs simplicity

✅ Improves generalization

❌ Extra computation

Moderate vs Strong Pruning ⚖️ How much

Moderate pruning:

- Keep useful sub-branches
- Balance accuracy & simplicity 🙂

Strong pruning:

- Aggressively cut → very shallow tree
- Easier to interpret, but higher bias 😬

Works for both Pre & Post:

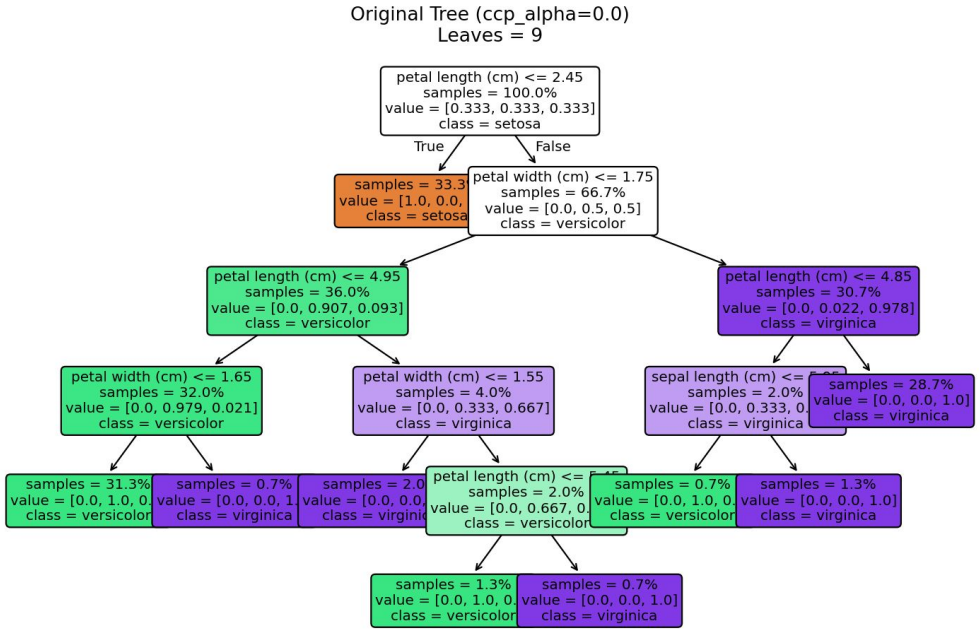
- Pre: adjust thresholds (strict vs loose)
- Post: choose small vs large

How to Implement Pruning ⚖️

- In any decision tree libraries, there is a built-in parameter called `ccp_alpha`
- It controls how much the tree is pruned
- Think of it like regularization in linear models:
- Best value is usually chosen by empirical study or cross-validation ⚖️

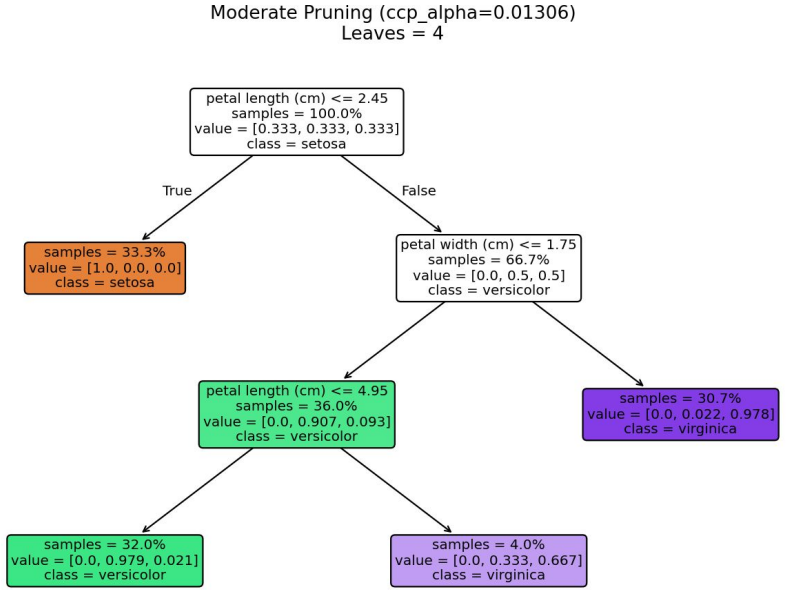
Original Tree 🌳

- Large tree grown fully
- Perfect fit to training data
- Risk: overfitting



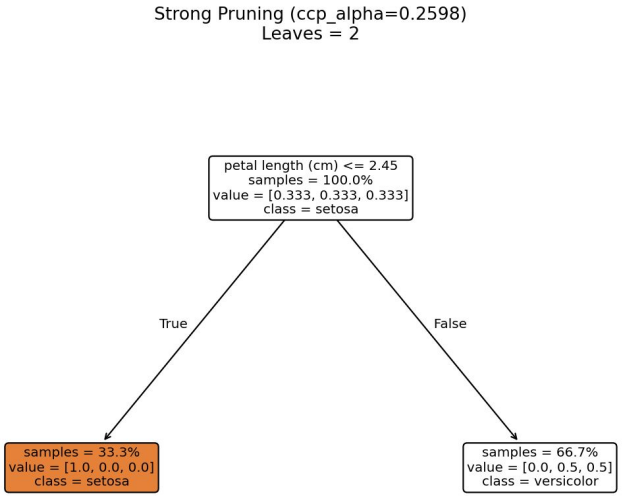
Moderate Pruning 🌱

- Remove weak branches
- Tree becomes smaller
- Slight accuracy loss on train, better test generalization



Strong Pruning 🌿

- Aggressive reduction of branches
- Tree is much simpler
- Easier to interpret



Decision Trees: Pros & Cons ⚖️

✅ Pros:

- Easy to understand & explain
- Works with tabular data
- Captures nonlinear interactions

❌ Cons:

- Prone to overfitting (high variance)
- Small changes in data → very different tree
- Weak standalone performance (needs ensembles)

Ensembles

Why Combine Models? 🤝

Single decision tree = unstable, high variance

Small changes in data → very different trees

💡 Idea: aggregate multiple trees to get more robust predictions

Analogy: 🌲 → 🌳🌳🌳

Bagging = Bootstrap Aggregation 👜

Train multiple models on bootstrap samples (resampling with replacement)

Average predictions (regression) or majority vote (classification)

Reduces variance without increasing bias much

Mathematical View 📐

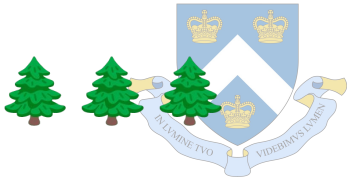
For regression: average across K models

$$f^{\text{bag}}(x) = \frac{1}{K} \sum_{k=1}^{K} f_k(x)$$

For classification: majority vote

Works best with unstable models (like decision trees 🌳)

Random Forest = Bagging + Random Features



At each split, we don’t look at all features, only a random few

This makes each tree different → expert on some small domains

When we average many such trees → predictions are more stable

That’s why Random Forest is a strong baseline in practice ✅

Simple Decision Tree Split Revisit


```
func choose_best_split(data) → (feature, threshold):
    best_split = None; best_gain  = -inf
    for feature in features:
        for threshold in possible_thresholds(feature):
            left, right = split(data, feature, threshold)
            if left or right is empty: continue
            gain = impurity(parent) - weighted_impurity(left, right)
            if gain > best_gain:
                best_gain = gain;  best_split = (feature, threshold)
    return best_split
```

Random Forest Pros & Cons

✅ Pros:

- Great out-of-the-box performance
- Handles tabular data well
- Robust to overfitting

❌ Cons:

- Slower than single trees
- Less interpretable
- Still limited for very high-dimensional sparse data

Boosting = Sequential Learning 🚀

Train models sequentially

Each new model focuses on errors of previous ones

Combines many weak learners → strong learner

Analogy: Coach correcting mistakes step by step

Idea of Gradient Boosting 🌱 → 🌳

Build trees sequentially, each new tree fixes errors of the previous ones.

Start with a simple model (seed prediction).

Each step: predict residuals/errors, fit a new weak learner.

Final model = weighted sum of all trees.

Start with Simple Residuals

In squared error regression:

- Initial prediction \hat{y}_i
- Compute residuals / errors:

$$r_i = y_i - \hat{y}_i$$

- Next tree is trained to predict these residuals

Generalize to Any Loss Function

For classification or other tasks, plain residuals are not enough 😫

We use gradient descent instead:

- Loss function L(y, F(x)) measures how far prediction F(x) is away from y
- Gradient tells us which direction reduces the loss fastest
- Thus we define pseudo-residuals

$$r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]$$

What Happens in Each Iteration?

Compute residuals (negative gradients).

Fit a weak learner (usually a small tree) to these residuals.

Update the model:

$$F_m(x) = F_{m-1}(x) + \nu \cdot \alpha_m h_m(x)$$

- h_m(x): new weak learner
- \alpha_m: weight for this learner
- \nu: learning rate (step size)

XGBoost / LightGBM ⚡

Engineering optimizations for speed and scalability

Key ideas:

- Regularization (to prevent overfitting)
- Handling missing values
- Parallel training

Popular in Kaggle competitions 🏆

Intuition 🎯

Think of a student learning over time:

- Day 1 → learns basics, makes many mistakes.
- Day 2 → focuses on yesterday's mistakes.
- Day 3 → focuses again on remaining mistakes.

Step by step, performance improves.

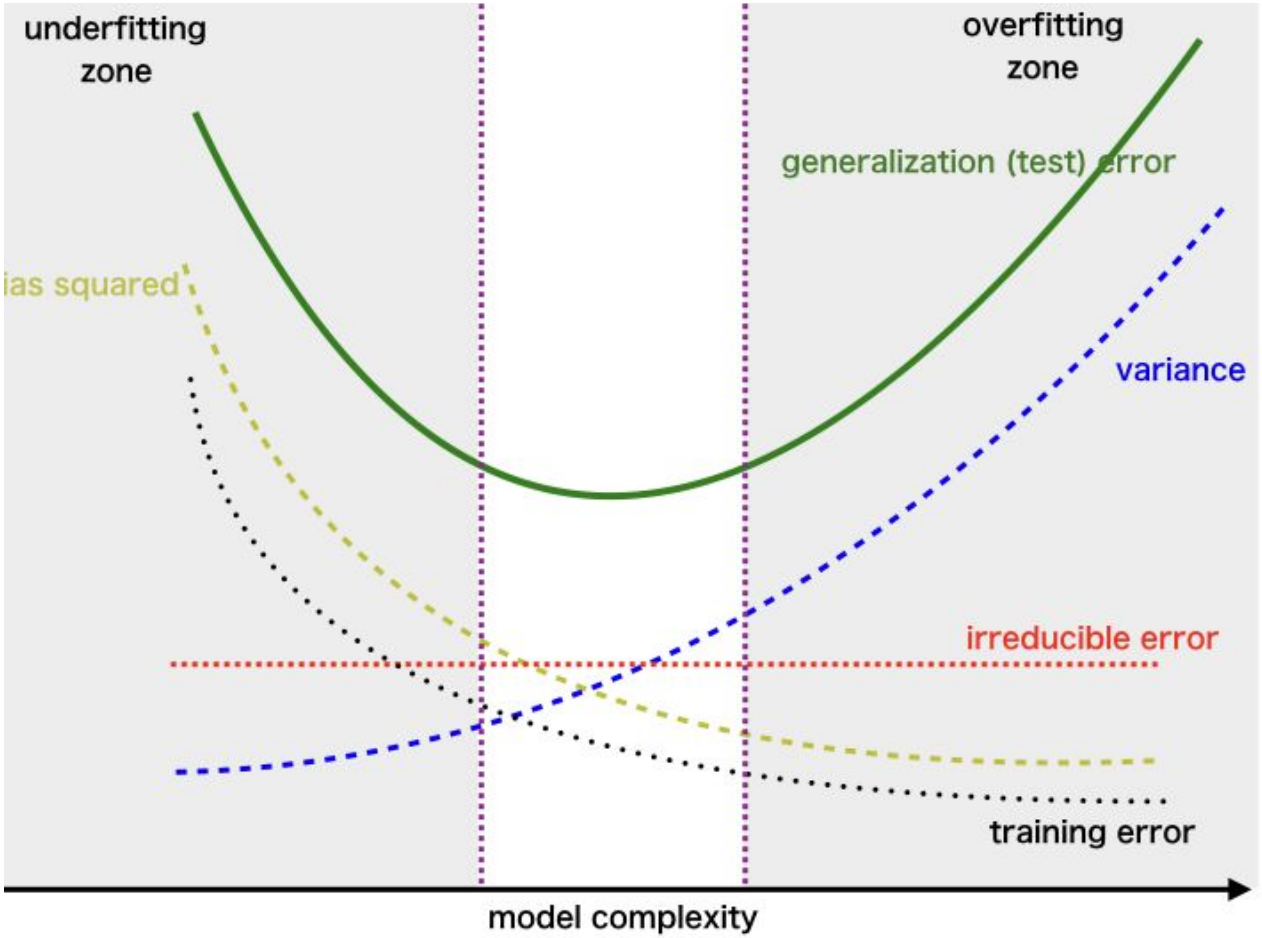
Gradient Boosting = Residual Learning + Gradient Descent

Key Features & Benefits 🚀

- Learning rate: controls step size, prevents overfitting.
- Number of trees: more trees = lower bias, risk of overfit.
- Depth of trees: shallow = weak learners (better generalization).
- Regularization: subsampling, shrinkage, pruning.

Boosting vs Bagging:

- Boosting = sequential, reduce bias.
- Bagging = parallel, reduce variance.


underfitting
zone
overfitting
zone
generalization (test) error
ias squared
variance
irreducible error
training error
model complexity

Decision Trees vs Ensembles 📊

Method	Strengths ✅	Weaknesses ❌
Decision Tree 🌳	Simple, interpretable, fast	Overfits, unstable
Bagging 🎲	Reduces variance, robust	Less interpretable
Random Forest 🌲🌲	Strong baseline, feature importance	Slower, less transparent
Boosting 🚀	High accuracy, flexible losses	Sensitive to parameters, less interpretable

Trees vs Deep Learning 🤖

Tree excels at tabular data (structured, mixed features)

Deep learning shines at unstructured data (images, text, audio)

In practice → ensembles wins on Kaggle tabular competitions 🏆

Rule of thumb 👍

- Tabular → Random Forest / XGBoost
- Image/Text → Neural Networks

Summary 📖

Decision Trees → splitting, pruning

Ensembles → Bagging, Random Forests, Boosting

Takeaway: ensembles make weak learners strong 💪