

Decision Trees Pruning

Nipun Batra and teaching staff

IIT Gandhinagar

September 3, 2025

Table of Contents

1. Pruning and Overfitting

Pruning and Overfitting

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex
- **Perfect training accuracy:** Each leaf contains single training example

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex
- **Perfect training accuracy:** Each leaf contains single training example
- **But:** Poor generalization to new data

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex
- **Perfect training accuracy:** Each leaf contains single training example
- **But:** Poor generalization to new data
- **Symptoms:**

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex
- **Perfect training accuracy:** Each leaf contains single training example
- **But:** Poor generalization to new data
- **Symptoms:**
 - High training accuracy, low test accuracy

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex
- **Perfect training accuracy:** Each leaf contains single training example
- **But:** Poor generalization to new data
- **Symptoms:**
 - High training accuracy, low test accuracy
 - Very deep trees with many leaves

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex
- **Perfect training accuracy:** Each leaf contains single training example
- **But:** Poor generalization to new data
- **Symptoms:**
 - High training accuracy, low test accuracy
 - Very deep trees with many leaves
 - Rules that are too specific to training data

The Problem: Overfitting in Decision Trees

- **Unpruned trees:** Can grow very deep and complex
- **Perfect training accuracy:** Each leaf contains single training example
- **But:** Poor generalization to new data
- **Symptoms:**
 - High training accuracy, low test accuracy
 - Very deep trees with many leaves
 - Rules that are too specific to training data
- **Solution:** Pruning to control model complexity

Pre-pruning (Early Stopping)

Stop growing tree before it becomes too complex:

- **Maximum depth:** Limit tree depth (e.g., `max_depth = 5`)

Advantages: Simple, computationally efficient

Disadvantages: May stop too early, miss good splits later

Pre-pruning (Early Stopping)

Stop growing tree before it becomes too complex:

- **Maximum depth:** Limit tree depth (e.g., `max_depth = 5`)
- **Minimum samples per split:** Don't split if node has $< N$ samples

Advantages: Simple, computationally efficient

Disadvantages: May stop too early, miss good splits later

Pre-pruning (Early Stopping)

Stop growing tree before it becomes too complex:

- **Maximum depth:** Limit tree depth (e.g., `max_depth = 5`)
- **Minimum samples per split:** Don't split if node has $< N$ samples
- **Minimum samples per leaf:** Ensure each leaf has $\geq M$ samples

Advantages: Simple, computationally efficient

Disadvantages: May stop too early, miss good splits later

Pre-pruning (Early Stopping)

Stop growing tree before it becomes too complex:

- **Maximum depth:** Limit tree depth (e.g., `max_depth = 5`)
- **Minimum samples per split:** Don't split if node has $< N$ samples
- **Minimum samples per leaf:** Ensure each leaf has $\geq M$ samples
- **Maximum features:** Consider only subset of features at each split

Advantages: Simple, computationally efficient

Disadvantages: May stop too early, miss good splits later

Pre-pruning (Early Stopping)

Stop growing tree before it becomes too complex:

- **Maximum depth:** Limit tree depth (e.g., `max_depth = 5`)
- **Minimum samples per split:** Don't split if node has $< N$ samples
- **Minimum samples per leaf:** Ensure each leaf has $\geq M$ samples
- **Maximum features:** Consider only subset of features at each split
- **Minimum impurity decrease:** Only split if improvement $>$ threshold

Advantages: Simple, computationally efficient

Disadvantages: May stop too early, miss good splits later

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**
 1. Grow complete tree on training data

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**

1. Grow complete tree on training data
2. Use validation set to evaluate subtree performance

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**

1. Grow complete tree on training data
2. Use validation set to evaluate subtree performance
3. Remove branches that don't improve validation accuracy

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**

1. Grow complete tree on training data
2. Use validation set to evaluate subtree performance
3. Remove branches that don't improve validation accuracy
4. Repeat until no beneficial removals remain

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**
 1. Grow complete tree on training data
 2. Use validation set to evaluate subtree performance
 3. Remove branches that don't improve validation accuracy
 4. Repeat until no beneficial removals remain
- **Cost Complexity Pruning:** Minimize $\text{Error} + \alpha \times \text{Tree Size}$

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**
 1. Grow complete tree on training data
 2. Use validation set to evaluate subtree performance
 3. Remove branches that don't improve validation accuracy
 4. Repeat until no beneficial removals remain
- **Cost Complexity Pruning:** Minimize Error + $\alpha \times \text{Tree Size}$
- **Advantages:** More thorough, can recover from early stopping mistakes

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm:**
 1. Grow complete tree on training data
 2. Use validation set to evaluate subtree performance
 3. Remove branches that don't improve validation accuracy
 4. Repeat until no beneficial removals remain
- **Cost Complexity Pruning:** Minimize Error + $\alpha \times \text{Tree Size}$
- **Advantages:** More thorough, can recover from early stopping mistakes
- **Disadvantages:** More computationally expensive

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_{\alpha}(T) = R(T) + \alpha|T|$

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_{\alpha}(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_{\alpha}(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)
 - $|T|$: Number of leaves

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_{\alpha}(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)
 - $|T|$: Number of leaves
 - α : Complexity penalty parameter

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_{\alpha}(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)
 - $|T|$: Number of leaves
 - α : Complexity penalty parameter
- **Weakest Link:** At each pruning step, compute:

$$g(t) = \frac{R(t) - R(T_t)}{|T_t| - 1}$$

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_\alpha(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)
 - $|T|$: Number of leaves
 - α : Complexity penalty parameter
- **Weakest Link:** At each pruning step, compute:

$$g(t) = \frac{R(t) - R(T_t)}{|T_t| - 1}$$

- $g(t)$: The α value at which subtree rooted at node t should be pruned

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_\alpha(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)
 - $|T|$: Number of leaves
 - α : Complexity penalty parameter
- **Weakest Link:** At each pruning step, compute:

$$g(t) = \frac{R(t) - R(T_t)}{|T_t| - 1}$$

- $g(t)$: The α value at which subtree rooted at node t should be pruned
- $R(t)$: Impurity of node t , treating it as leaf node

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_\alpha(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)
 - $|T|$: Number of leaves
 - α : Complexity penalty parameter
- **Weakest Link:** At each pruning step, compute:

$$g(t) = \frac{R(t) - R(T_t)}{|T_t| - 1}$$

- $g(t)$: The α value at which subtree rooted at node t should be pruned
- $R(t)$: Impurity of node t , treating it as leaf node
- $R(T_t)$: Total impurity of subtree rooted at node t

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function:** $R_\alpha(T) = R(T) + \alpha|T|$
 - $R(T)$: Total impurity (training error)
 - $|T|$: Number of leaves
 - α : Complexity penalty parameter
- **Weakest Link:** At each pruning step, compute:

$$g(t) = \frac{R(t) - R(T_t)}{|T_t| - 1}$$

- $g(t)$: The α value at which subtree rooted at node t should be pruned
- $R(t)$: Impurity of node t , treating it as leaf node
- $R(T_t)$: Total impurity of subtree rooted at node t
- $|T_t|$: Number of leaves in subtree rooted at node t

Cost Complexity Pruning: Algorithm Steps

Iterative pruning process:

- **Process:**

Cost Complexity Pruning: Algorithm Steps

Iterative pruning process:

- **Process:**
 1. Start with full tree ($\alpha = 0$)

Cost Complexity Pruning: Algorithm Steps

Iterative pruning process:

- **Process:**
 1. Start with full tree ($\alpha = 0$)
 2. Compute $g(t)$ for all internal nodes

Cost Complexity Pruning: Algorithm Steps

Iterative pruning process:

- **Process:**

1. Start with full tree ($\alpha = 0$)
2. Compute $g(t)$ for all internal nodes
3. Prune node with smallest $g(t)$ (weakest link)

Cost Complexity Pruning: Algorithm Steps

Iterative pruning process:

- **Process:**

1. Start with full tree ($\alpha = 0$)
2. Compute $g(t)$ for all internal nodes
3. Prune node with smallest $g(t)$ (weakest link)
4. Repeat until only root remains

Cost Complexity Pruning: Algorithm Steps

Iterative pruning process:

- **Process:**

1. Start with full tree ($\alpha = 0$)
2. Compute $g(t)$ for all internal nodes
3. Prune node with smallest $g(t)$ (weakest link)
4. Repeat until only root remains
5. Use cross-validation to select optimal α

Bias-Variance Trade-off in Trees

- **Unpruned trees:**

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)
 - Prone to overfitting

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)
 - Prone to overfitting
- **Heavily pruned trees:**

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)
 - Prone to overfitting
- **Heavily pruned trees:**
 - High bias (may miss important patterns)

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)
 - Prone to overfitting
- **Heavily pruned trees:**
 - High bias (may miss important patterns)
 - Low variance (more stable predictions)

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)
 - Prone to overfitting
- **Heavily pruned trees:**
 - High bias (may miss important patterns)
 - Low variance (more stable predictions)
 - Risk of underfitting

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)
 - Prone to overfitting
- **Heavily pruned trees:**
 - High bias (may miss important patterns)
 - Low variance (more stable predictions)
 - Risk of underfitting
- **Optimal pruning:** Balances bias and variance

Bias-Variance Trade-off in Trees

- **Unpruned trees:**
 - Low bias (can fit complex patterns)
 - High variance (sensitive to training data changes)
 - Prone to overfitting
- **Heavily pruned trees:**
 - High bias (may miss important patterns)
 - Low variance (more stable predictions)
 - Risk of underfitting
- **Optimal pruning:** Balances bias and variance
- **Cross-validation:** Essential for finding this balance

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters
- **Validation curves:** Plot training/validation error vs. tree complexity

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters
- **Validation curves:** Plot training/validation error vs. tree complexity
- **Common parameters** (sklearn):

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters
- **Validation curves:** Plot training/validation error vs. tree complexity
- **Common parameters (sklearn):**
 - `max_depth`: Start with 3-10

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters
- **Validation curves:** Plot training/validation error vs. tree complexity
- **Common parameters (sklearn):**
 - `max_depth`: Start with 3-10
 - `min_samples_split`: Try 10-100

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters
- **Validation curves:** Plot training/validation error vs. tree complexity
- **Common parameters (sklearn):**
 - `max_depth`: Start with 3-10
 - `min_samples_split`: Try 10-100
 - `min_samples_leaf`: Try 5-50

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters
- **Validation curves:** Plot training/validation error vs. tree complexity
- **Common parameters (sklearn):**
 - `max_depth`: Start with 3-10
 - `min_samples_split`: Try 10-100
 - `min_samples_leaf`: Try 5-50
 - `ccp_alpha`: Use for cost complexity pruning

Practical Pruning Guidelines

- **Start simple:** Begin with restrictive pre-pruning parameters
- **Cross-validation:** Always use CV to select pruning parameters
- **Validation curves:** Plot training/validation error vs. tree complexity
- **Common parameters (sklearn):**
 - `max_depth`: Start with 3-10
 - `min_samples_split`: Try 10-100
 - `min_samples_leaf`: Try 5-50
 - `ccp_alpha`: Use for cost complexity pruning
- **Domain knowledge:** Consider interpretability requirements