Decision Trees: Overfitting

CS229: Machine Learning
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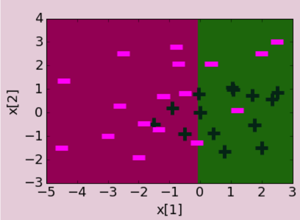
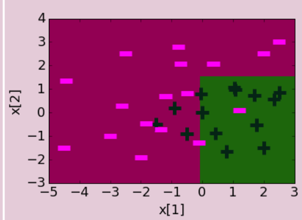
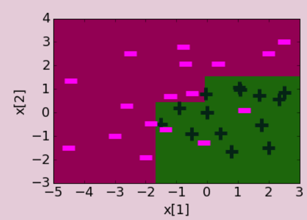
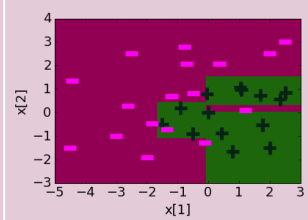
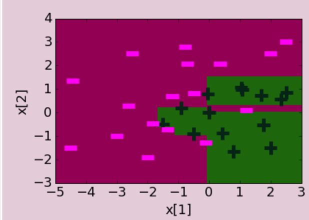
Slides include content developed by and co-developed with Emily Fox

Overfitting in decision trees

What happens when we increase depth?

Training error reduces with depth

Tree depth	depth = 1	depth = 2	depth = 3	depth = 5	depth = 10
Training error	0.22	0.13	0.10	0.03	0.00
Decision boundary					

Two approaches to picking simpler trees

1. **Early Stopping:**
   Stop the learning algorithm **before** tree becomes too complex

2. **Pruning:**
   Simplify the tree **after** the learning algorithm terminates

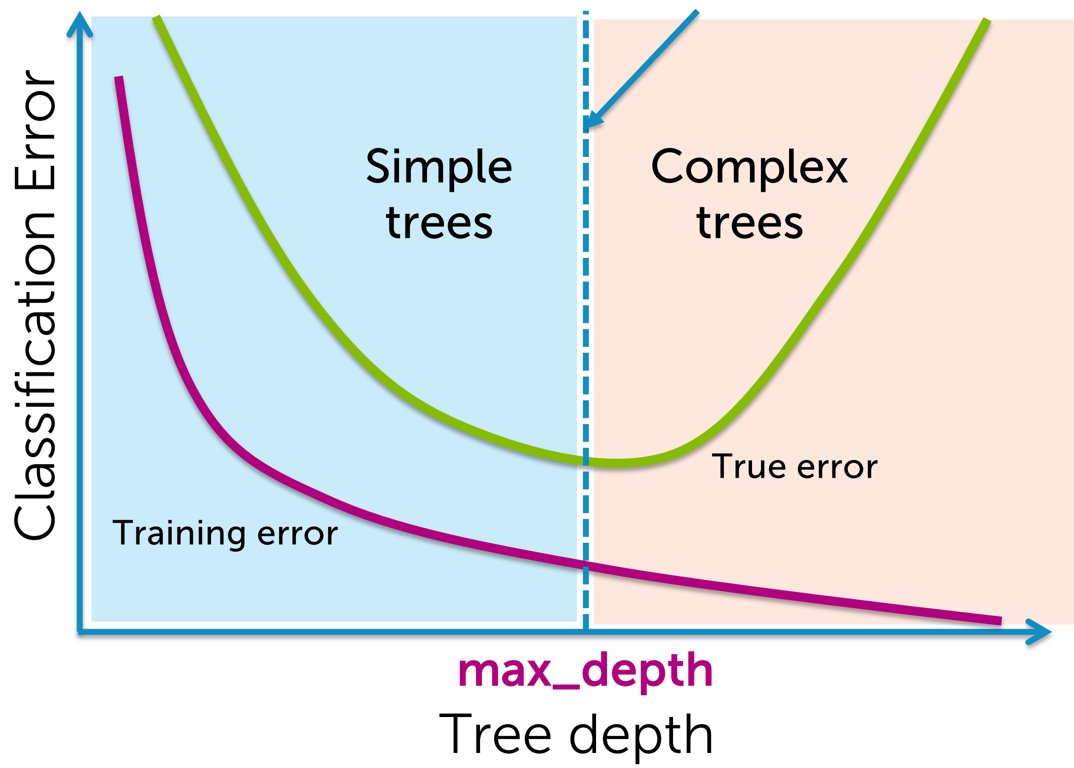
Technique 1: Early stopping

- Stopping conditions (recap):
  1. All examples have the same target value
  2. No more features to split on

- Early stopping conditions:
  1. Limit tree depth (choose *max_depth* using validation set)
  2. Do not consider splits that do not cause a sufficient decrease in classification error
  3. Do not split an intermediate node which contains too few data points

Challenge with early stopping condition 1

Hard to know exactly when to stop



Also, might want some branches of tree to go deeper while others remain shallow

Early stopping condition 2: Pros and Cons

- Pros:
  - A reasonable heuristic for early stopping to avoid useless splits

- Cons:
  - Too short sighted: We may miss out on “good” splits may occur right after “useless” splits
  - Saw this with “xor” example

Two approaches to picking simpler trees

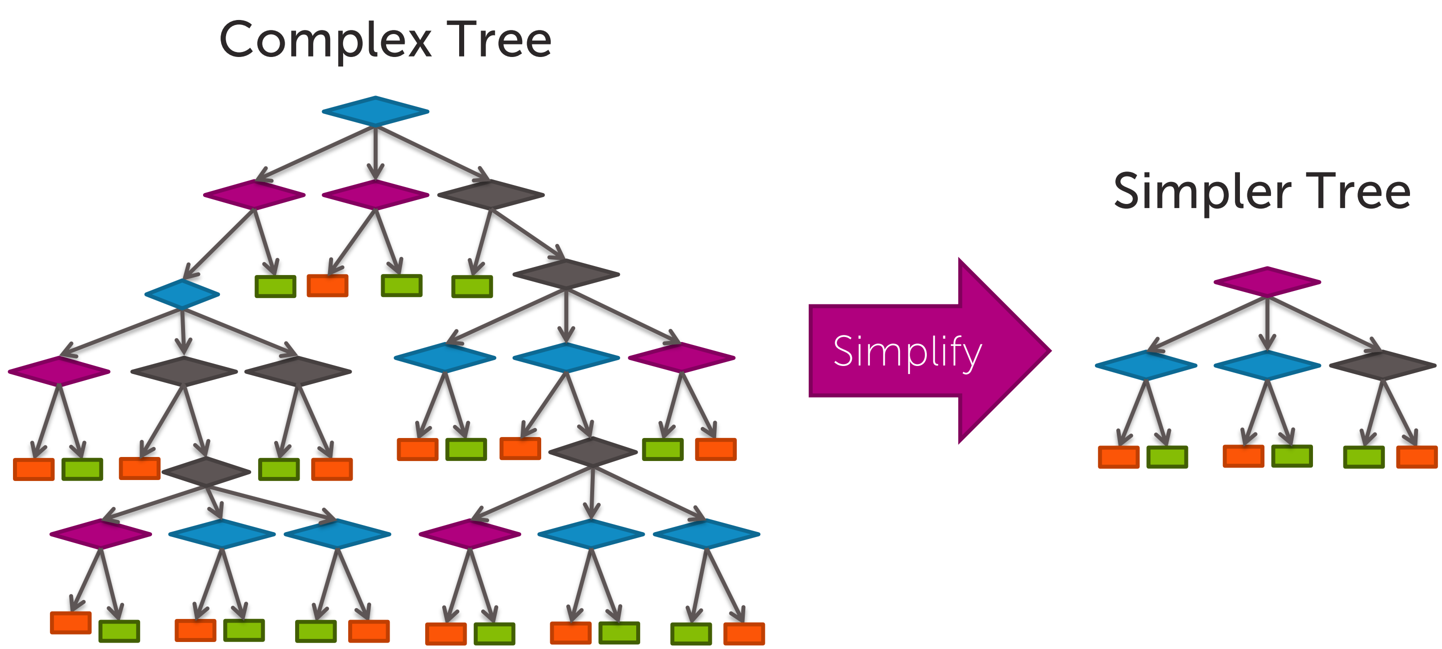
1. **Early Stopping:**
   Stop the learning algorithm **before** tree becomes too complex

2. **Pruning:**
   Simplify the tree **after** the learning algorithm terminates

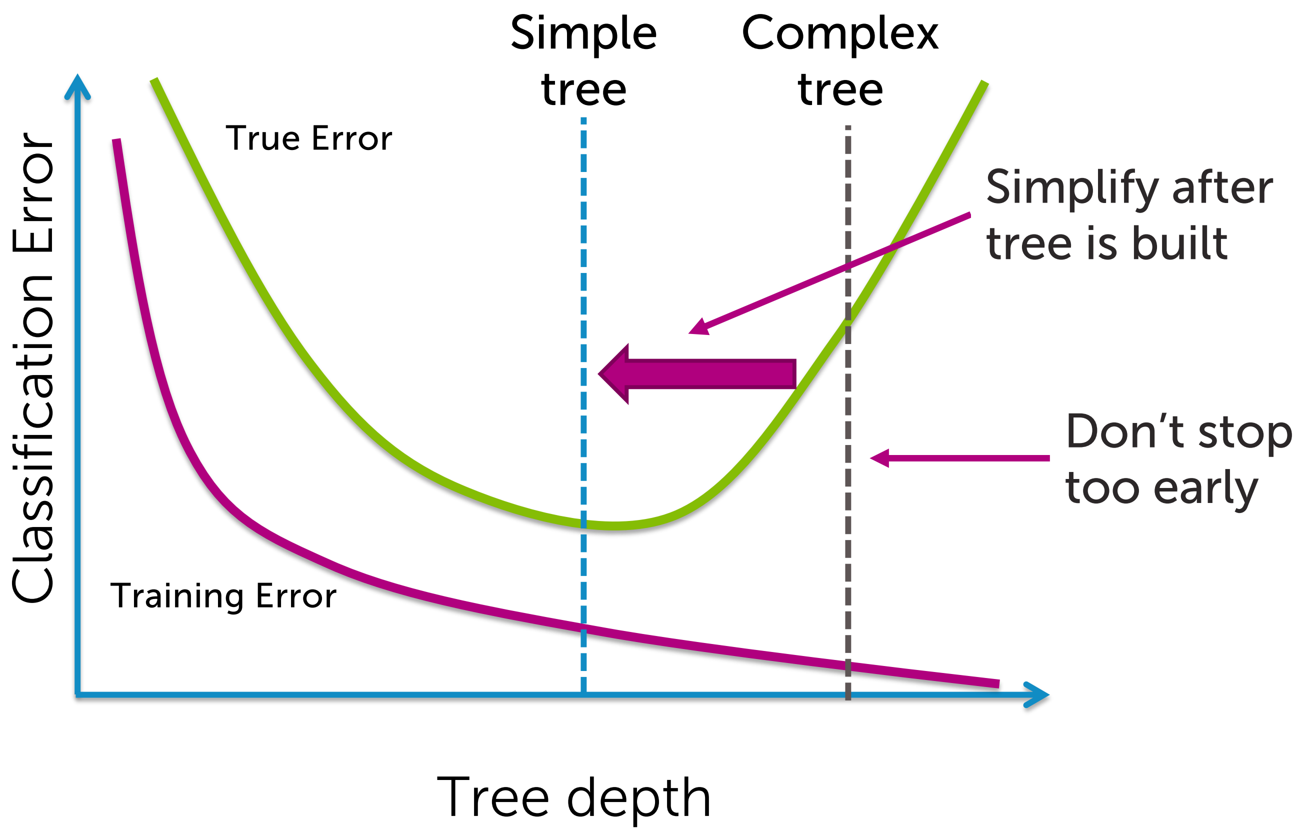
Complements early stopping

Pruning: *Intuition*

Train a complex tree, simplify later



Pruning motivation



Scoring trees: Desired total quality format

Want to balance:

i. How well tree fits data

ii. Complexity of tree

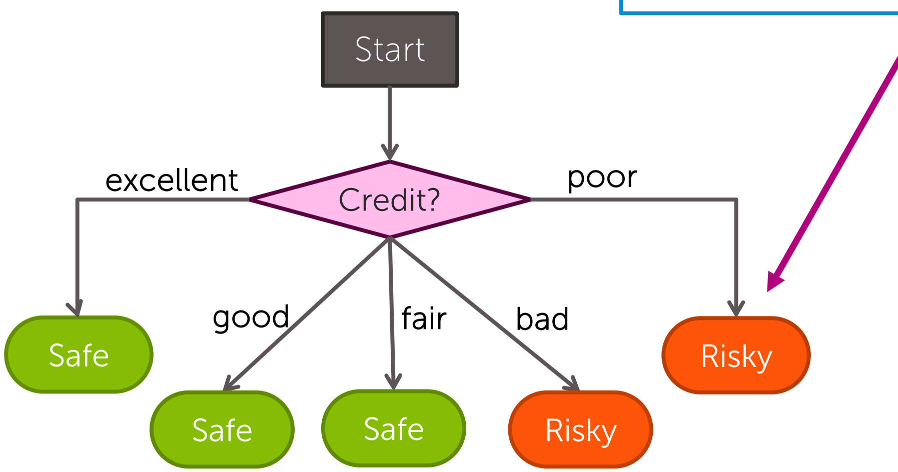
want to balance

Total cost =

measure of fit + measure of complexity

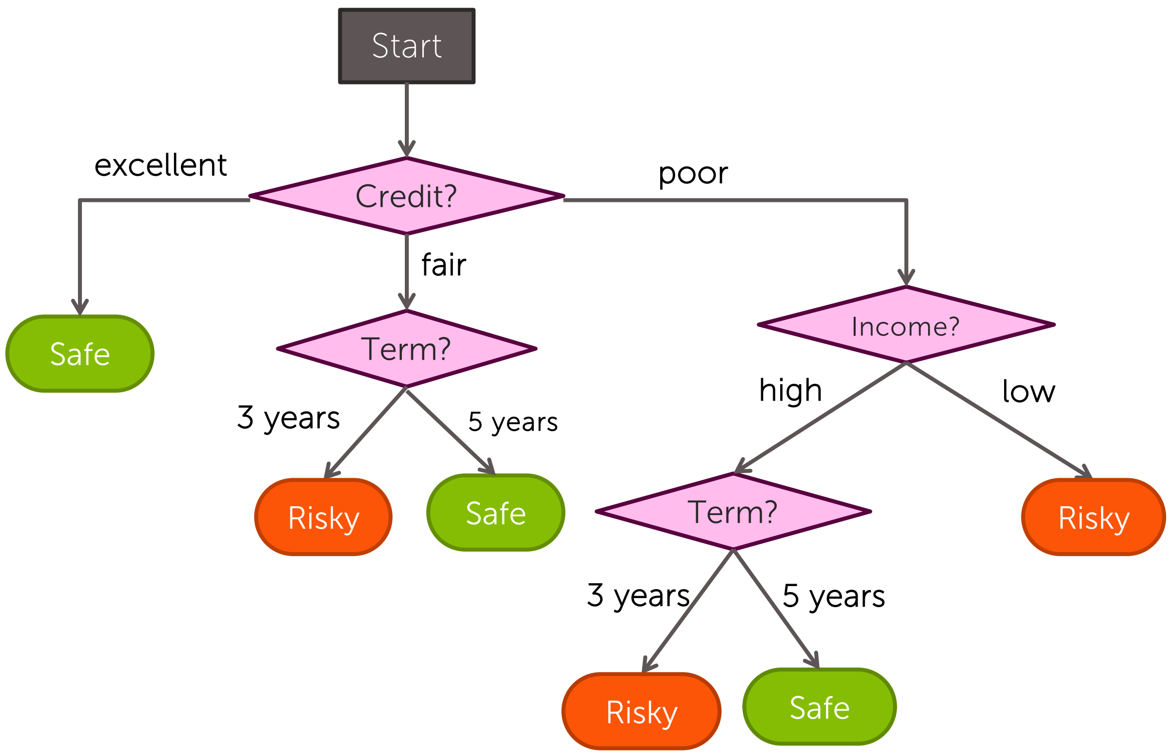
Simple measure of complexity of tree

$\boxed{L(T) = \text{\# of leaf nodes}}$



Balance simplicity & predictive power

Too complex, risk of overfitting



Too simple, high classification error

Balancing fit and complexity

$$\text{Total cost } C(T) = \text{Error}(T) + \lambda\, L(T)$$

tuning parameter

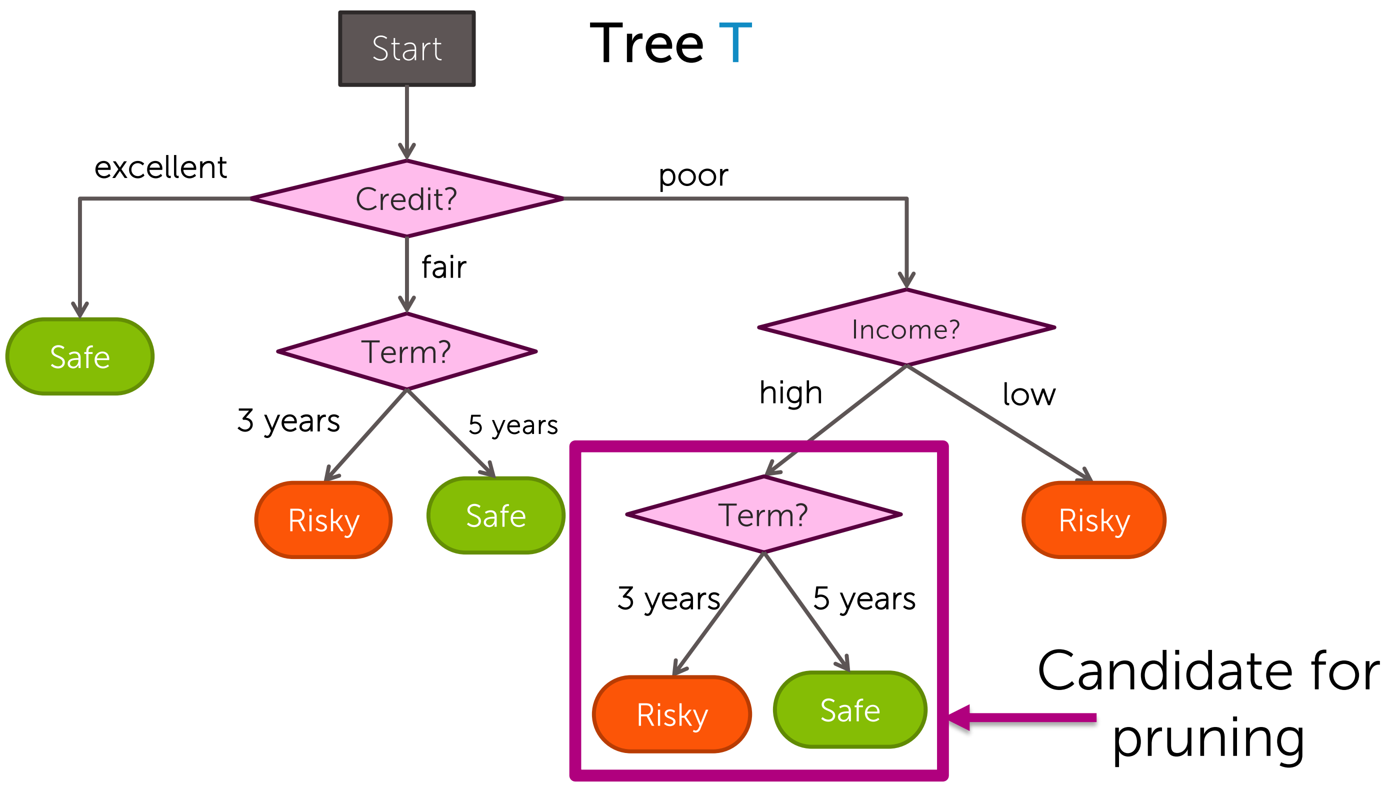
If $\lambda=0$:

If $\lambda=\infty$:

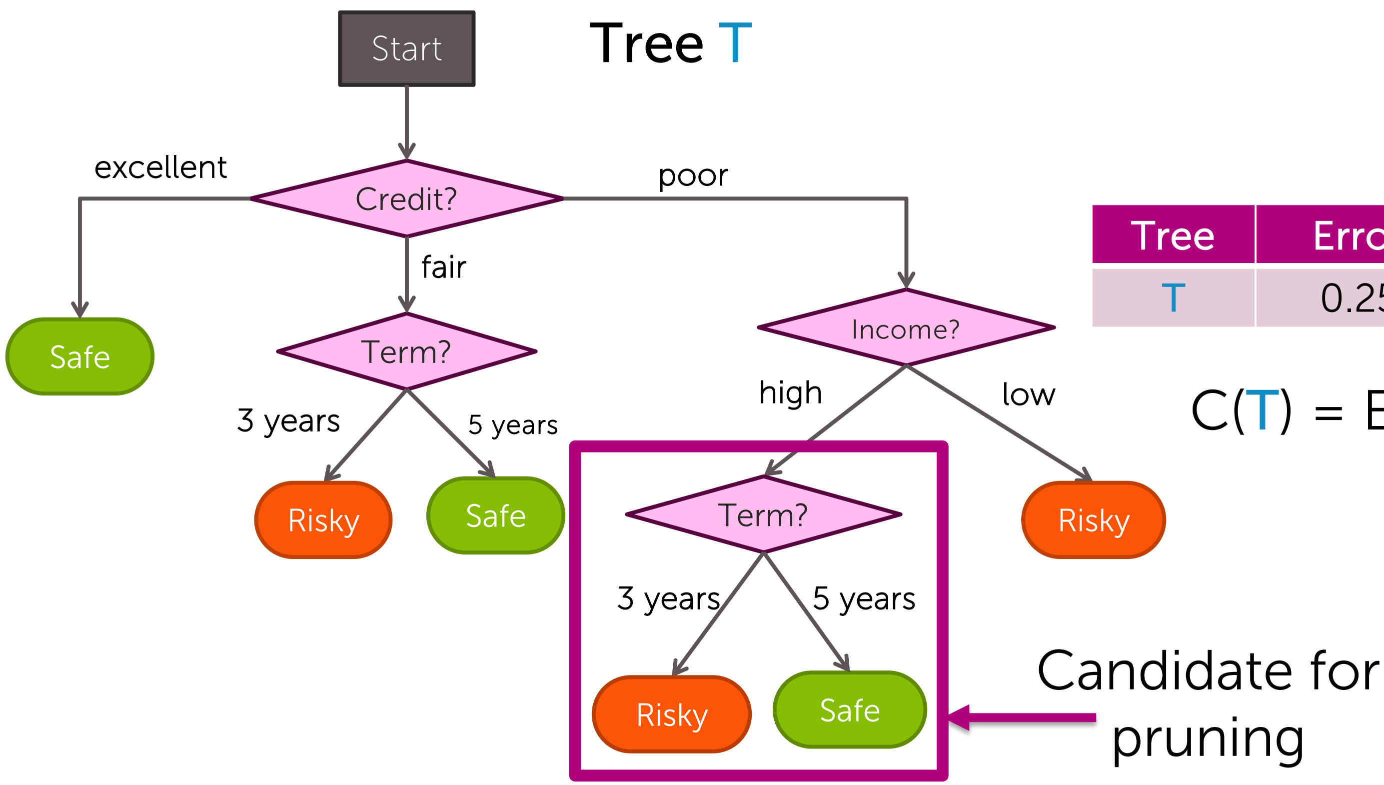
If λ in between:

Tree pruning algorithm

Step 1: Consider a split



Step 2: Compute total cost C(T) of split

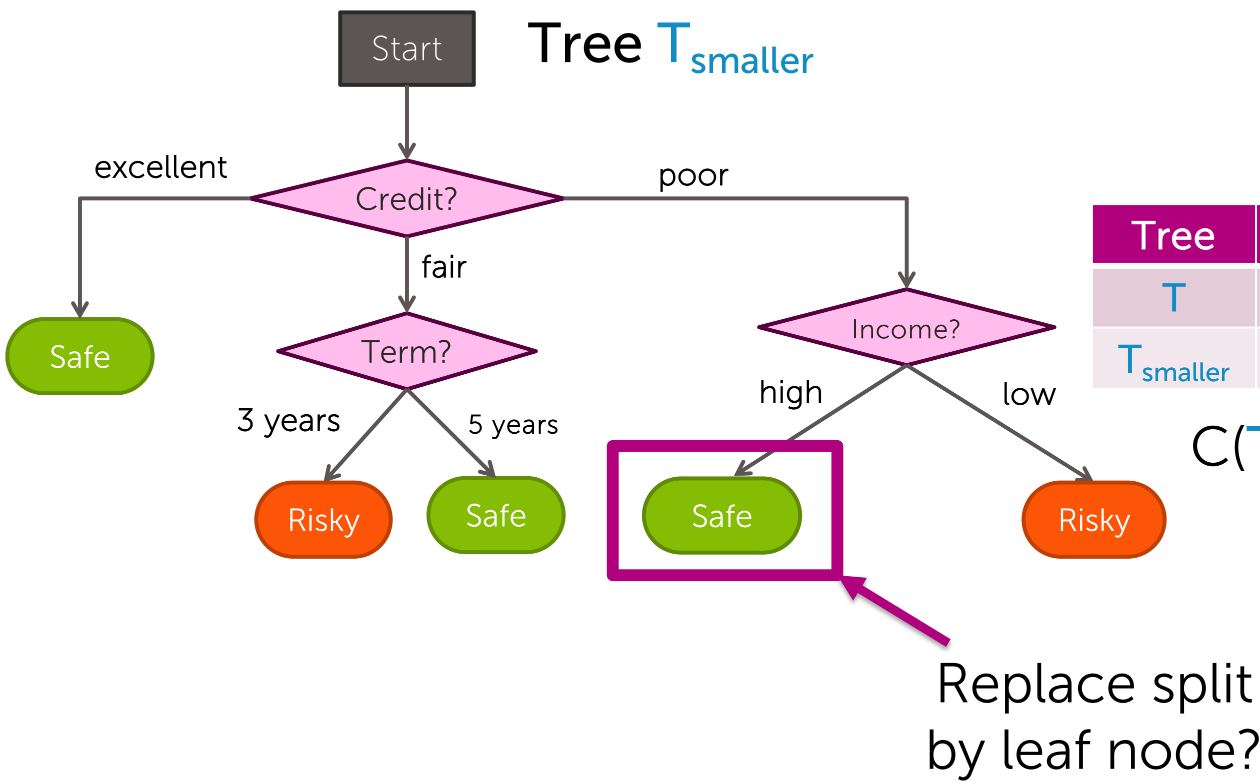


$\lambda = 0.3$

Tree	Error	#Leaves	Total
T	0.25	6	0.43

$$C(T) = \text{Error}(T) + \lambda\, L(T)$$

Step 2: "Undo" the splits on Tsmaller



$\lambda = 0.3$

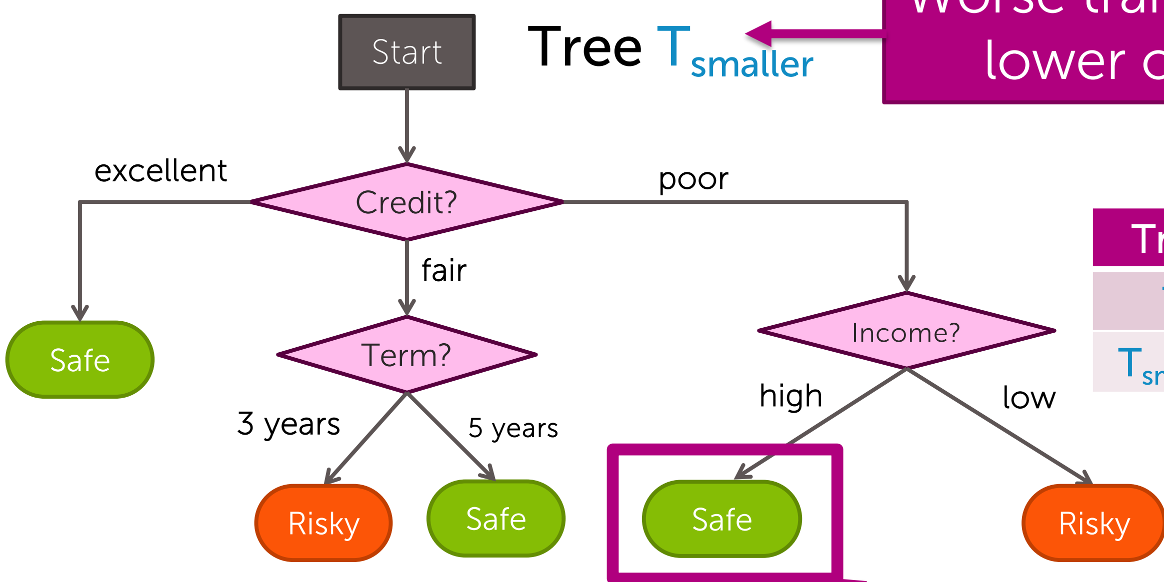
Tree	Error	#Leaves	Total
T	0.25	6	0.43
$T_{smaller}$	0.26	5	0.41

$$C(T) = \text{Error}(T) + \lambda\, L(T)$$

Prune if total cost is lower: $C(T_{smaller}) \leq C(T)$

Tree $T_{smaller}$

Worse training error but lower overall cost



$\lambda = 0.3$

Tree	Error	#Leaves	Total
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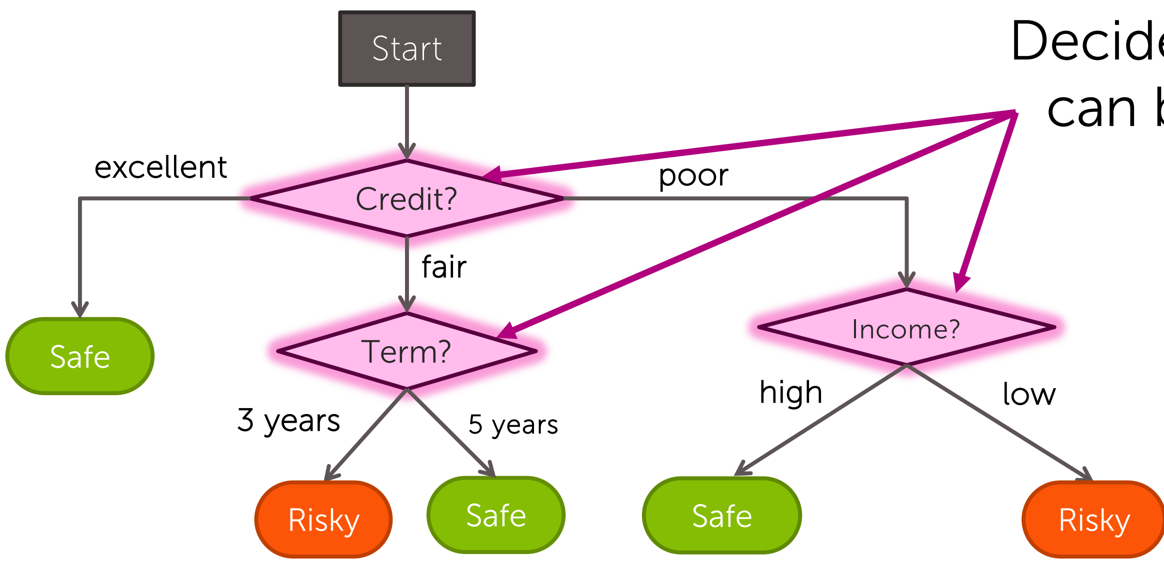
$T_{smaller}$	0.26	5	0.41

$$C(T) = \text{Error}(T) + \lambda\, L(T)$$

Replace split by leaf node? ← YES!

Step 5: Repeat Steps 1-4 for every split



Decide if each split can be "pruned"

Summary of overfitting in decision trees

What you can do now…

- Identify when overfitting in decision trees
- Prevent overfitting with early stopping
  - Limit tree depth
  - Do not consider splits that do not reduce classification error
  - Do not split intermediate nodes with only few points
- Prevent overfitting by pruning complex trees
  - Use a total cost formula that balances classification error and tree complexity
  - Use total cost to merge potentially complex trees into simpler ones