



Overfitting



in decision trees

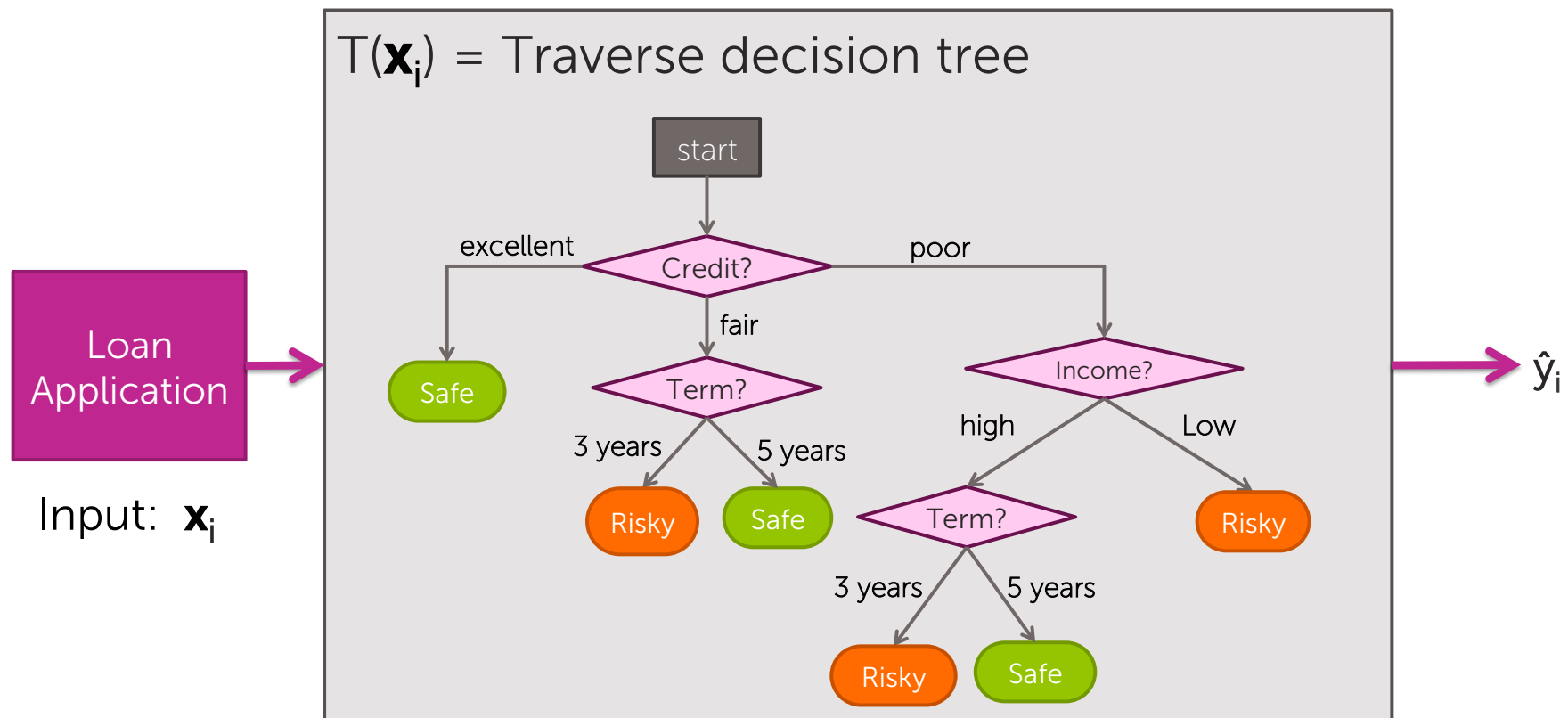
Emily Fox & Carlos Guestrin
Machine Learning Specialization
University of Washington

Review of loan default prediction

Loan
Applications

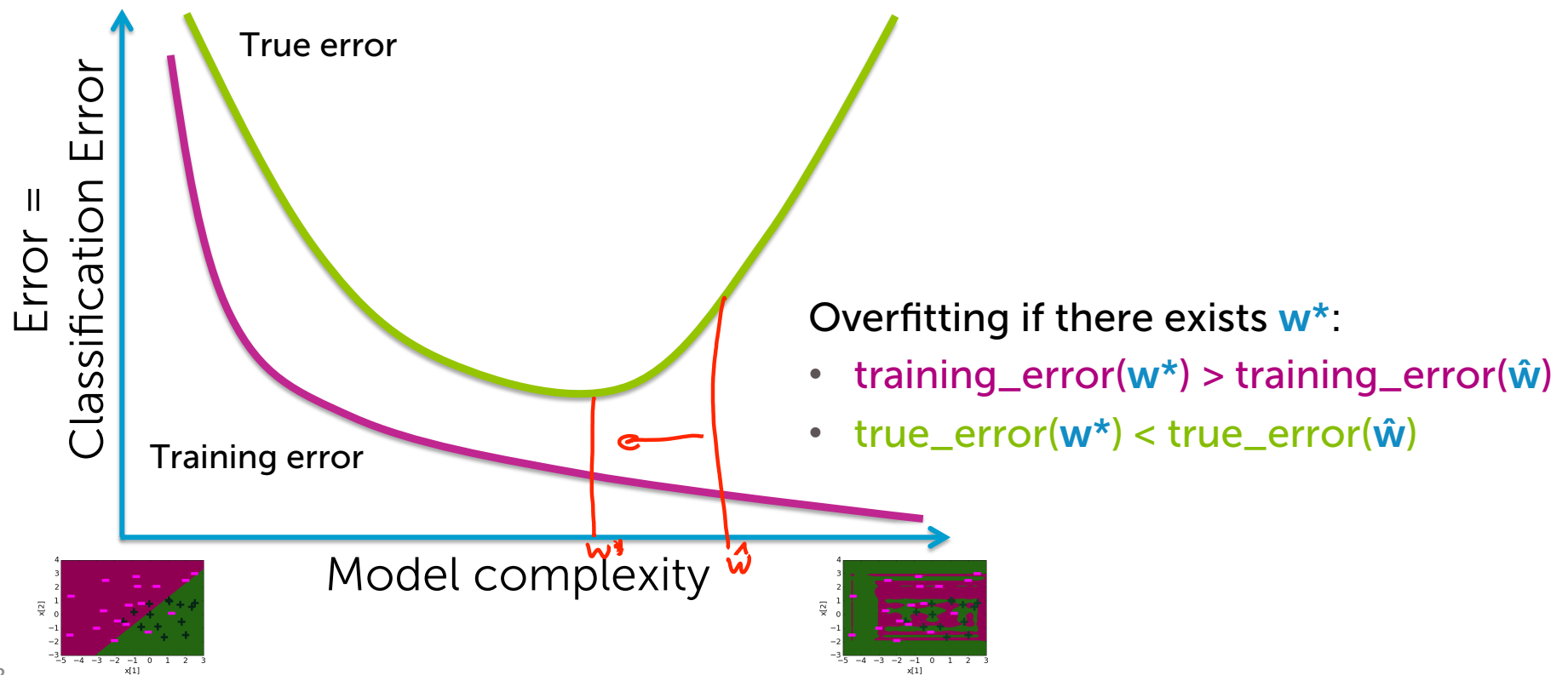


Decision tree review

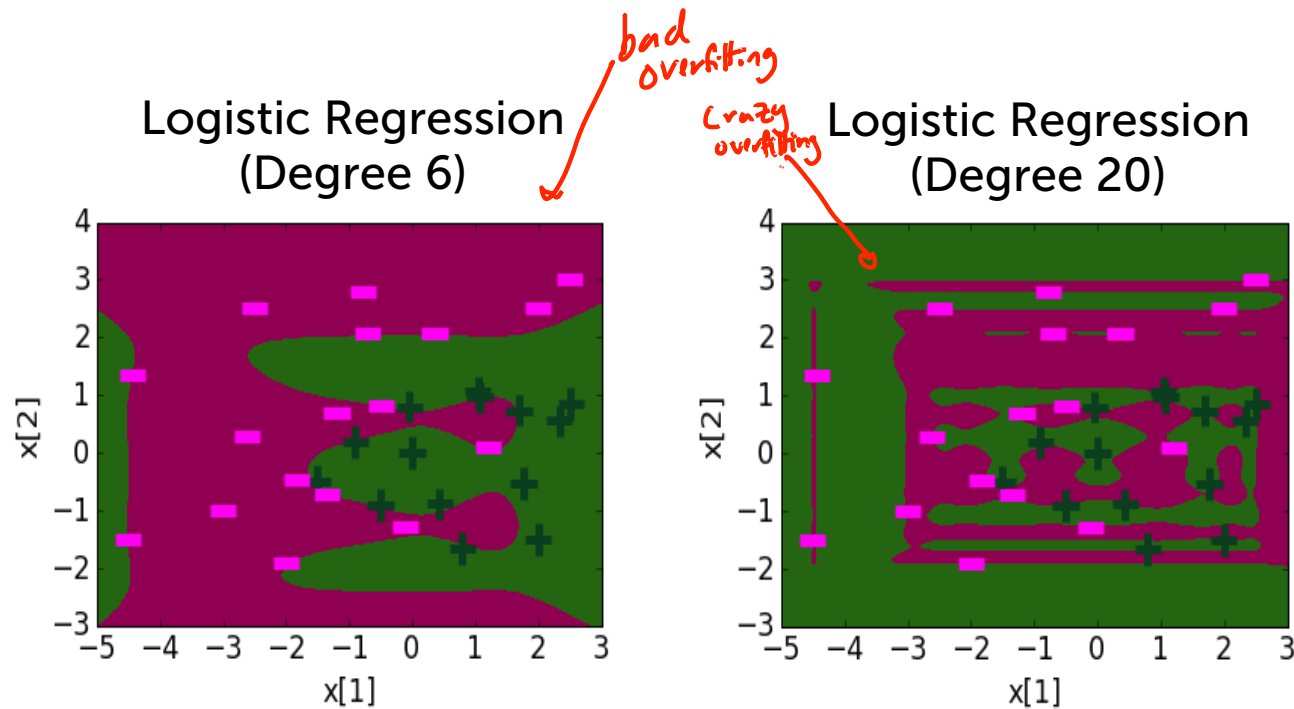


Overfitting review

Overfitting in logistic regression

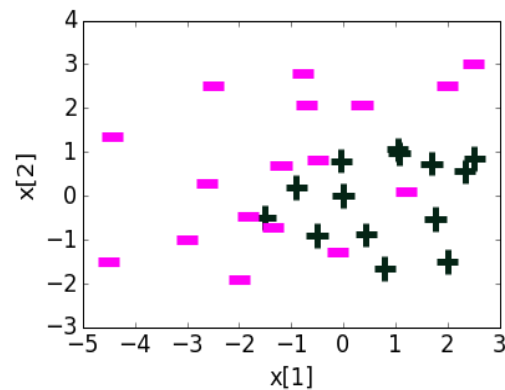


Overfitting → Overconfident predictions

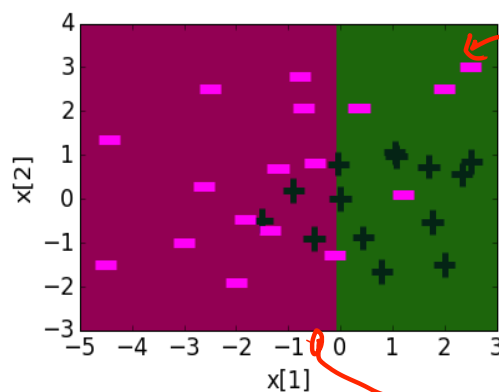
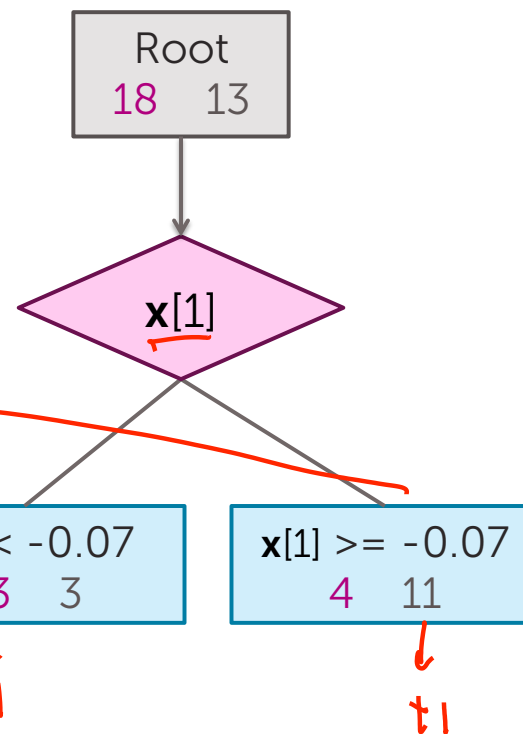


Overfitting in decision trees

Decision stump (Depth 1): Split on $x[1]$



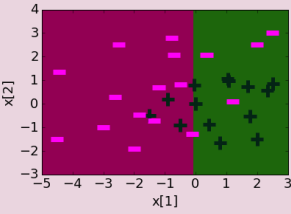
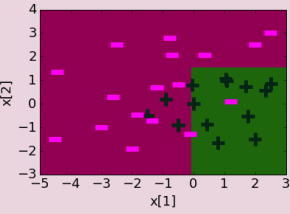
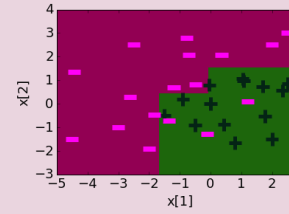
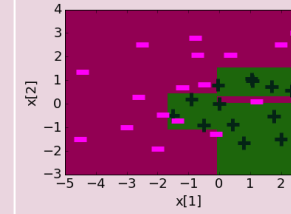
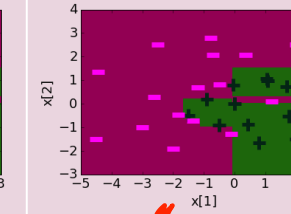
y values
- +



What happens when we increase depth?

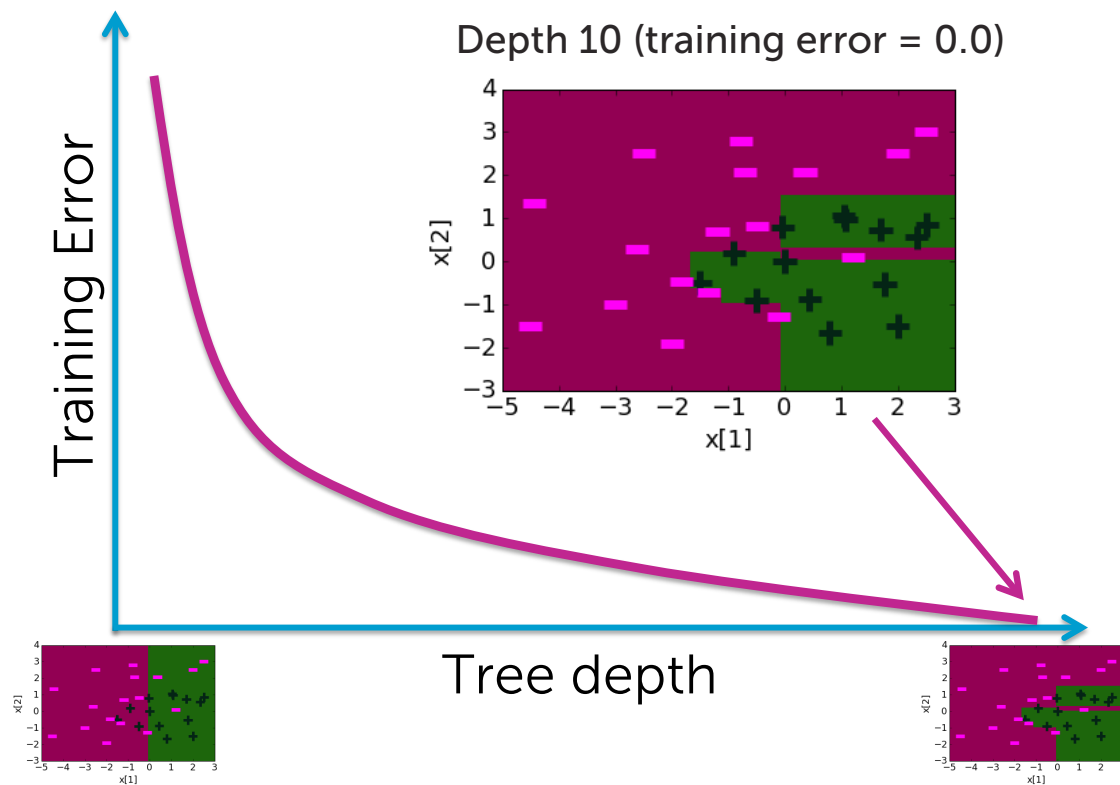
Training error reduces with depth

Big warning!!

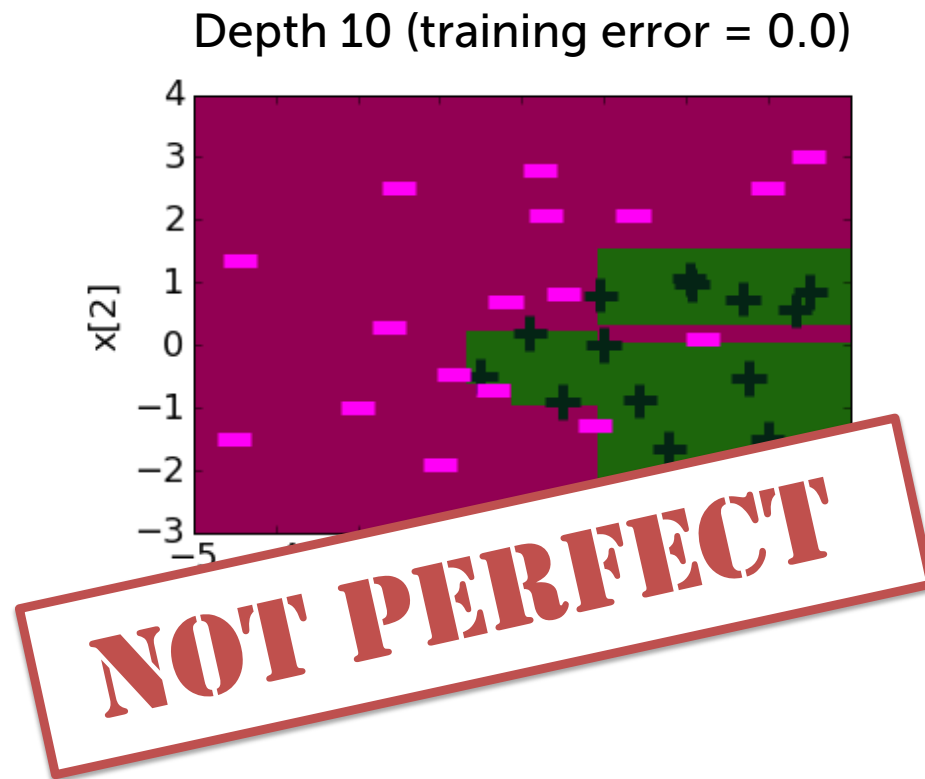
Tree depth	depth = 1	depth = 2	depth = 3	depth = 5	depth = 10
<u>Training error</u>	<u>0.22</u>	<u>0.13</u>	<u>0.10</u>	0.03	<u>0.00</u>
Decision boundary					

complexity of decision boundary

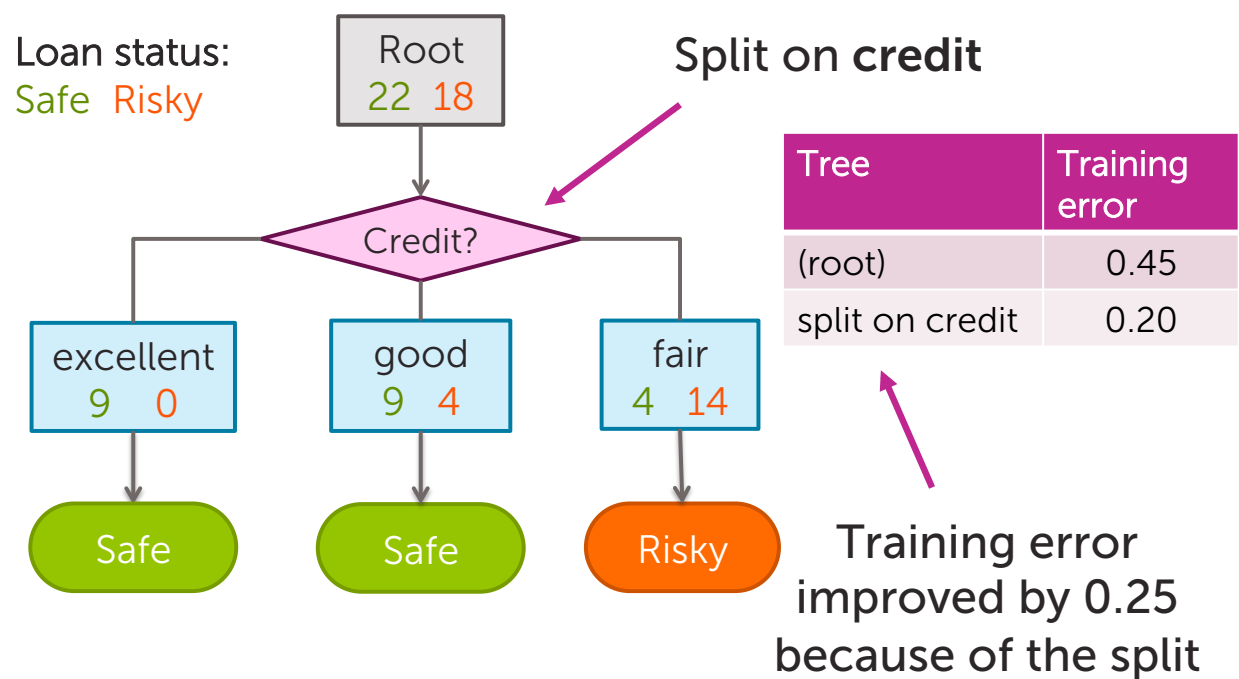
Deeper trees → lower training error



Training error = 0: Is this model perfect?



Why training error reduces with depth?

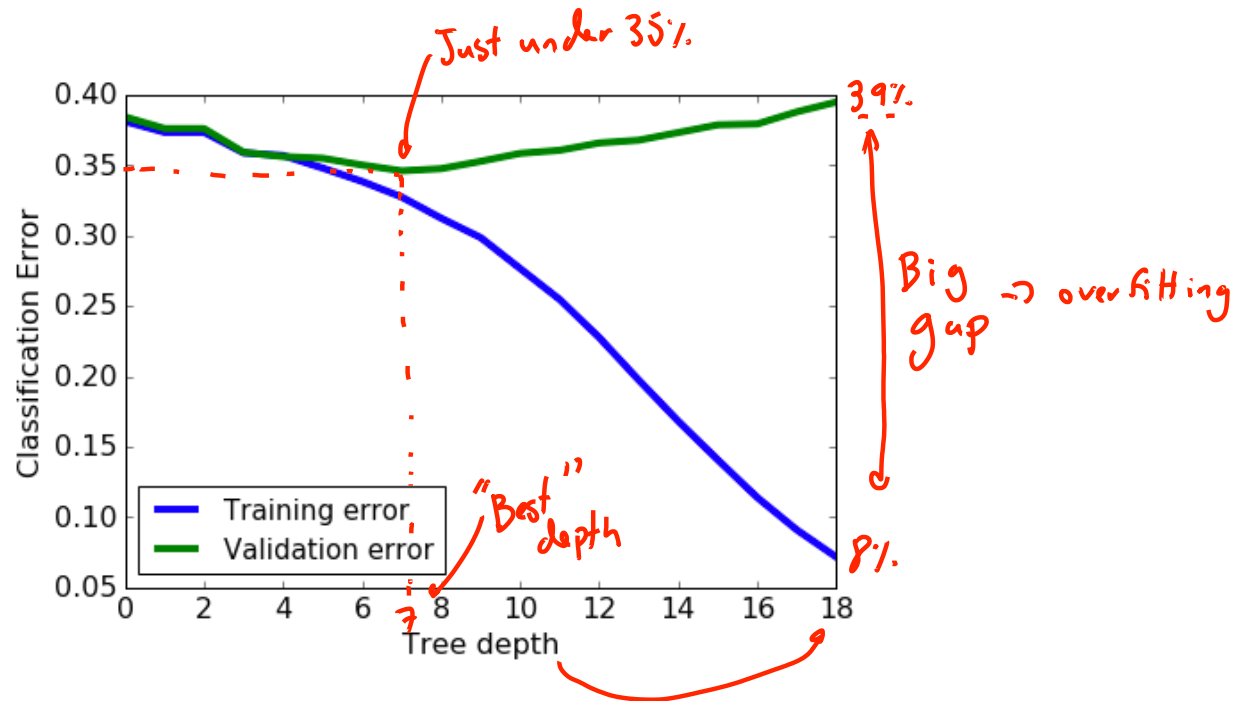


Feature split selection algorithm

- Given a subset of data M (a node in a tree)
- For each feature $h_i(\mathbf{x})$:
 1. Split data of M according to feature $h_i(\mathbf{x})$
 2. Compute classification error split
- Chose feature $h^*(\mathbf{x})$ with lowest classification error

By design, each split
reduces training error

Decision trees overfitting on loan data



Principle of Occam's razor:
Simpler trees are better

Principle of Occam's Razor



*"Among competing hypotheses, the one with fewest assumptions should be selected",
William of Occam, 13th Century*

Symptoms: S_1 and S_2

Diagnosis 1: 2 diseases

Two diseases D_1 and D_2 where
 D_1 explains S_1 , D_2 explains S_2

OR

SIMPLER

Diagnosis 2: 1 disease

Disease D_3 explains both
symptoms S_1 and S_2

Occam's Razor for decision trees

When two trees have similar classification error on the validation set, pick the simpler one

Complexity	Train error	Validation error
Simple	0.23	0.24
Moderate	0.12	0.15
Complex	0.07	0.15
Super complex	0	0.18

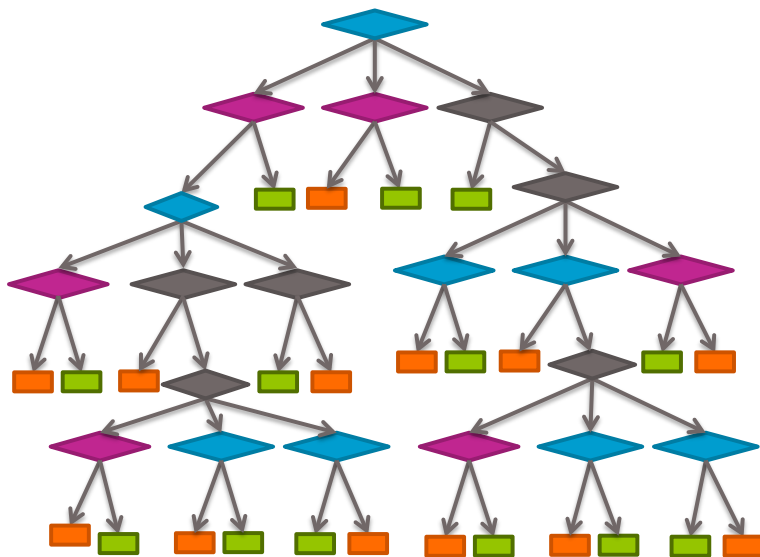
Same validation error

pick

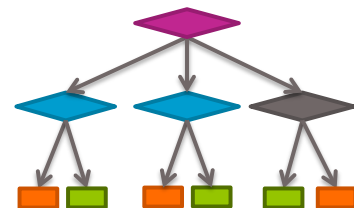
bad!

Overfit

Which tree is simpler?



OR

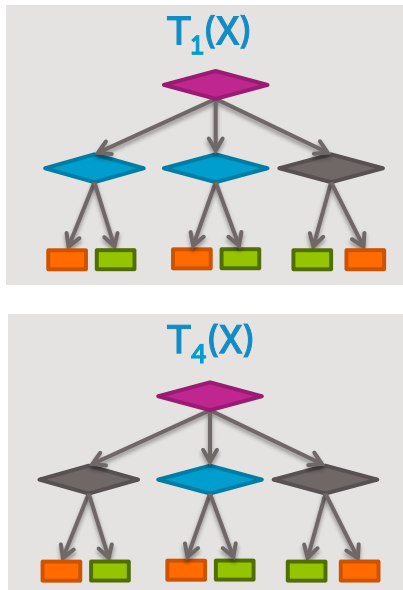


SIMPLER

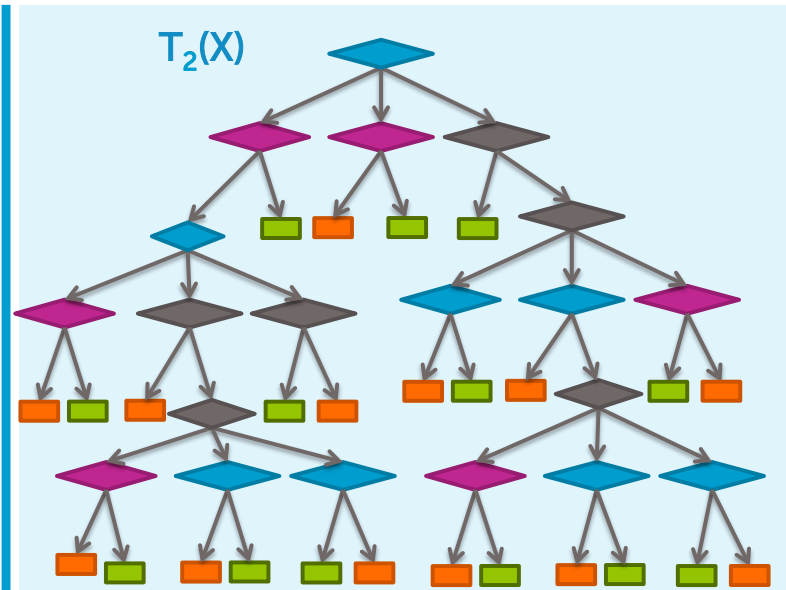
Modified tree learning problem

Find a “**simple**” decision tree with low classification error

Simple trees



Complex trees





How do we pick simpler trees?

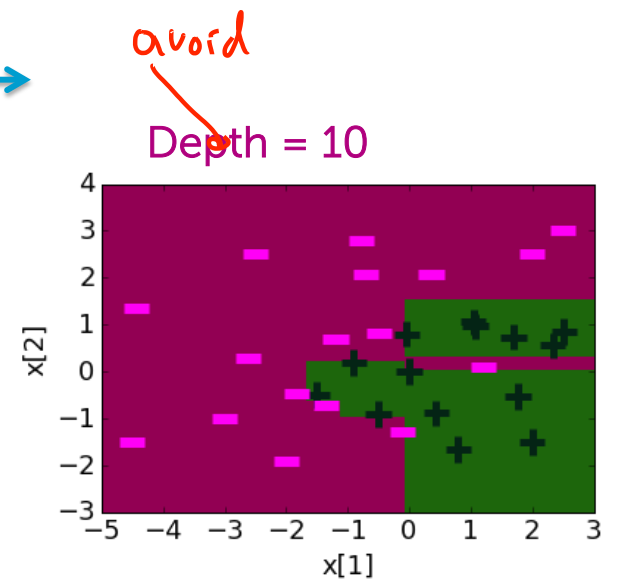
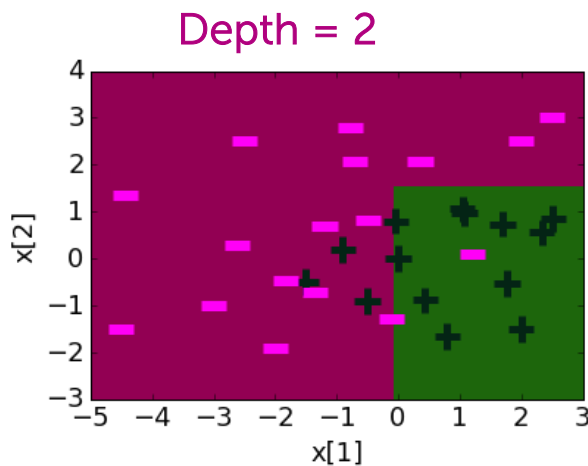
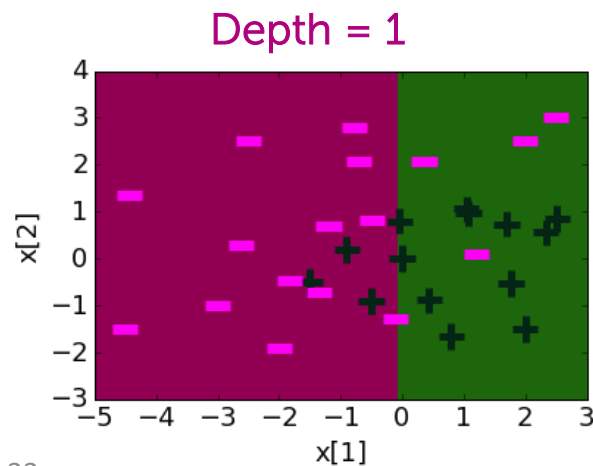
1. **Early Stopping:** Stop learning algorithm **before** tree become too complex
2. **Pruning:** Simplify tree **after** learning algorithm terminates



Early stopping for learning decision trees

Deeper trees → Increasing complexity

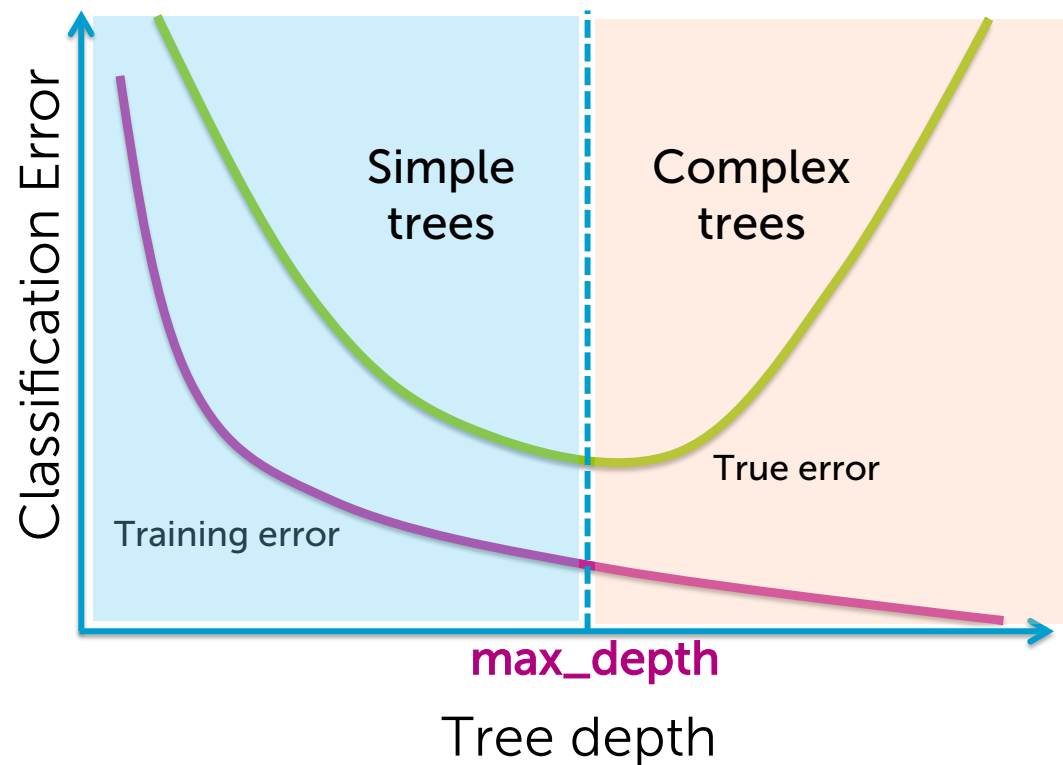
Model complexity increases with depth



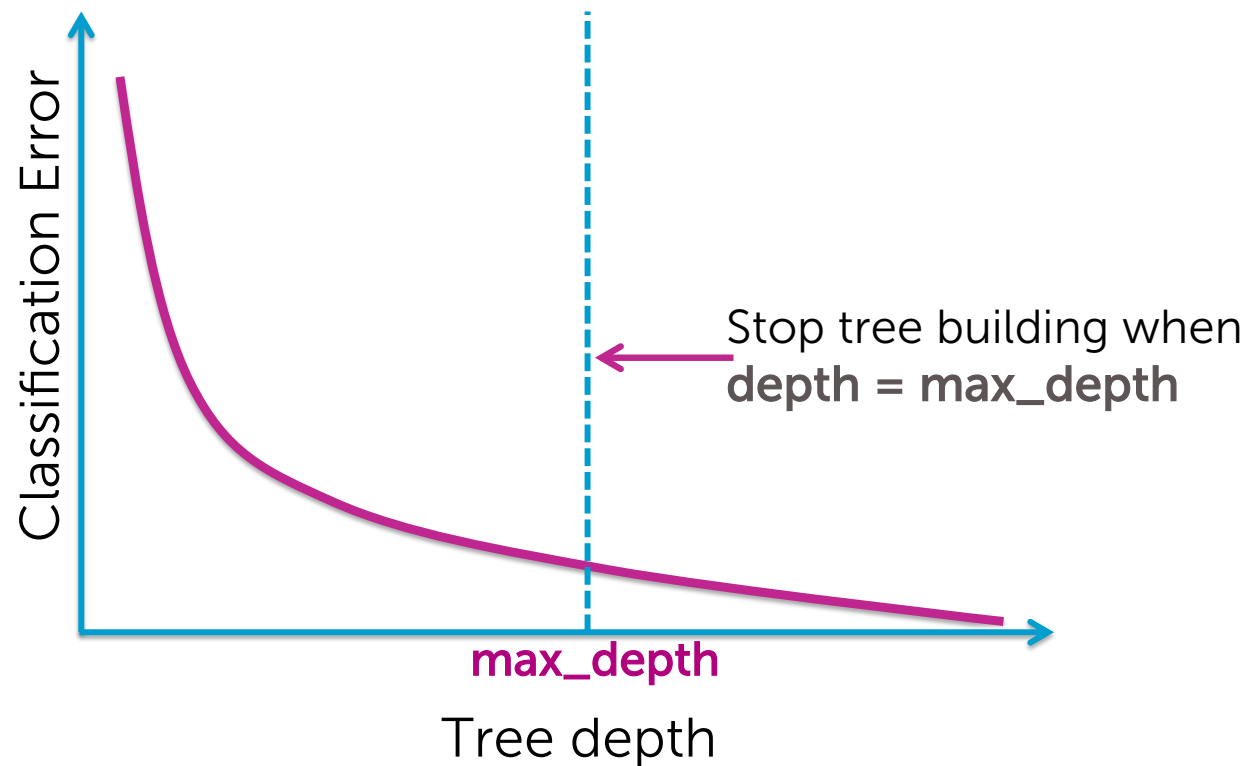


Early stopping condition 1:
Limit the depth of a tree

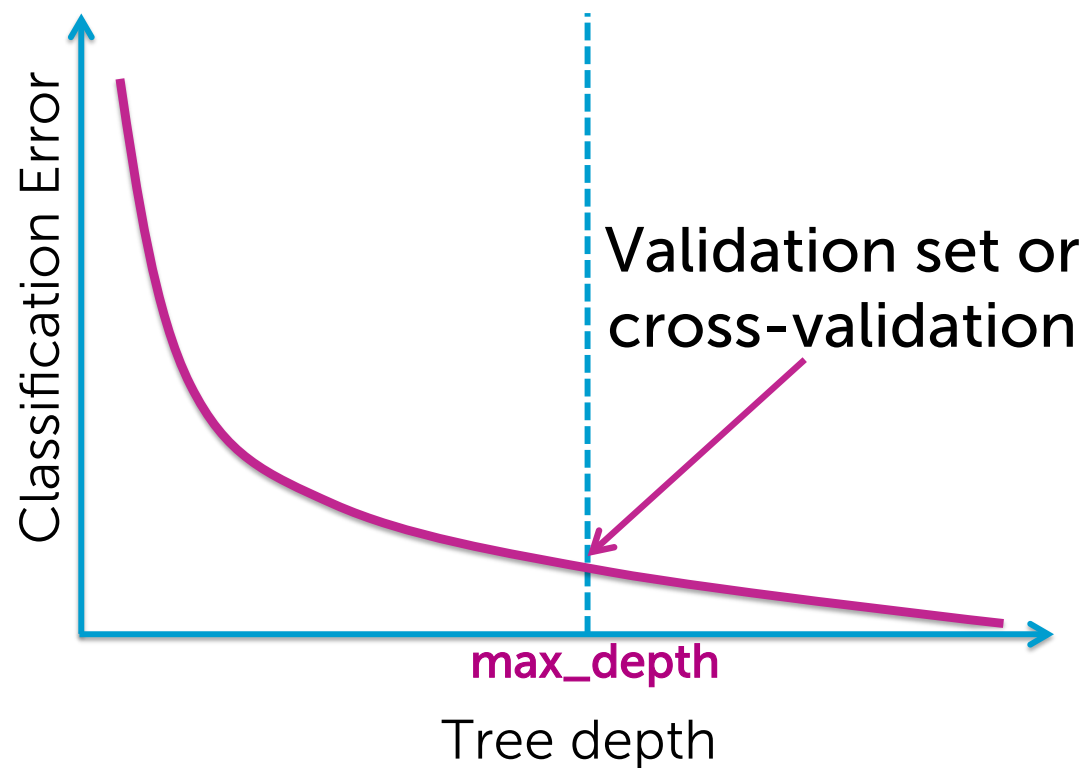
Restrict tree learning to shallow trees?



Early stopping condition 1: Limit depth of tree



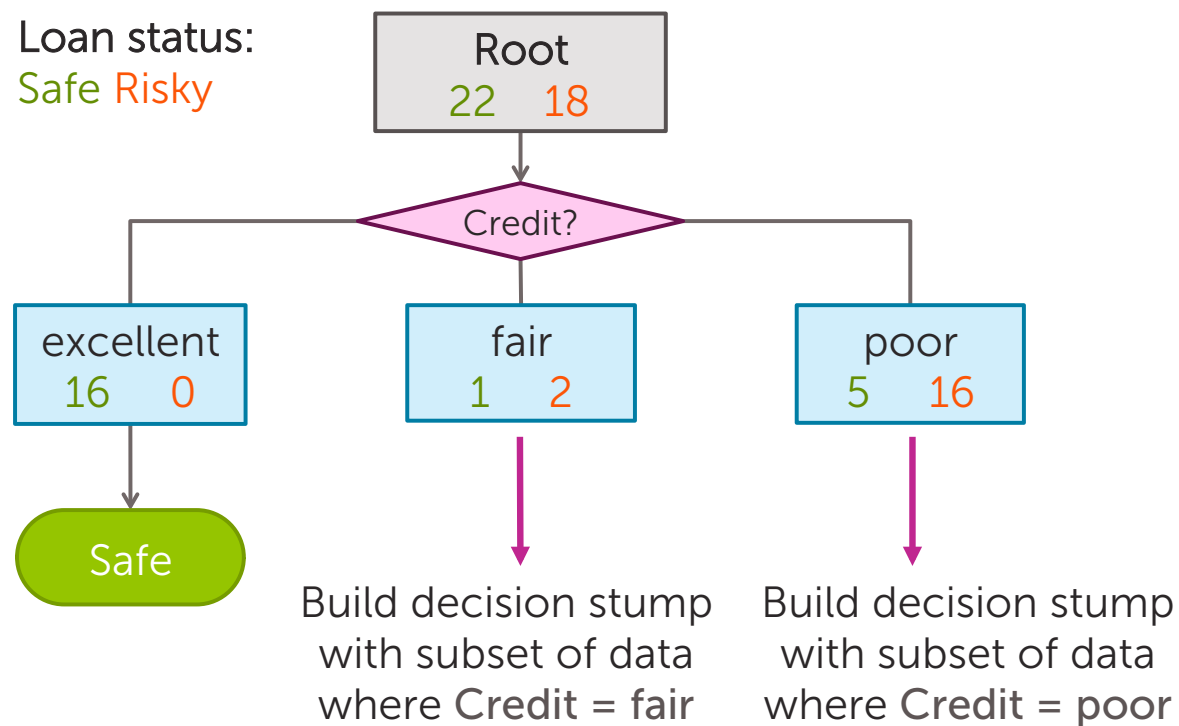
Picking value for `max_depth`???



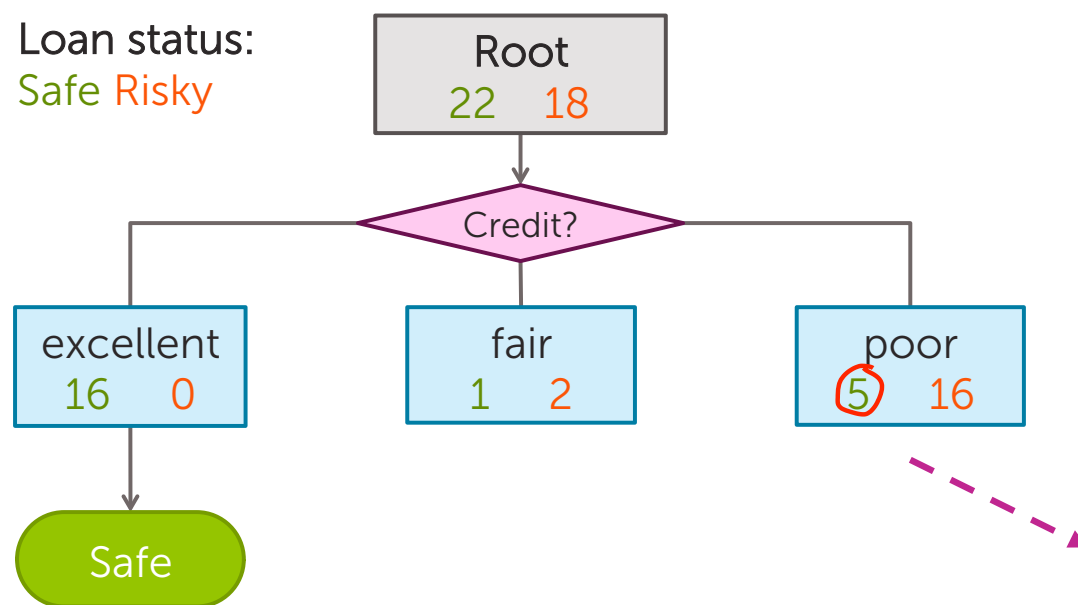


Early stopping condition 2:
*Use classification error to
limit depth of tree*

Decision tree recursion review



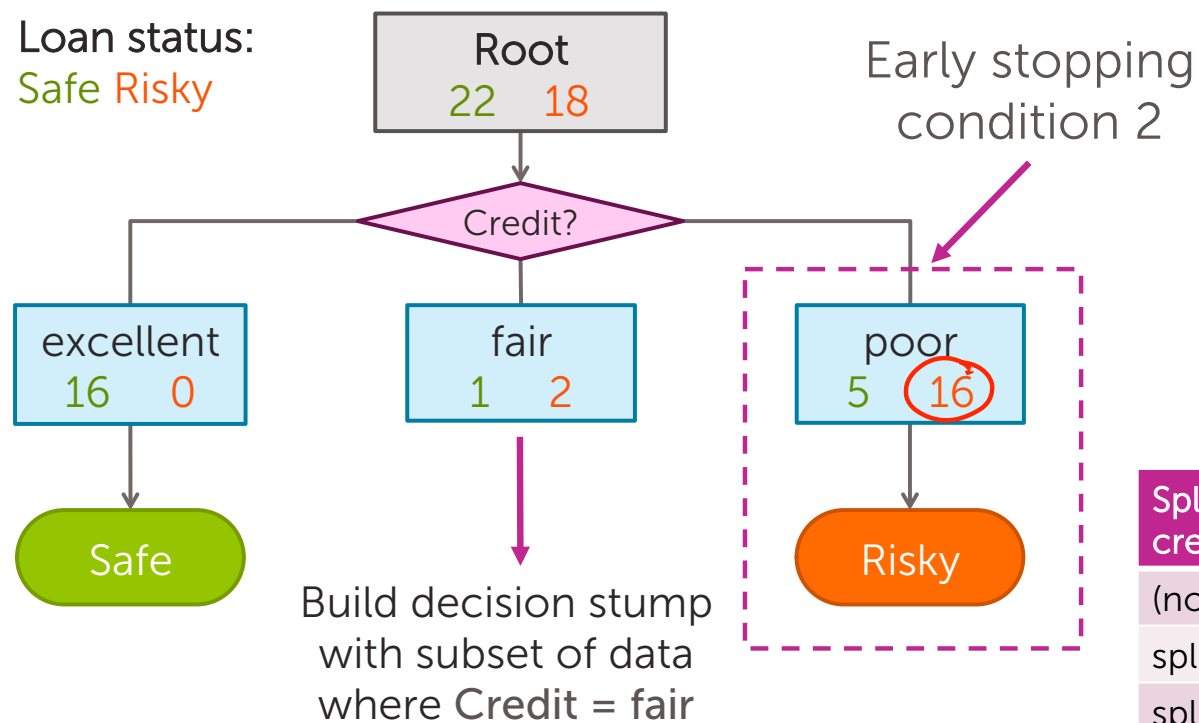
Split selection for credit=poor



No split improves
classification error
→ Stop!

Splits for credit=poor	Classification error
(no split)	<u>0.24</u>
split on term	<u>0.24</u>
split on income	<u>0.24</u>

Early stopping condition 2: No split improves classification error



Splits for credit=poor	Classification error
(no split)	0.24
split on term	0.24
split on income	0.24



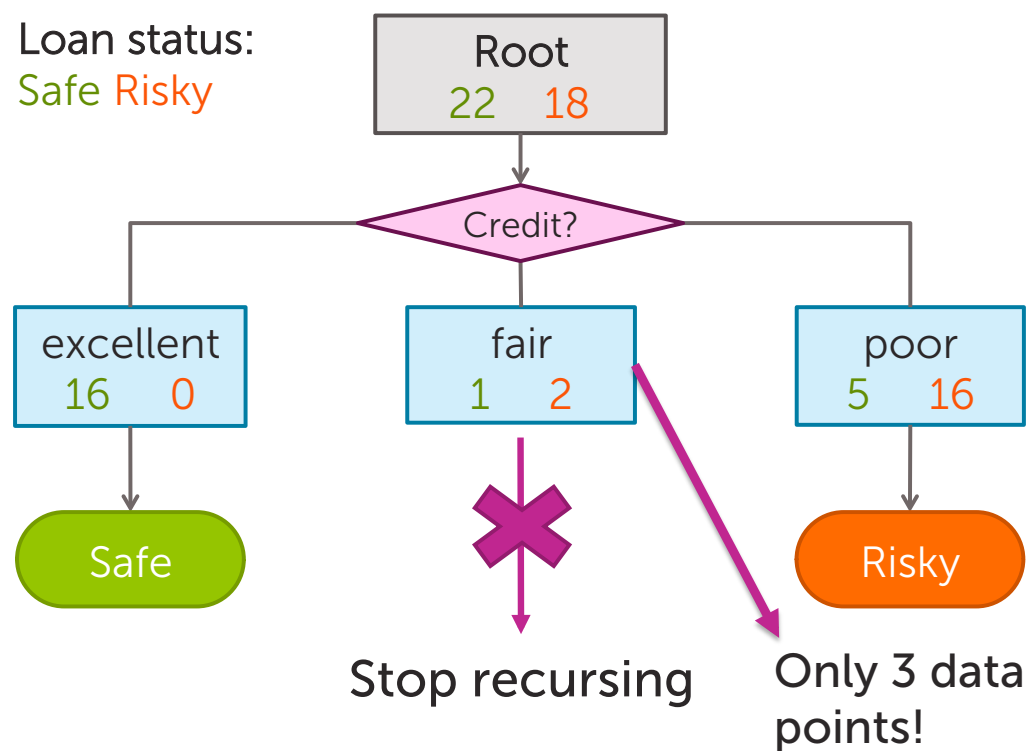
Practical notes about stopping when classification error doesn't decrease

1. Typically, add magic parameter ϵ
 - Stop if error doesn't decrease by more than ϵ
2. Some pitfalls to this rule (see pruning section)
3. Very useful in practice

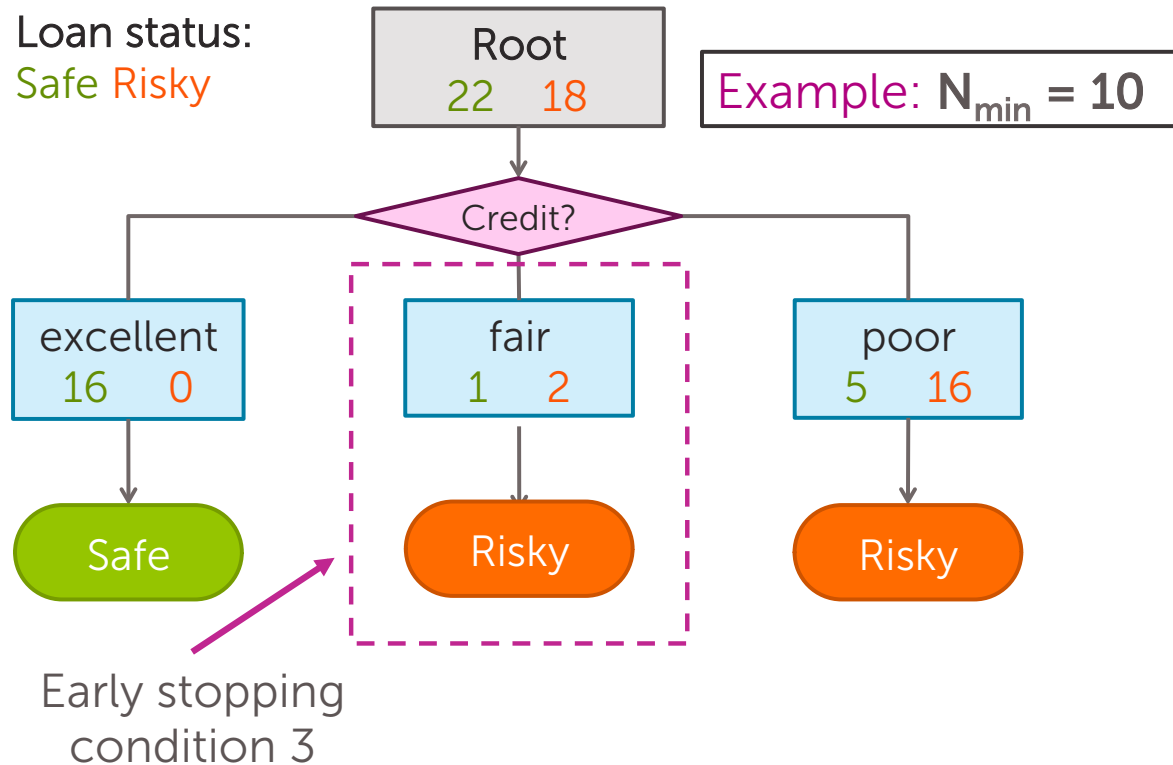


Early stopping condition 3:
*Stop if number of data points
contained in a node is too small*

Can we trust nodes with very few points?



Early stopping condition 3: Stop when data points in a node $\leq N_{\min}$





Summary of decision trees with early stopping



Early stopping: Summary

1. **Limit tree depth:** Stop splitting after a certain depth
2. **Classification error:** Do not consider any split that does not cause a sufficient decrease in classification error
3. **Minimum node "size":** Do not split an intermediate node which contains too few data points

Greedy decision tree learning

- **Step 1:** Start with an empty tree
- **Step 2:** Select a feature to split data
- For each split of the tree:

- **Step 3:** If nothing more to, make predictions ← Majority

- **Step 4:** Otherwise, go to **Step 2** & continue (recurse) on this split

Previous module

Stopping conditions 1 & 2
or
Early stopping conditions 1, 2 & 3

Recursion

Overfitting in Decision Trees: *Pruning*

OPTIONAL



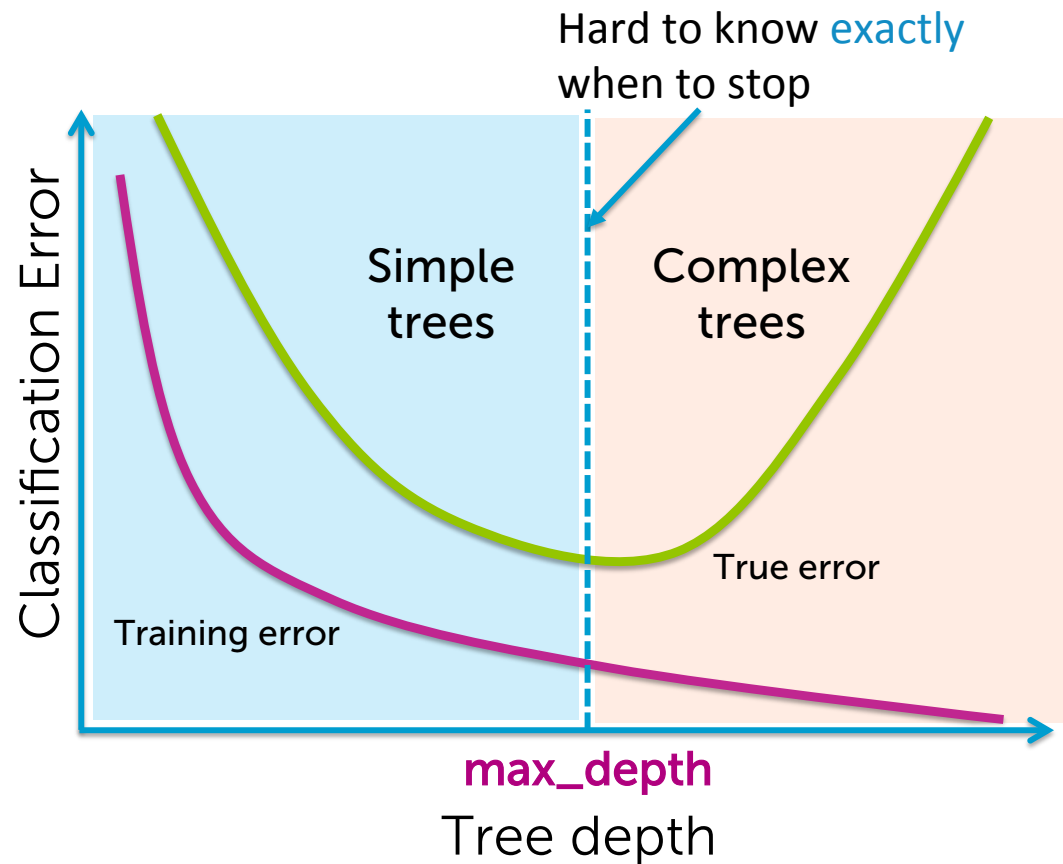
Stopping condition summary

- Stopping condition:
 1. All examples have the same target value
 2. No more features to split on
- Early stopping conditions:
 1. Limit tree depth
 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

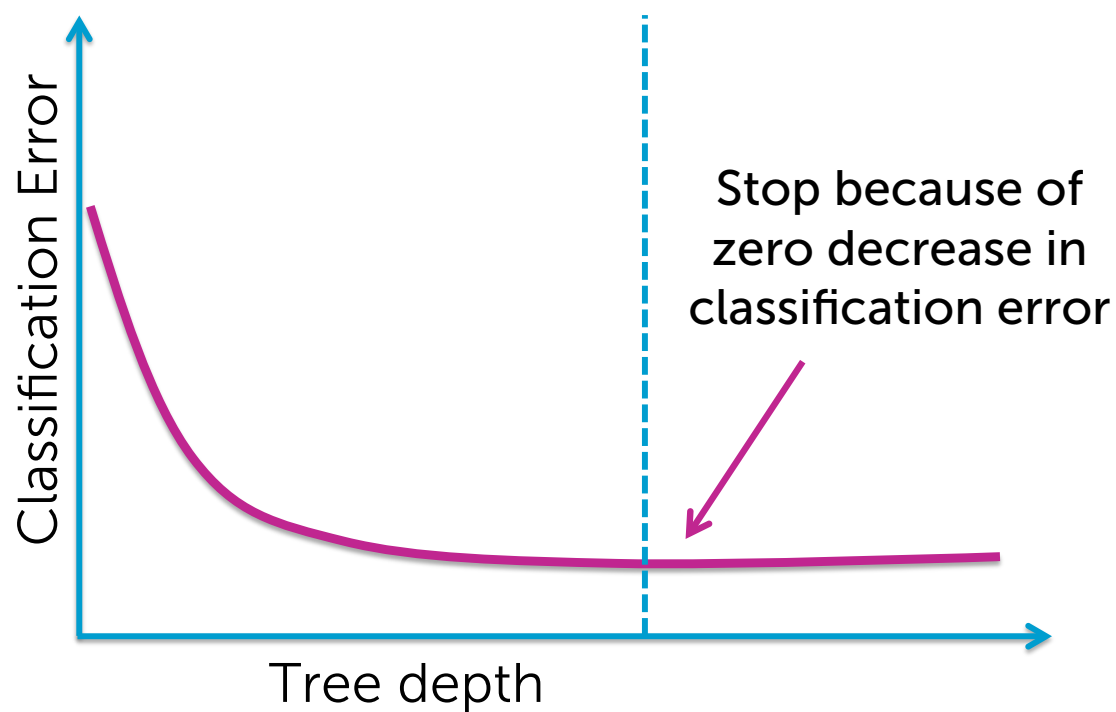


Exploring some challenges with early stopping conditions

Challenge with early stopping condition 1



Is early stopping condition 2 a good idea?



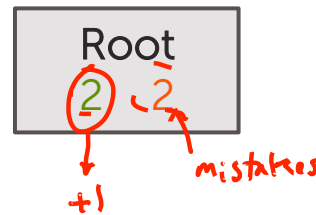
Early stopping condition 2:

Don't stop if error doesn't decrease???

$$y = \mathbf{x}[1] \text{ xor } \mathbf{x}[2]$$

$\mathbf{x}[1]$	$\mathbf{x}[2]$	y
False	False	False
False	True	True
True	False	True
True	True	False

y values
True False



$$\text{Error} = \frac{2}{4} = 0.5$$

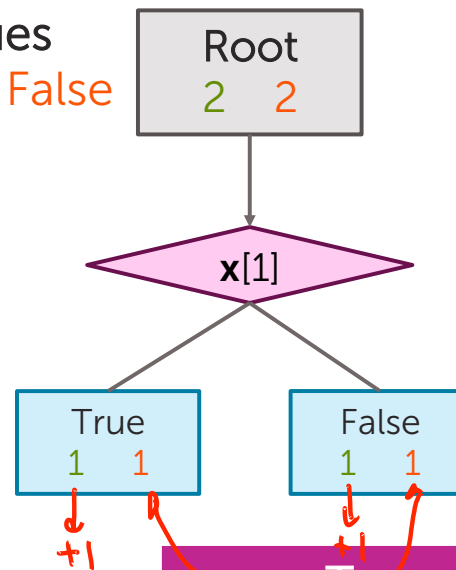
Tree	Classification error
(root)	0.5

Consider split on $x[1]$

$$y = x[1] \text{ xor } x[2]$$

$x[1]$	$x[2]$	y
False	False	False
False	True	True
True	False	True
True	True	False

y values
True False



$$\text{Error} = \frac{1+1}{4} = 0.5$$

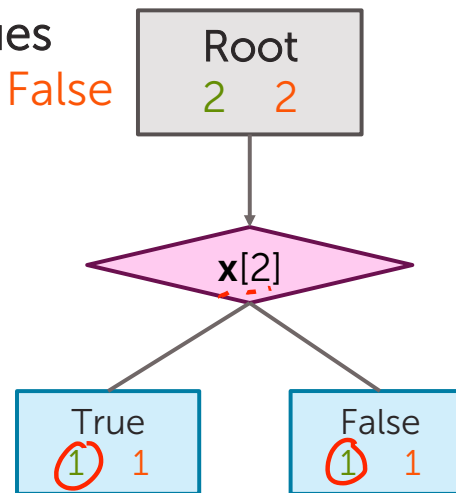
Tree	Classification error
(root)	0.5
Split on $x[1]$	0.5

Consider split on $x[2]$

$$y = x[1] \text{ xor } x[2]$$

$x[1]$	$x[2]$	y
False	False	False
False	True	True
True	False	True
True	True	False

y values
True False



$$\text{Error} = \frac{1 + 1}{4} = 0.5$$

Neither features
improve training error...
Stop now???

Tree	Classification error
(root)	0.5
Split on $x[1]$	0.5
Split on $x[2]$	0.5

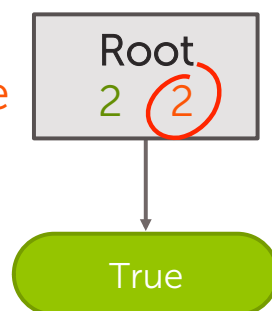
Same error

Final tree with early stopping condition 2

$$y = \mathbf{x}[1] \text{ xor } \mathbf{x}[2]$$

$\mathbf{x}[1]$	$\mathbf{x}[2]$	y
False	False	False
False	True	True
True	False	True
True	True	False

y values
True False



Tree	Classification error
with early stopping condition 2	0.5

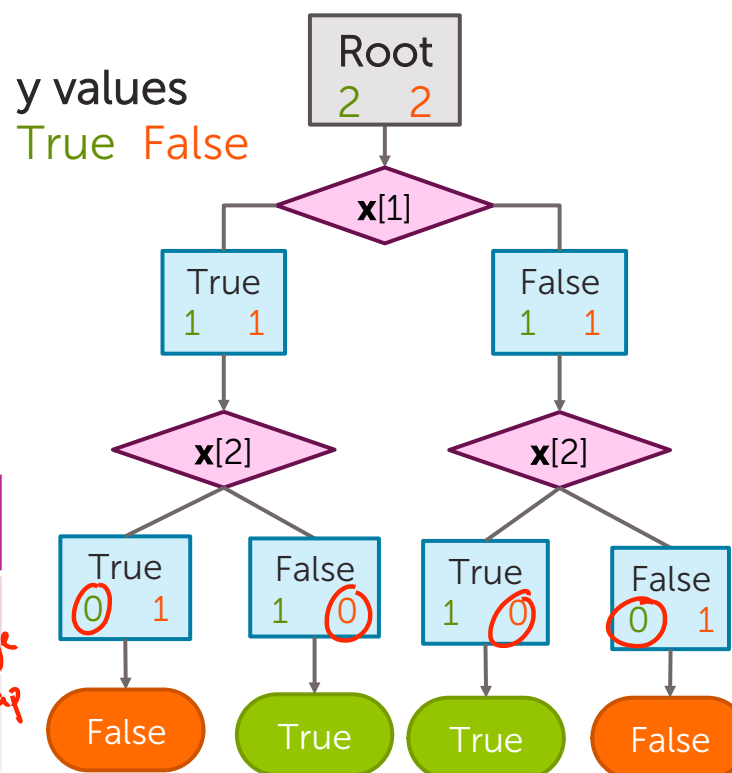
Without early stopping condition 2

$$y = \mathbf{x}[1] \text{ xor } \mathbf{x}[2]$$

$\mathbf{x}[1]$	$\mathbf{x}[2]$	y
False	False	False
False	True	True
True	False	True
True	True	False

Tree	Classification error
with early stopping condition 2	0.5
without early stopping condition 2	<u>0.0</u>

huge gap





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



Tree pruning



Two approaches to picking simpler trees

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

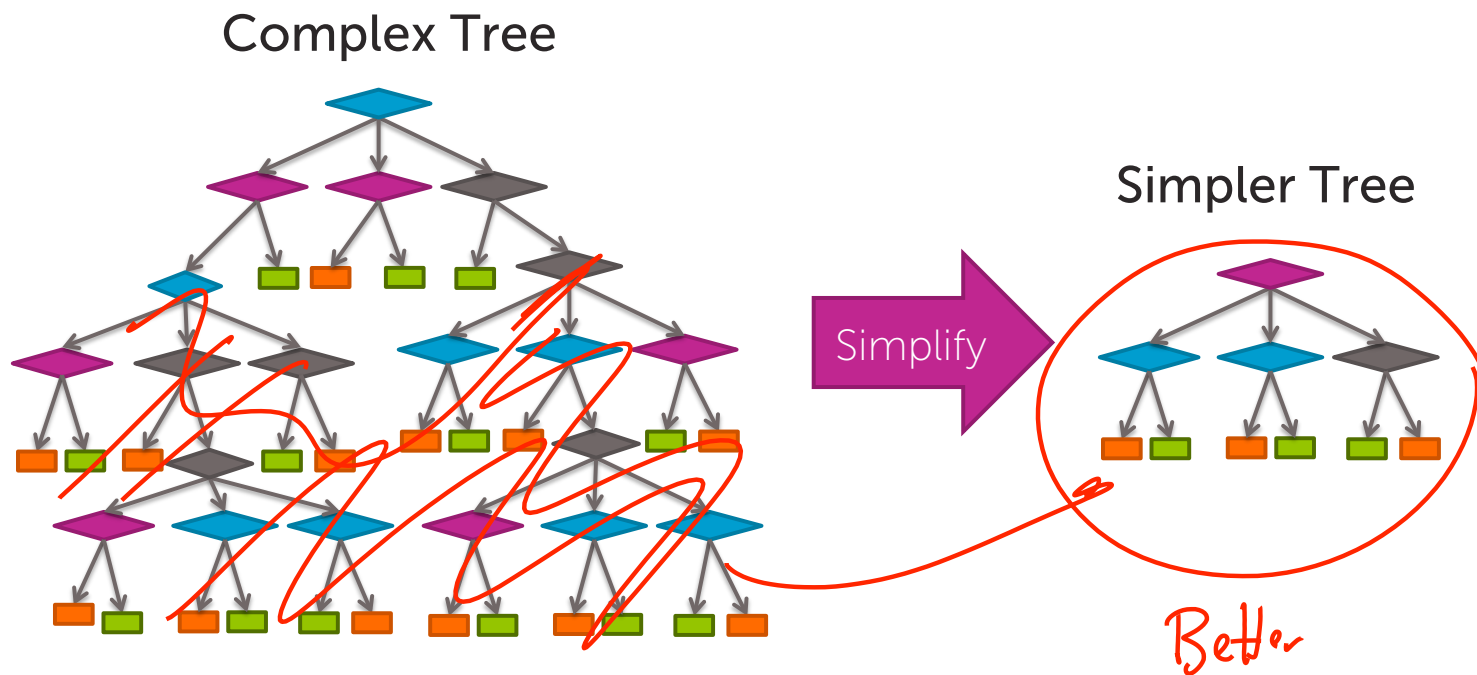
2. **Pruning:** Simplify the tree **after** the learning algorithm terminates



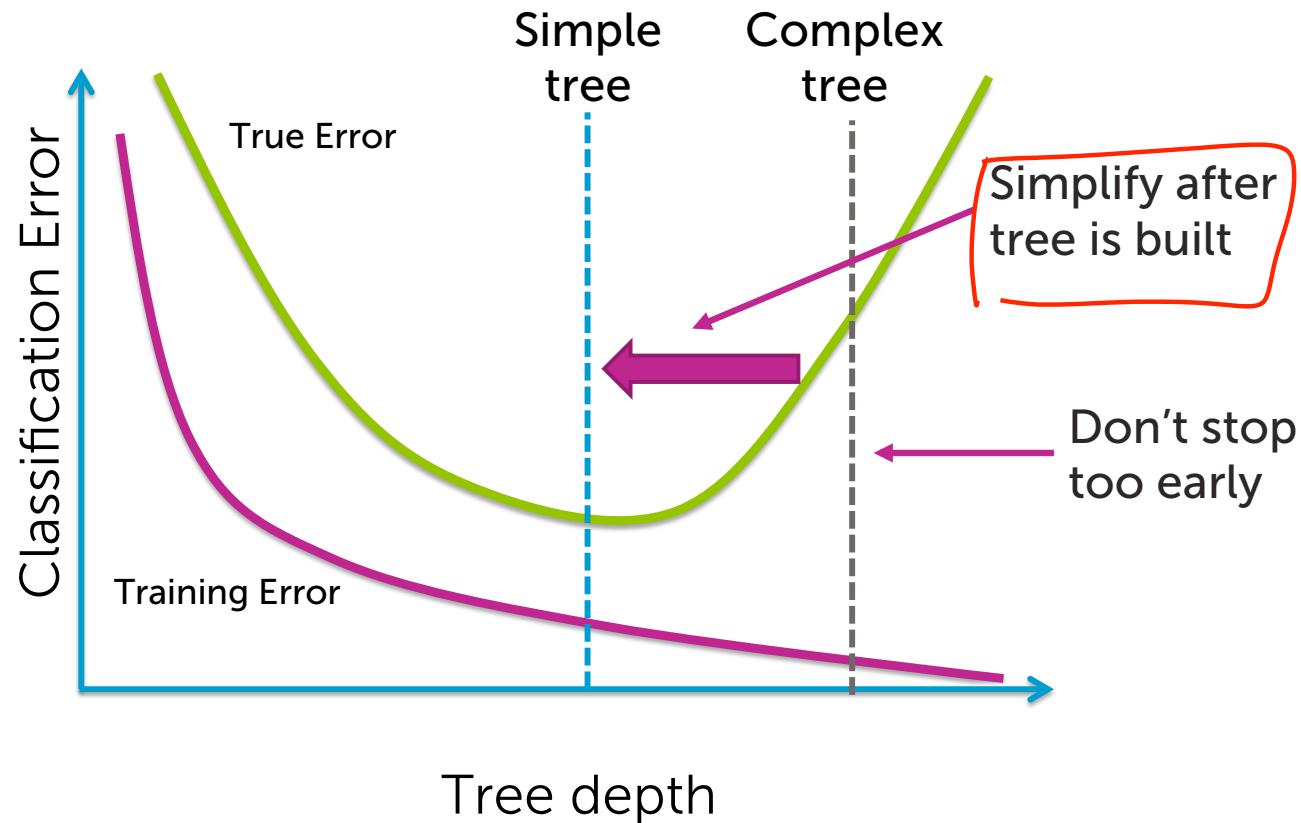
Complements early stopping

Pruning: *Intuition*

Train a complex tree, simplify later

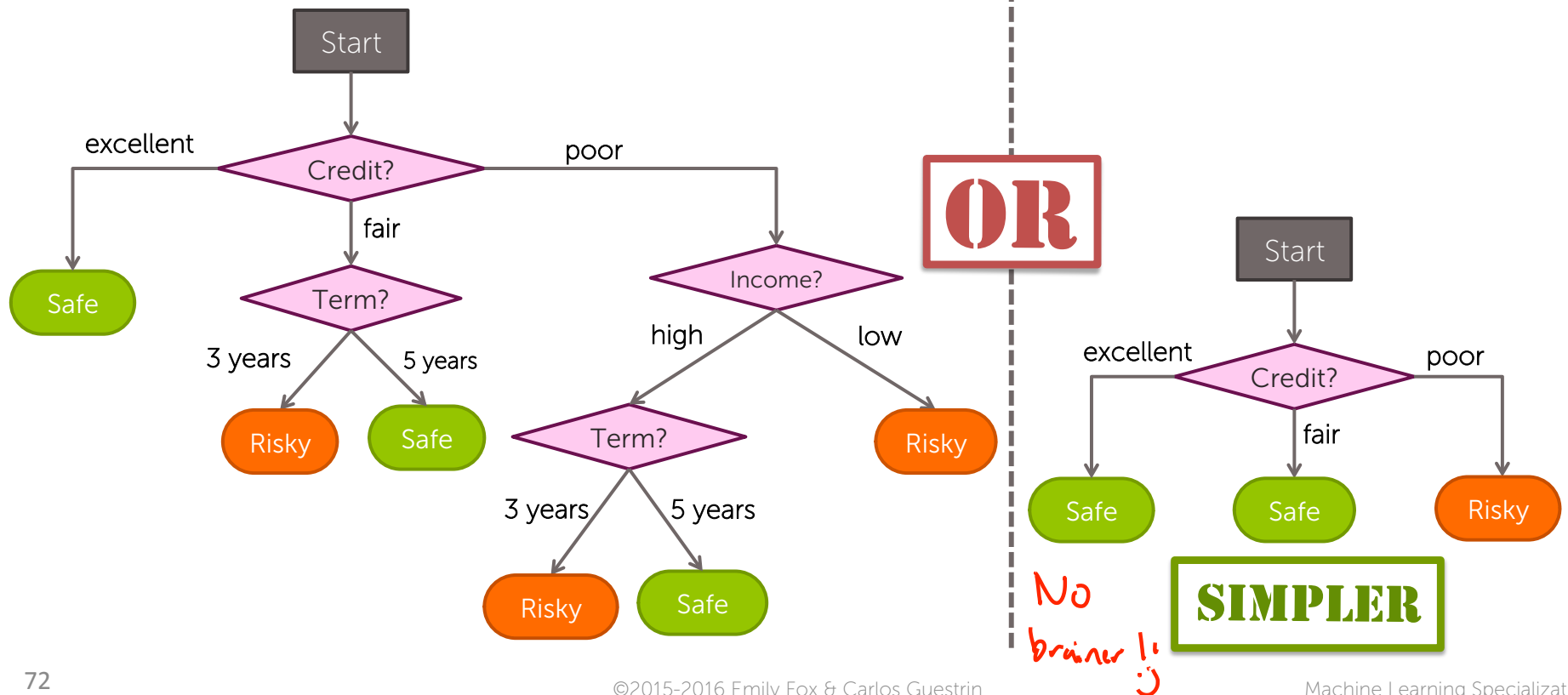


Pruning motivation



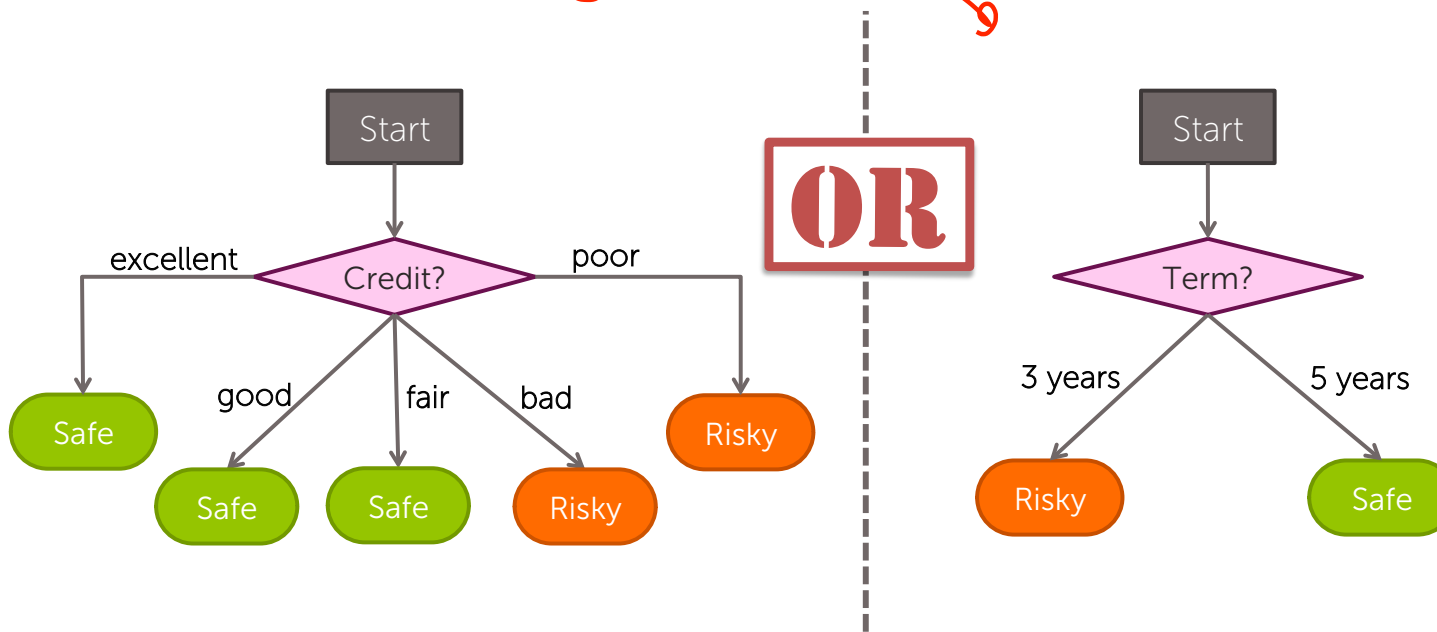
Example 1: Which tree is simpler?

Depth

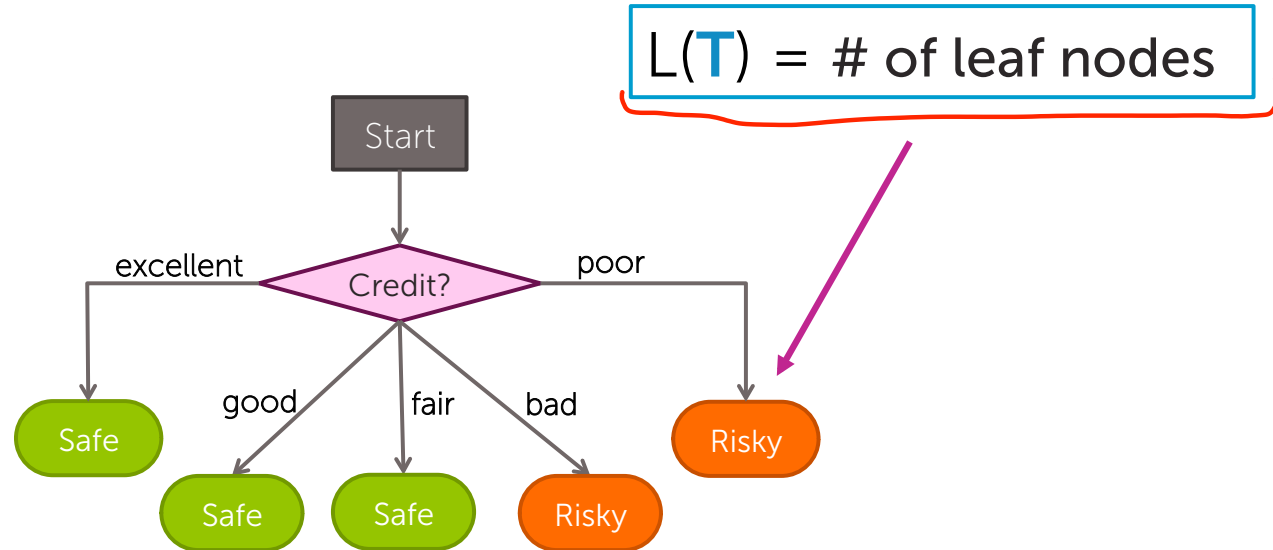


Example 2: Which tree is simpler???

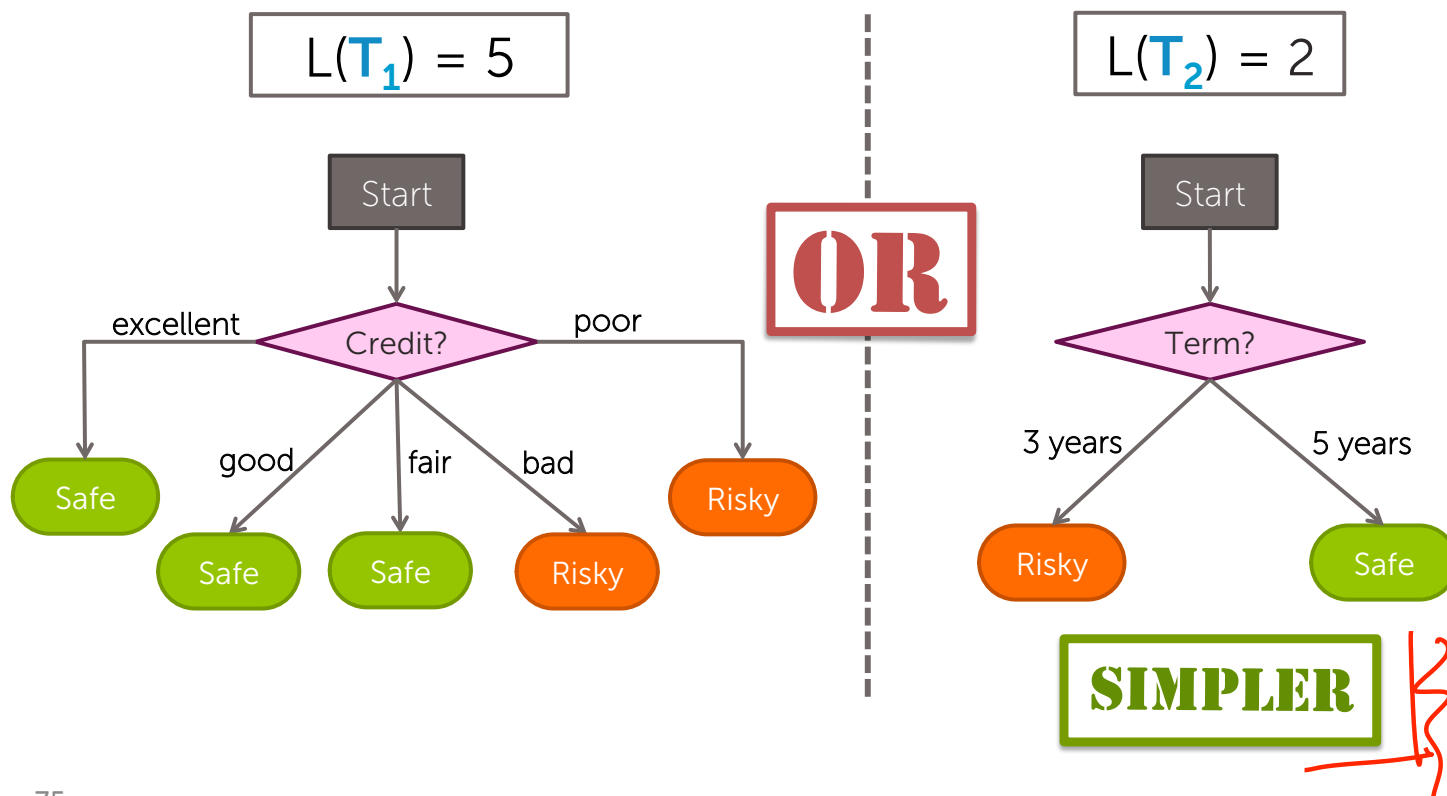
*Same Depth:
Simpler?*



Simple measure of complexity of tree



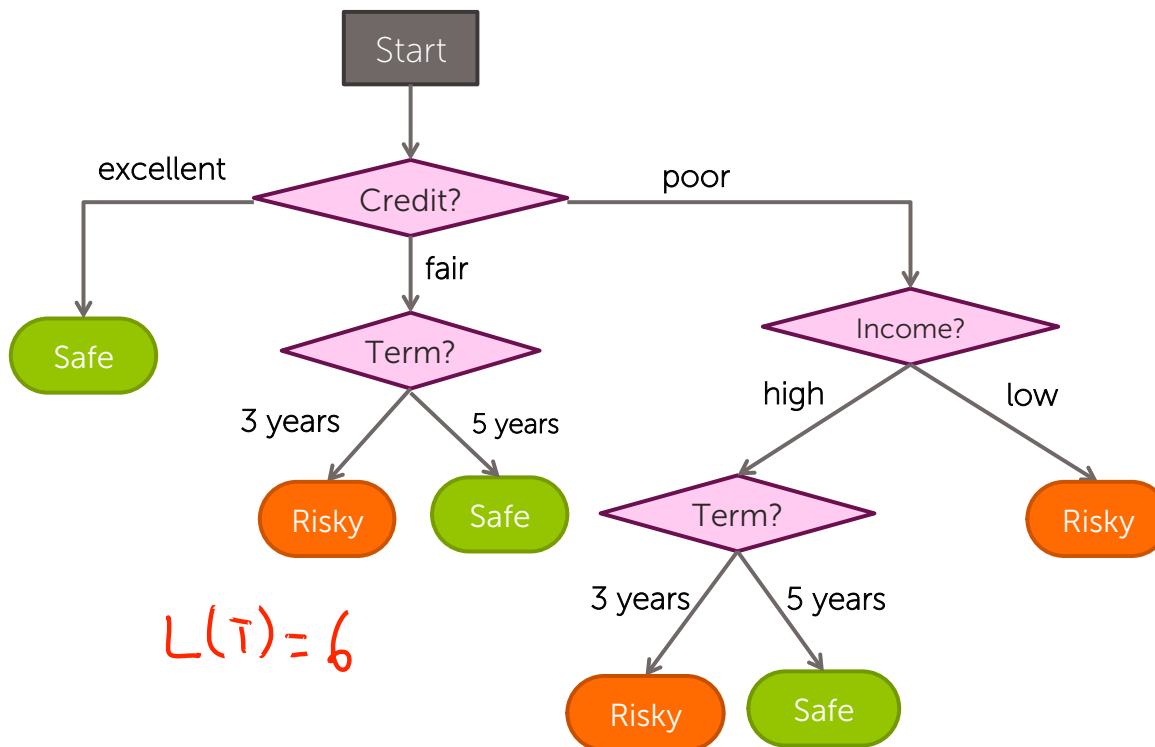
Which tree has lower $L(T)$?



Balance simplicity & predictive power

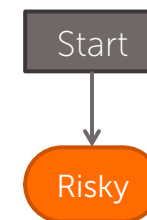
Too complex, risk of overfitting

solution in between



$$L(\bar{T}) = 6$$

Too simple, high classification error

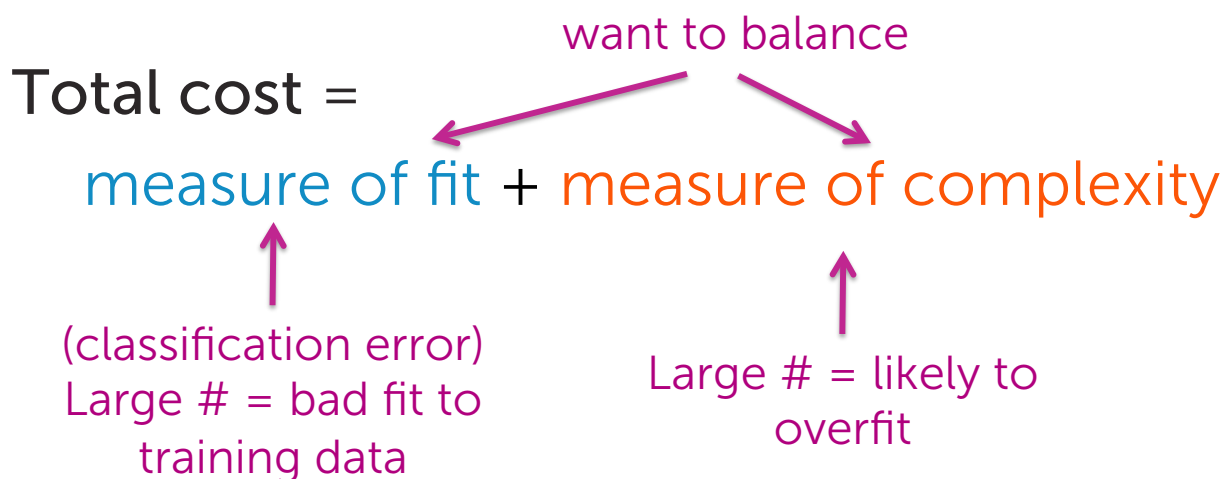


$$L(T) = 1$$

Desired total quality format

Want to balance:

- i. How well tree fits data
- ii. Complexity of tree



Consider specific total cost

$$\text{Total cost} = \underbrace{\text{classification error}}_{\text{Error}(\mathbf{T})} + \underbrace{\text{number of leaf nodes}}_{L(\mathbf{T})}$$

Balancing fit and complexity

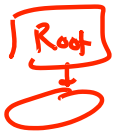
$$\text{Total cost } C(\mathbf{T}) = \text{Error}(\mathbf{T}) + \lambda L(\mathbf{T})$$

tuning parameter

If $\lambda = 0$:

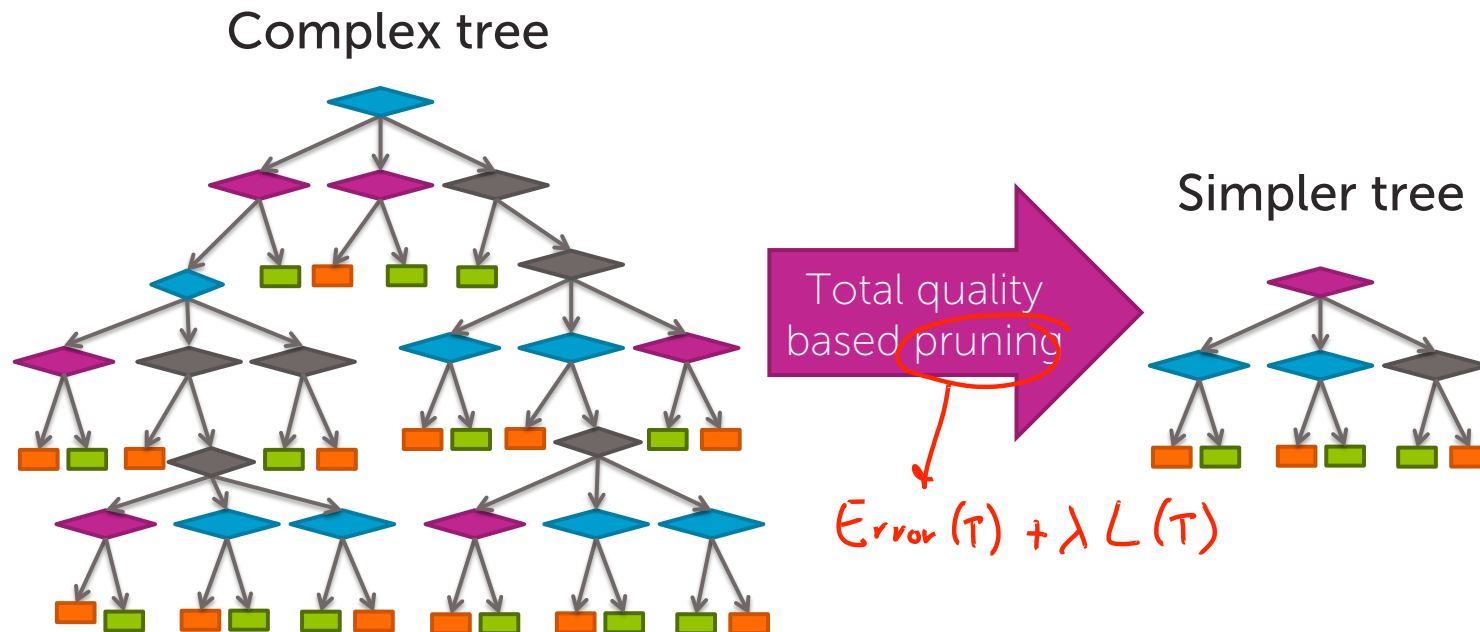
Standard decision tree learning

If $\lambda = \infty$:

∞ penalty \rightarrow  $\rightarrow \hat{y} = \text{Majority class}$

If λ in between: Balance fit & complexity

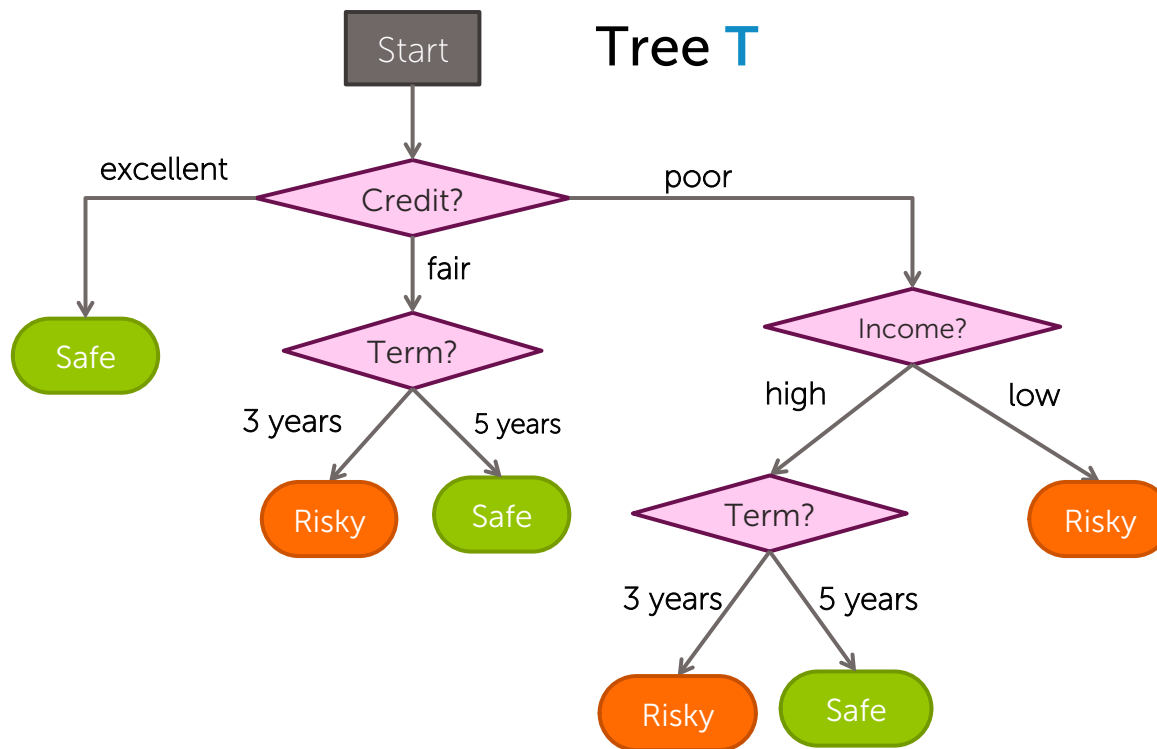
Use total cost to simplify trees



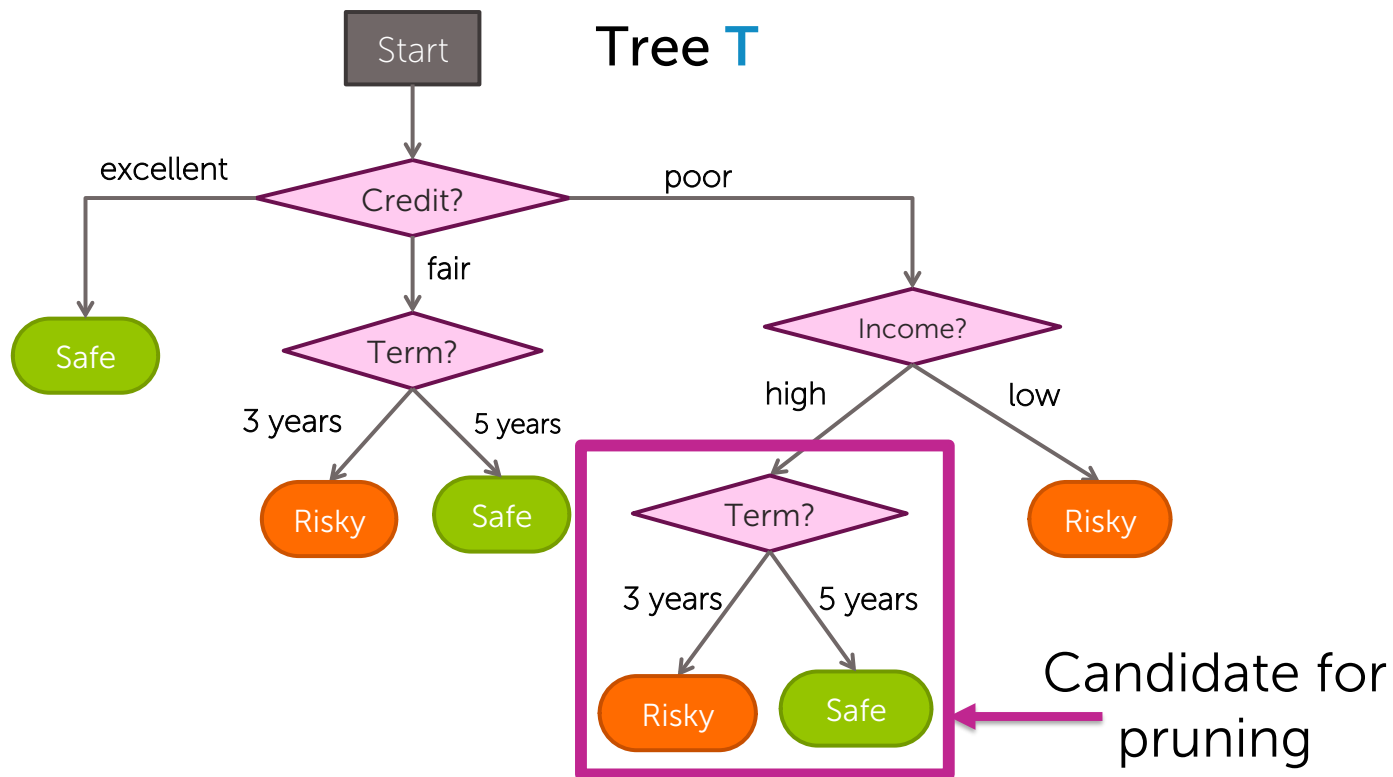


Tree pruning algorithm

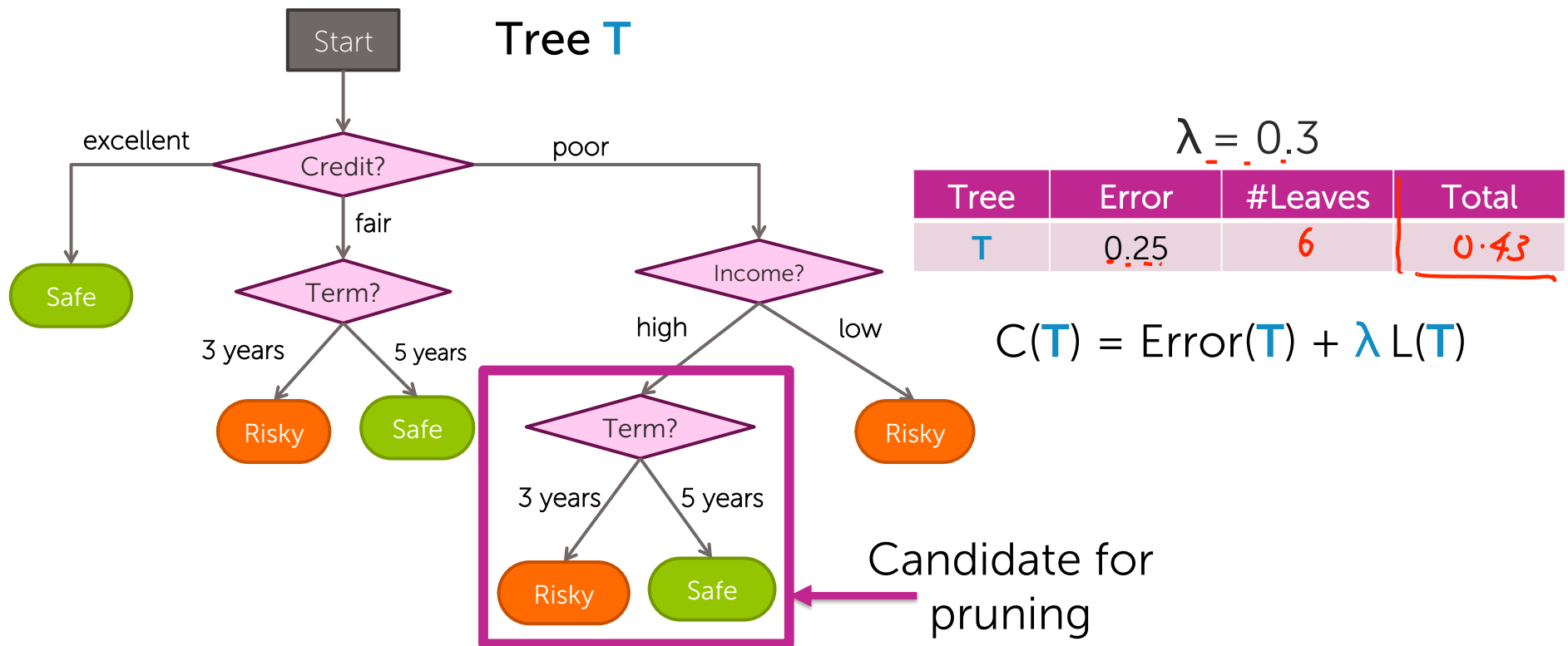
Pruning Intuition



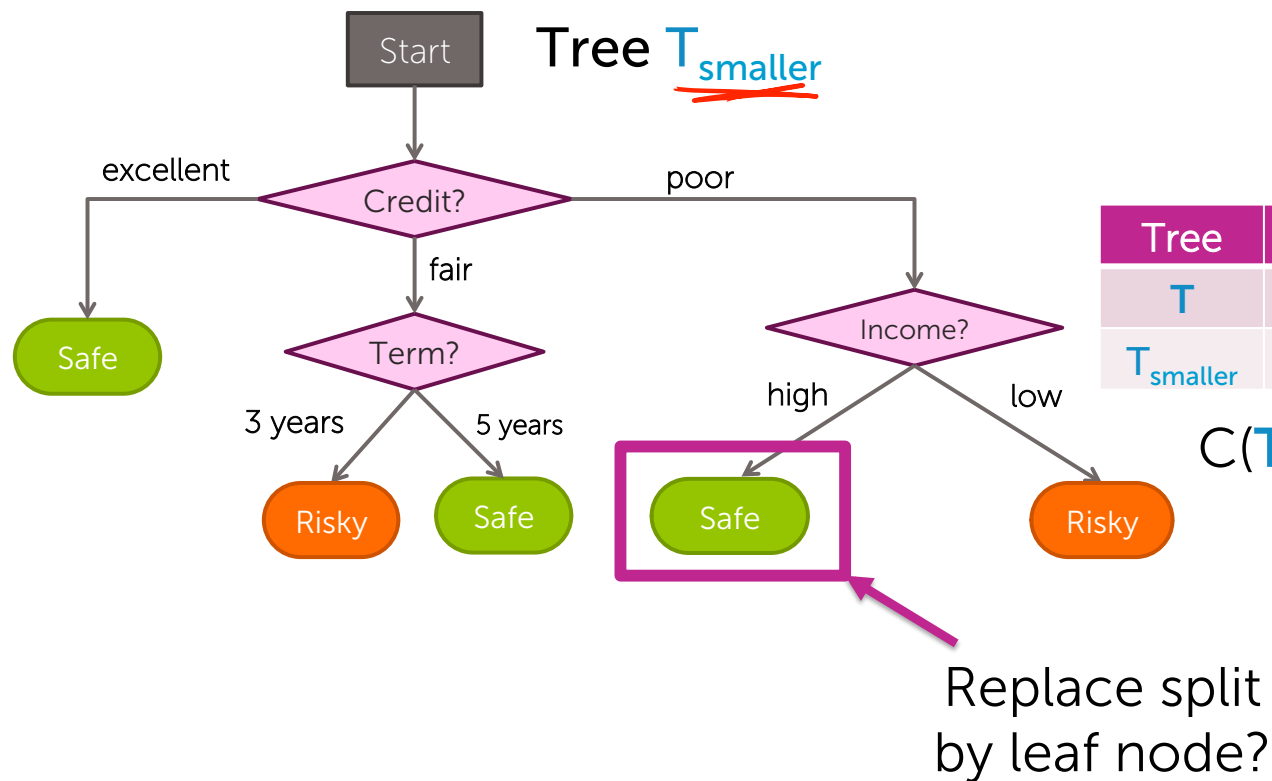
Step 1: Consider a split



Step 2: Compute total cost $C(\mathbf{T})$ of split



Step 2: “Undo” the splits on T_{smaller}

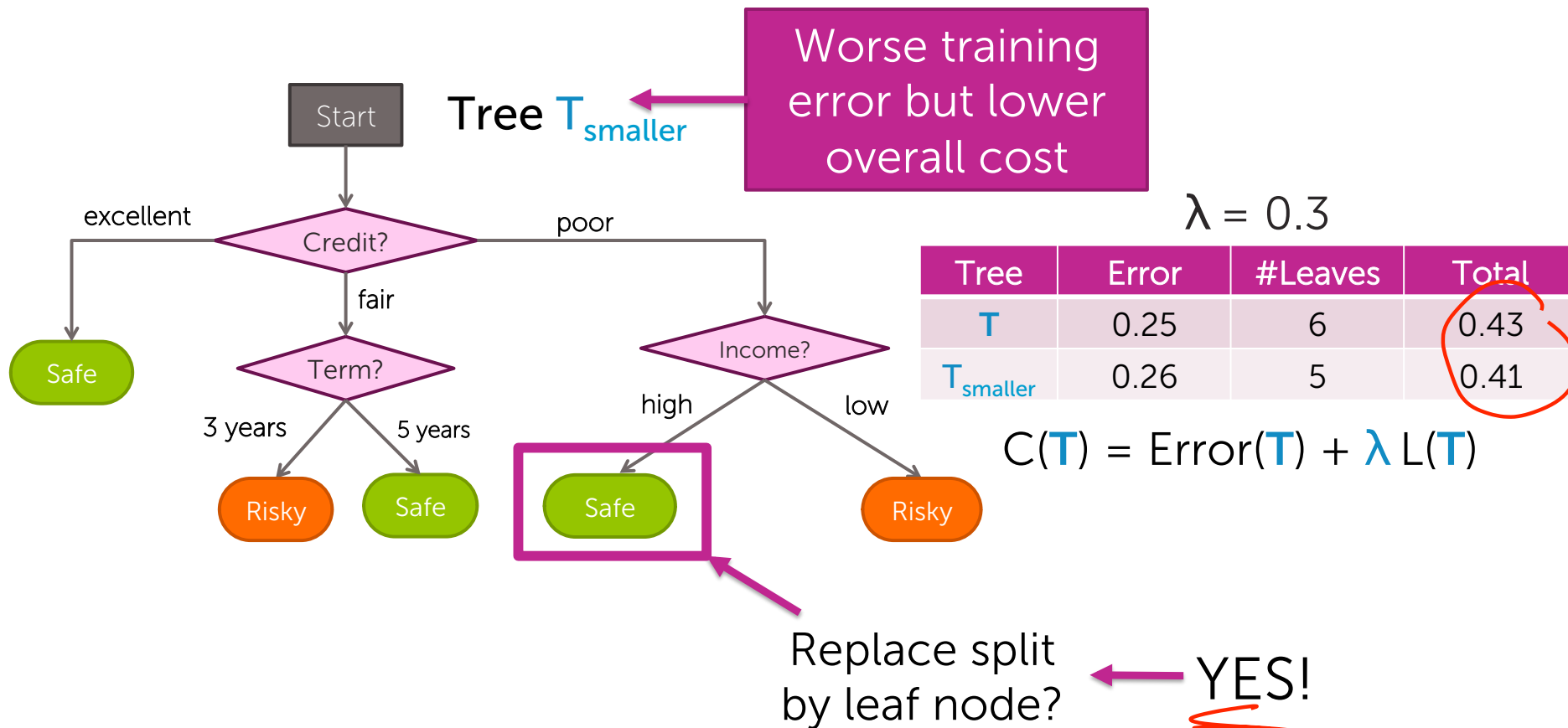


$\lambda = 0.3$

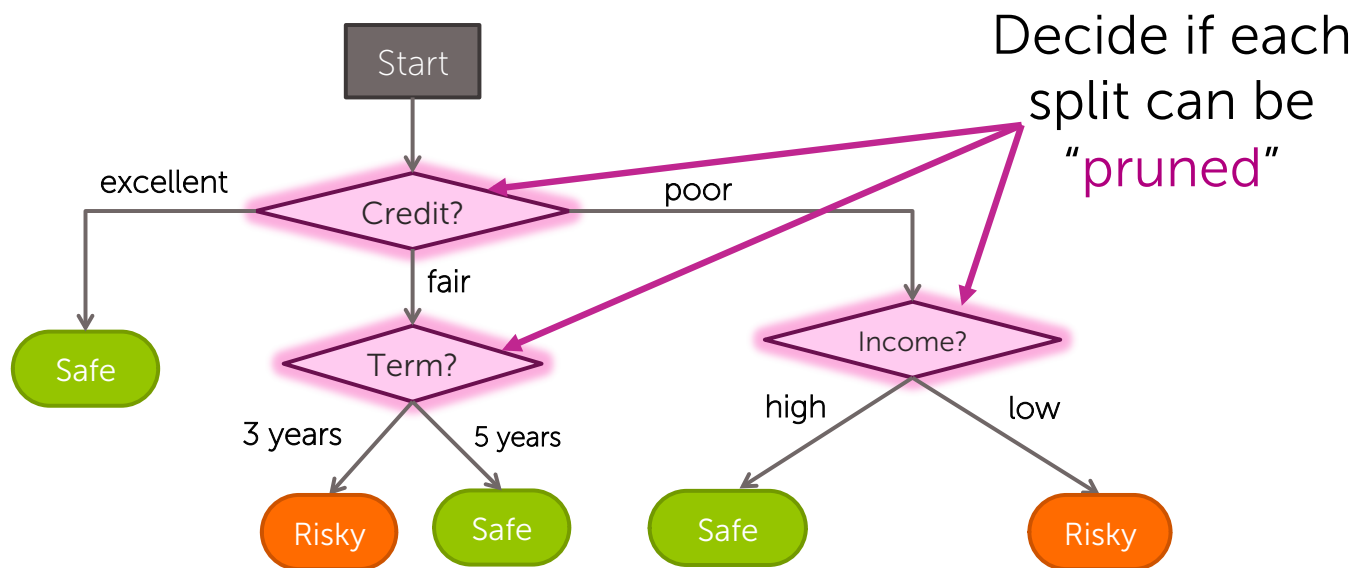
Tree	Error	#Leaves	Total
T	0.25	6	0.43
T_{smaller}	0.26	5	0.41

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

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



Step 5: Repeat Steps 1-4 for every split



Decision tree pruning algorithm

- Start at bottom of tree T and traverse up, apply *prune_split* to each decision node M
- *prune_split*(T, M):
 1. Compute total cost of tree T using
$$C(T) = \text{Error}(T) + \lambda L(T)$$
 2. Let T_{smaller} be tree after pruning subtree below M
 3. Compute total cost complexity of T_{smaller}
$$C(T_{\text{smaller}}) = \text{Error}(T_{\text{smaller}}) + \lambda L(T_{\text{smaller}})$$
 4. If $C(T_{\text{smaller}}) < C(T)$, prune to T_{smaller}



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

Thank you to Dr. Krishna Sridhar



Dr. Krishna Sridhar
Staff Data Scientist, Dato, Inc.