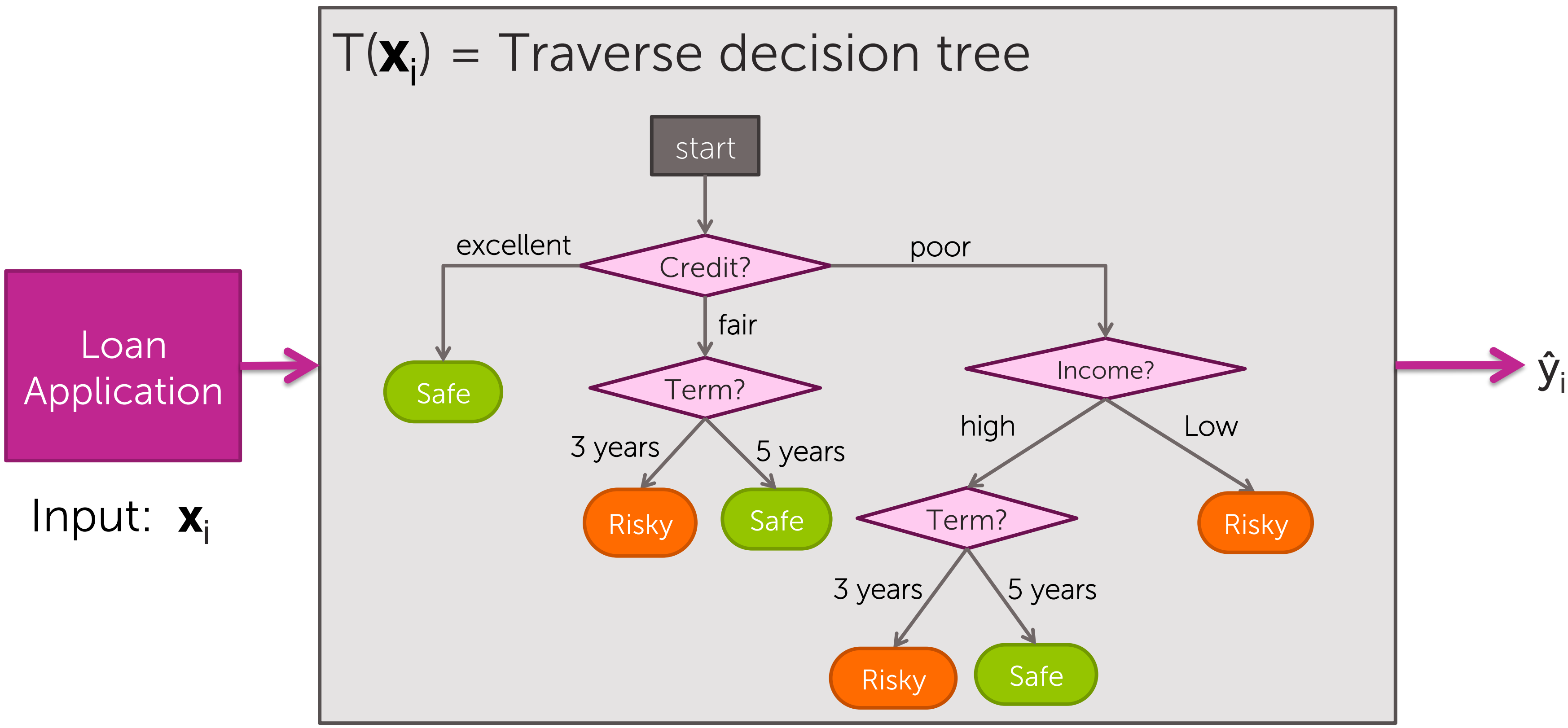
Overfitting in decision trees

Emily Fox & Carlos Guestrin
Machine Learning Specialization
University of Washington

Review of loan default prediction

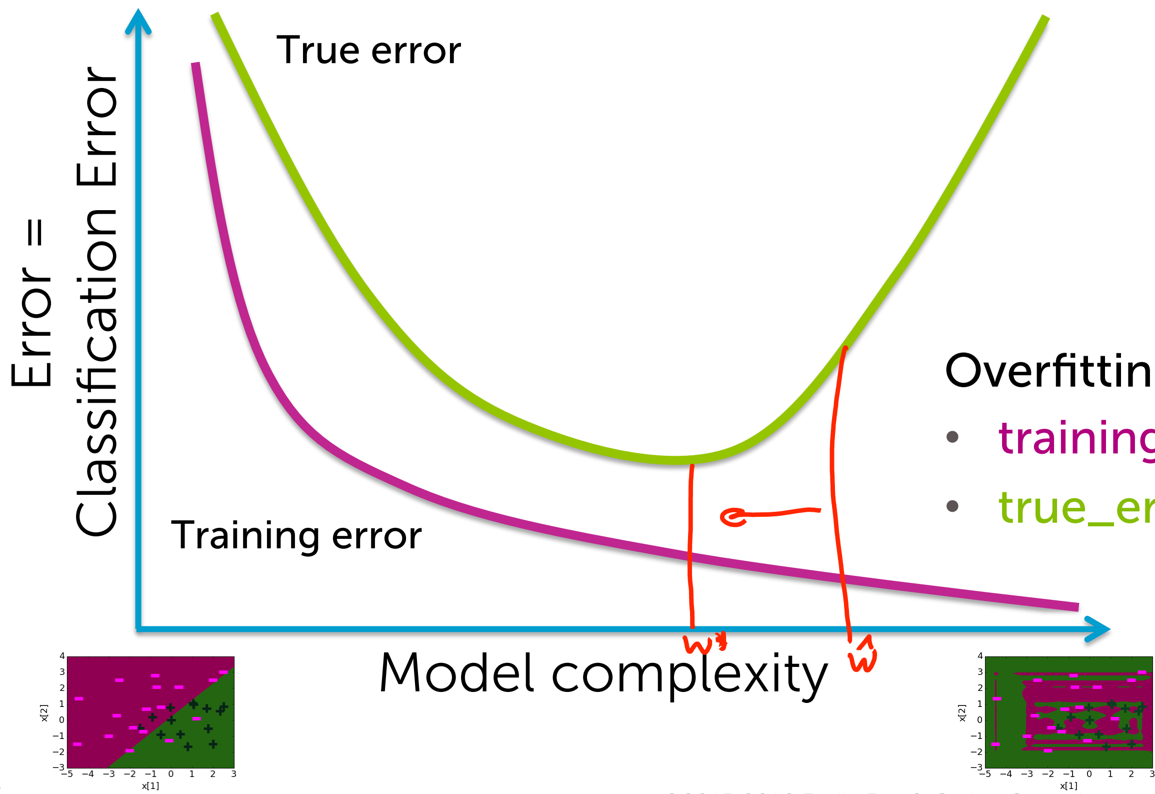
Decision tree review



Input: $\mathbf{x}_i$

Overfitting review

Overfitting in logistic regression



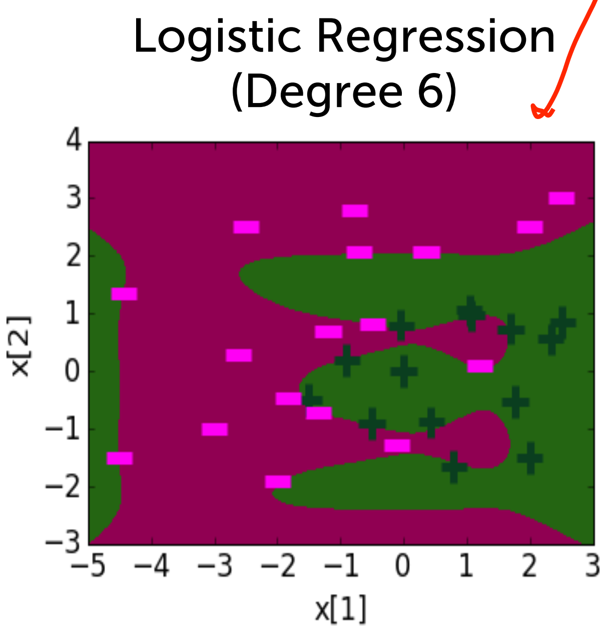
Overfitting if there exists **w***:

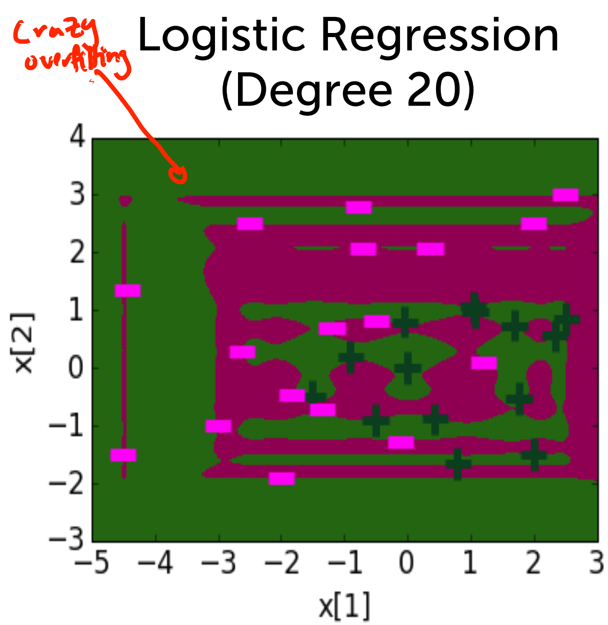
- training_error(**w***) > training_error(**ŵ**)
- true_error(**w***) < true_error(**ŵ**)

Overfitting → Overconfident predictions

bad overfitting

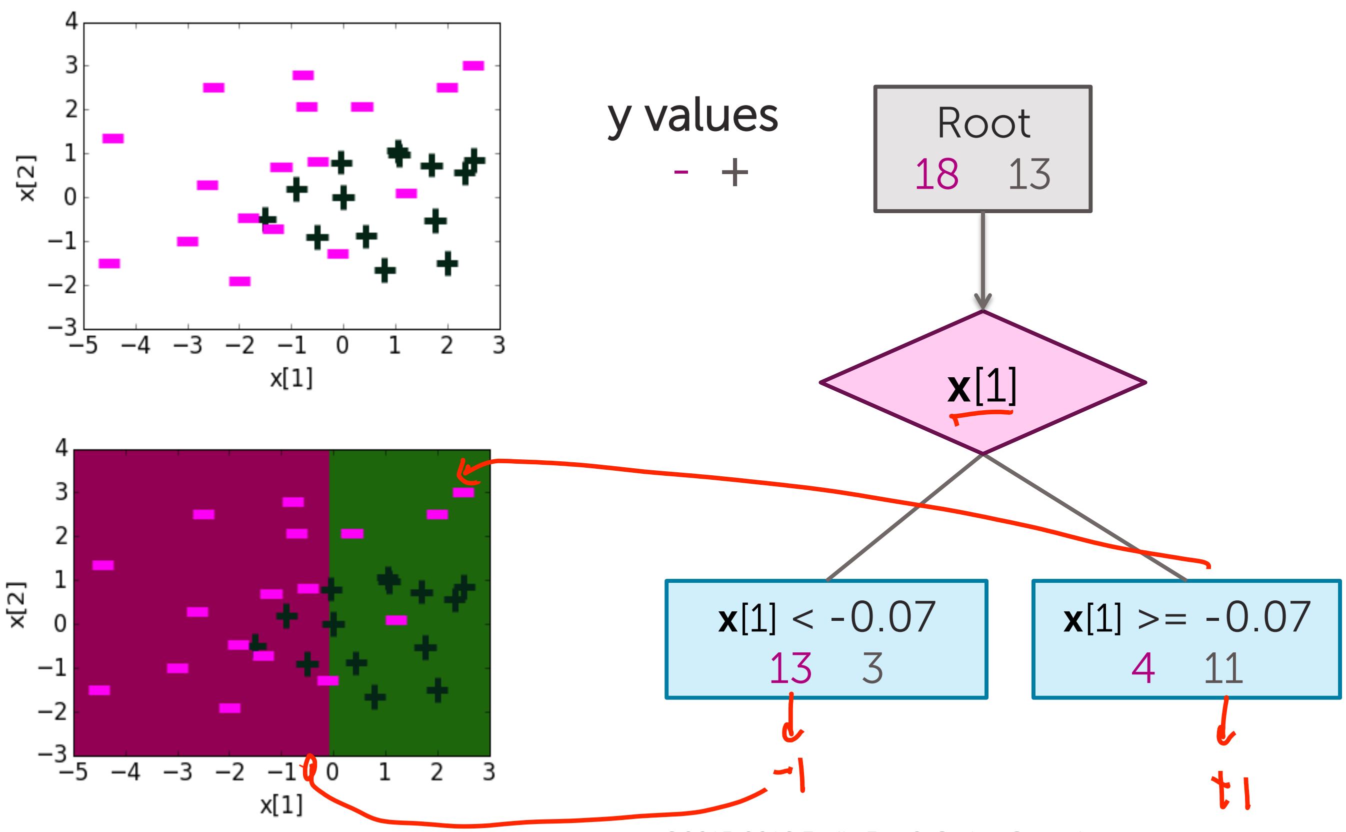
crazy overfitting





Overfitting in decision trees

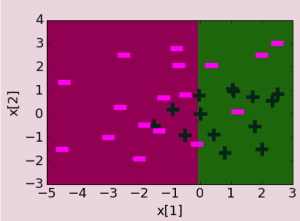
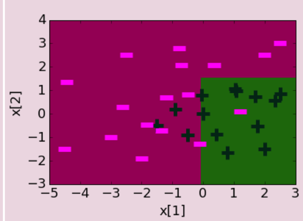
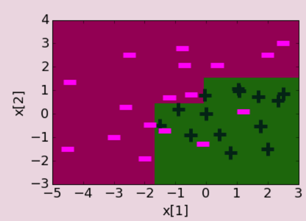
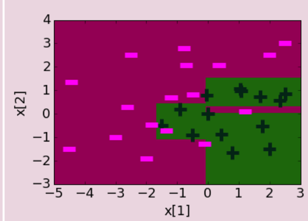
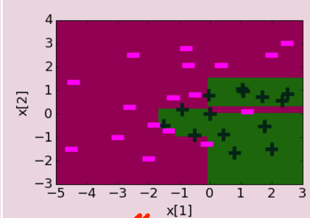
Decision stump (Depth 1): Split on **x**[1]



What happens when we increase depth?

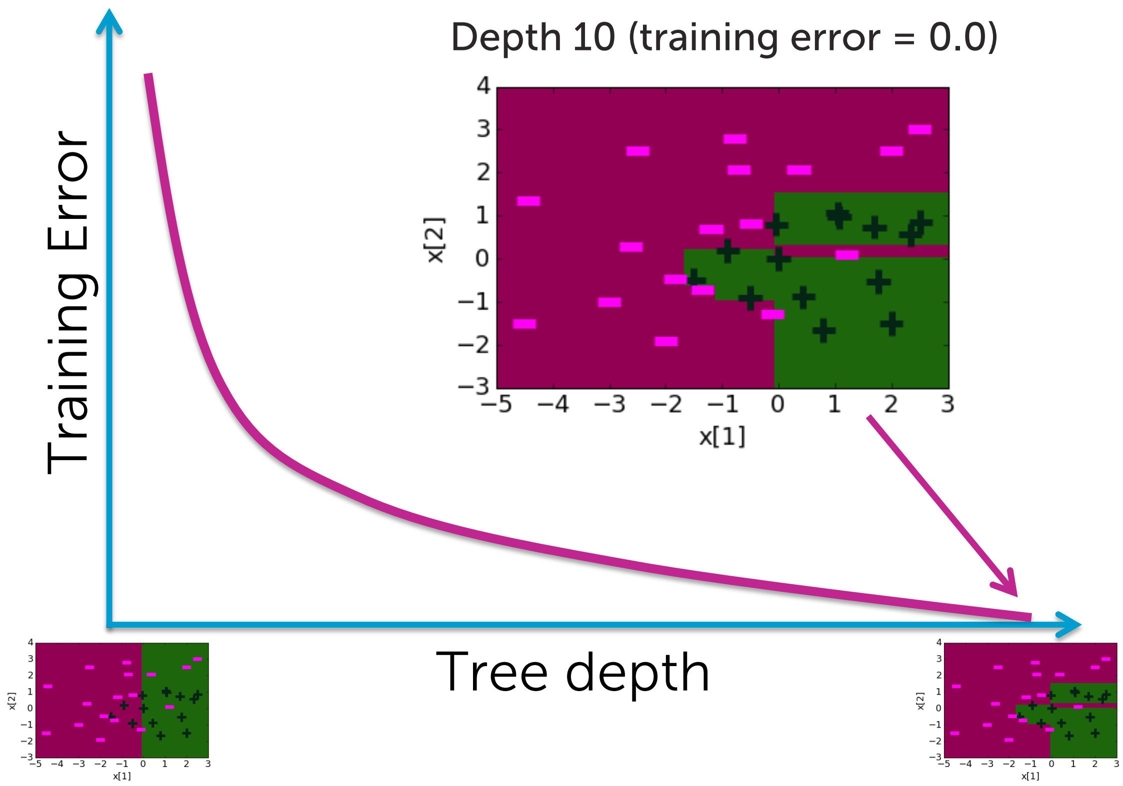
Training error reduces with depth

Big warning!!

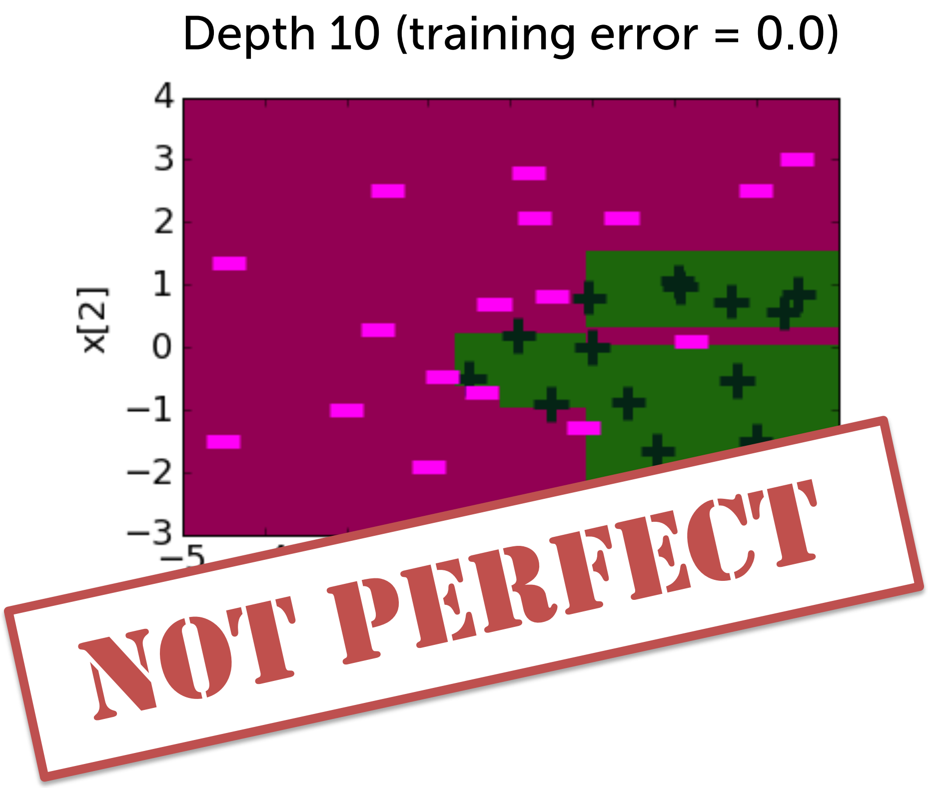
Tree depth	depth = 1	depth = 2	depth = 3	depth = 5	depth = 10
Training error	0.22	0.13	0.10	0.03	0.00
Decision boundary					

complexity of decision boundary

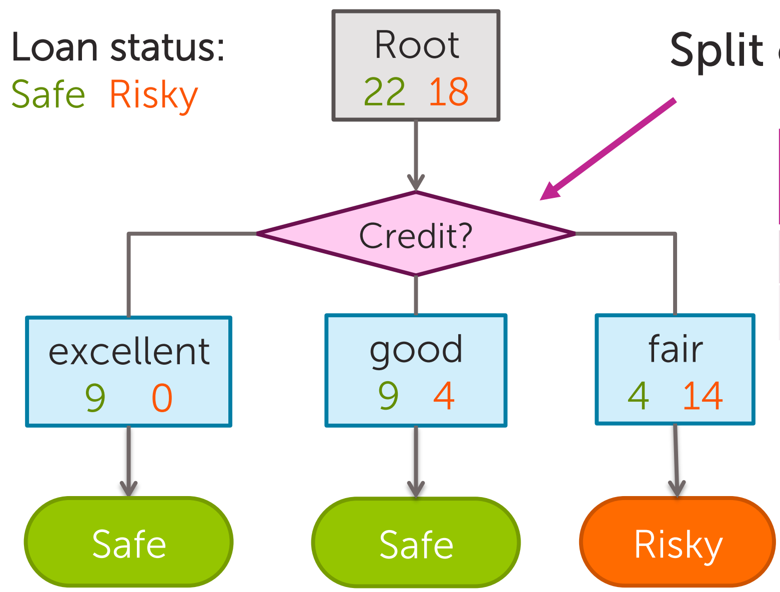
Deeper trees ➔ lower training error



Training error = 0: Is this model perfect?



Why training error reduces with depth?



Split on **credit**

Tree	Training error
(root)	0.45
split on credit	0.20

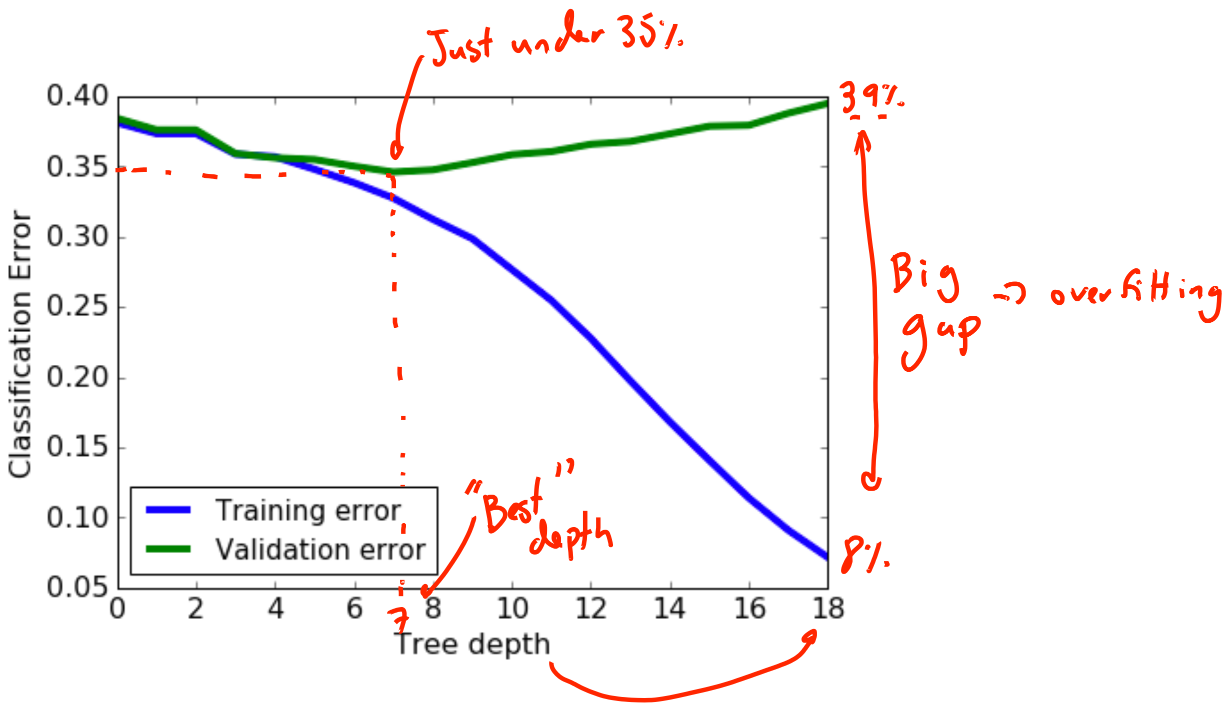
Training error improved by 0.25 because of the split

Feature split selection algorithm

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

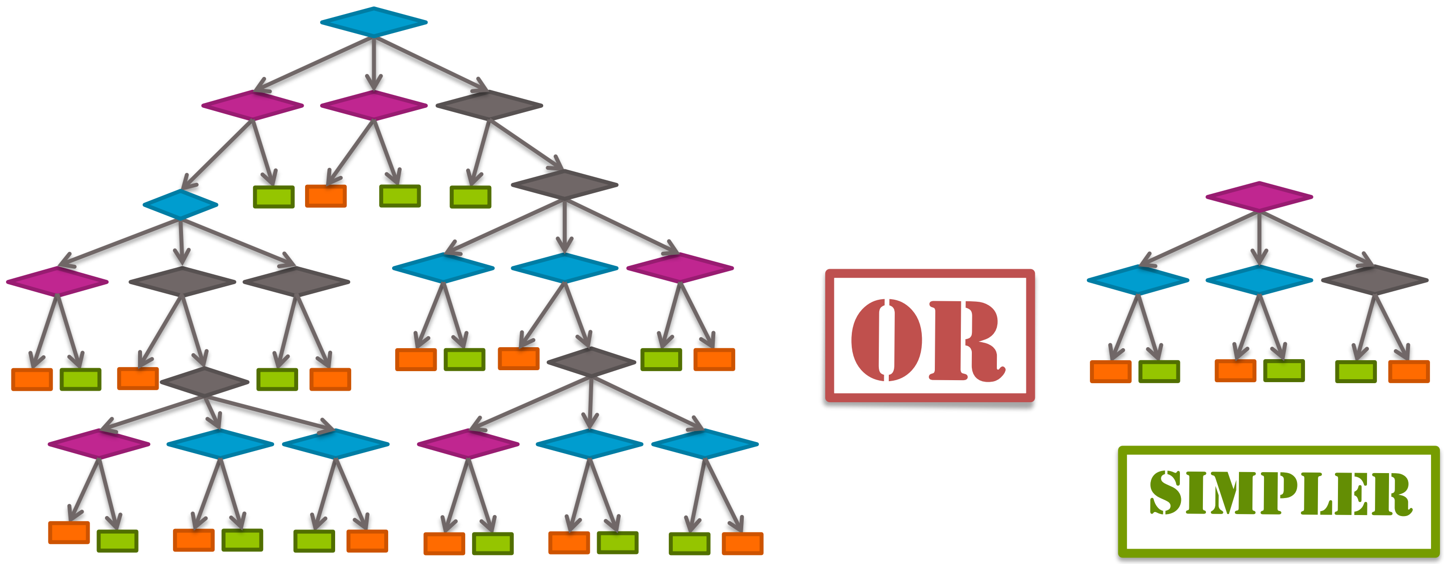
Same validation error

pick

bad!

Overfit

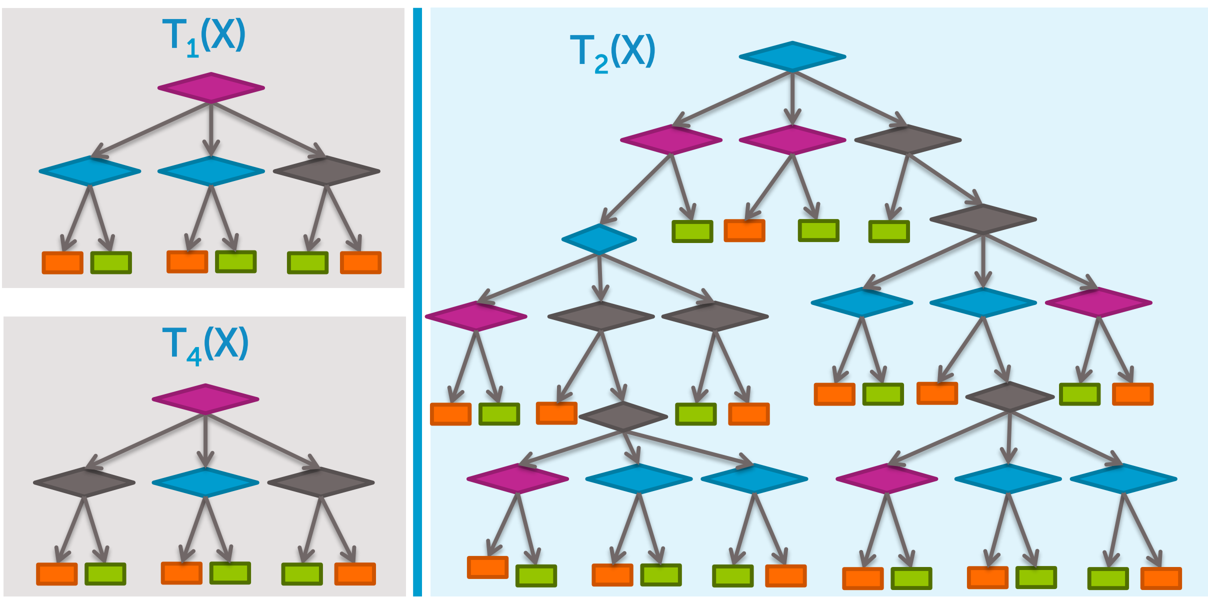
Which tree is simpler?



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

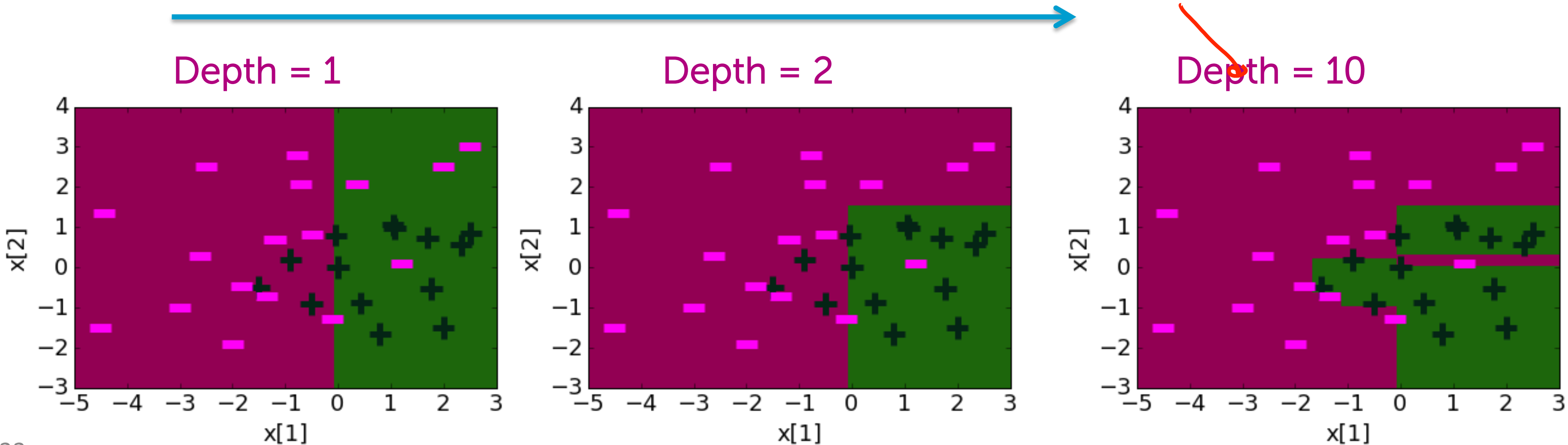
2. **Pruning:** Simplify tree **after** learning algorithm terminates

Early stopping for learning decision trees

Deeper trees → Increasing complexity

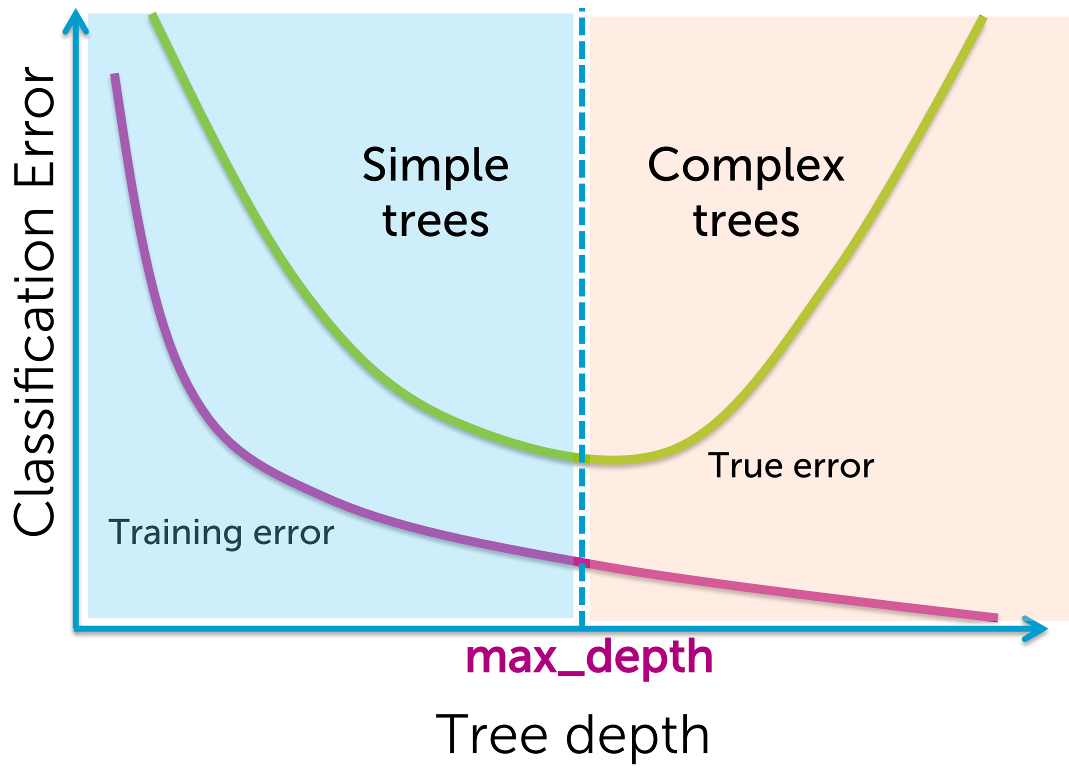
Model complexity increases with depth

avoid

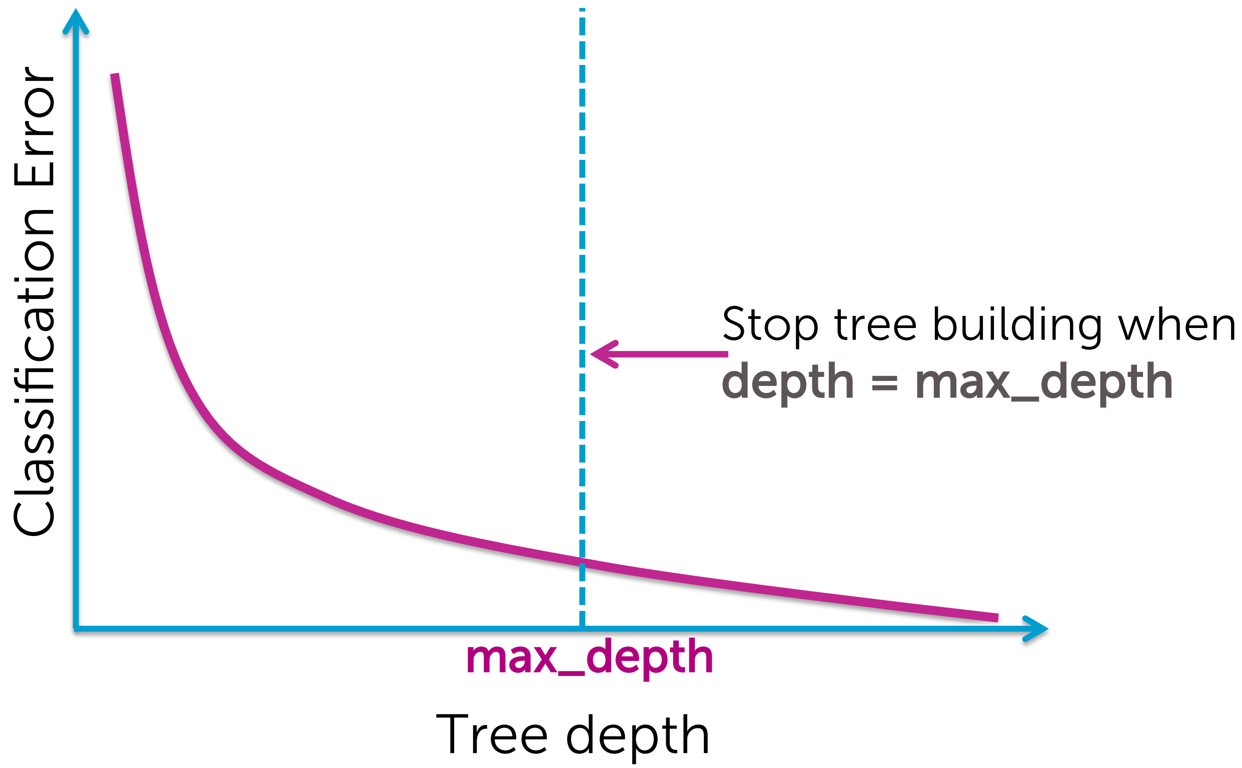


Early stopping condition 1: *Limit the depth of a tree*

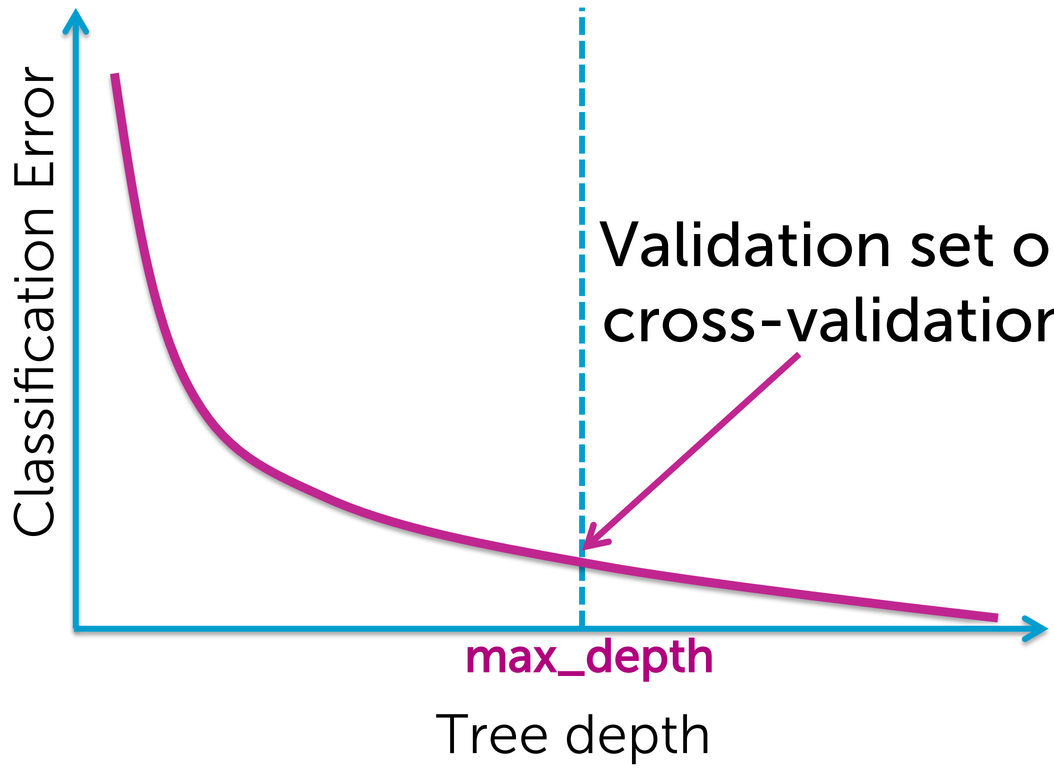
Restrict tree learning to shallow trees?



Early stopping condition 1: Limit depth of tree

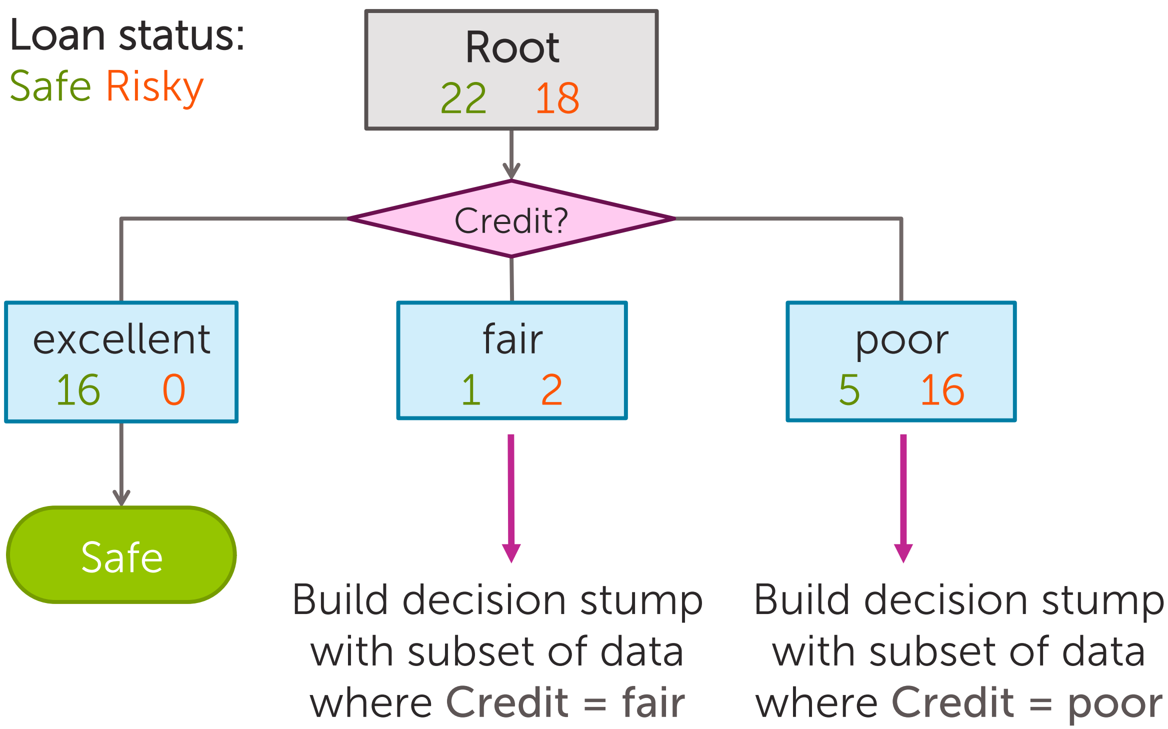


Picking value for max_depth???

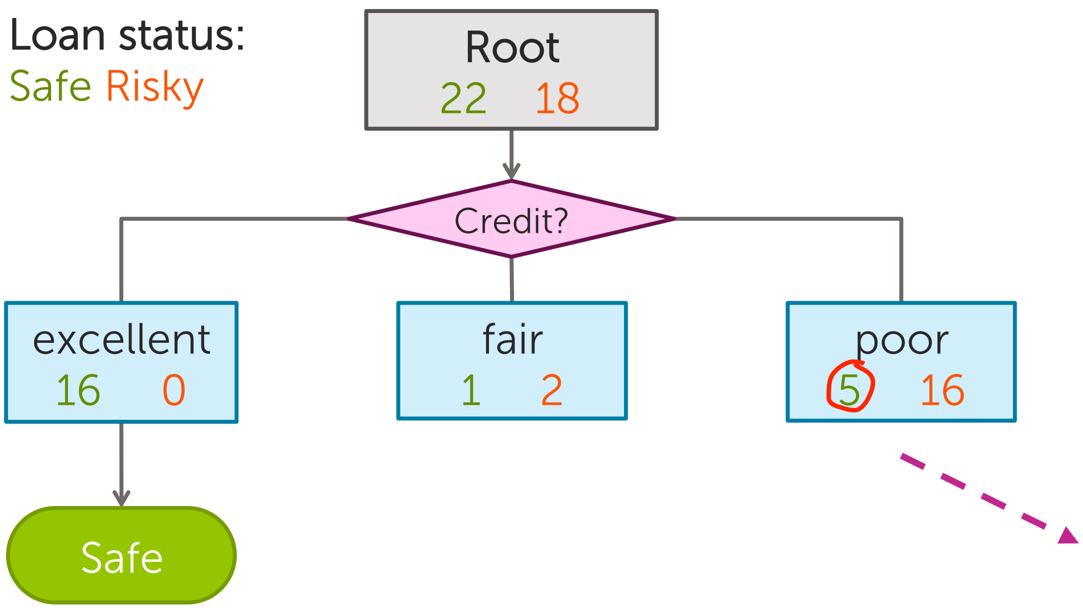


Early stopping condition 2: *Use classification error to limit depth of tree*

Decision tree recursion review



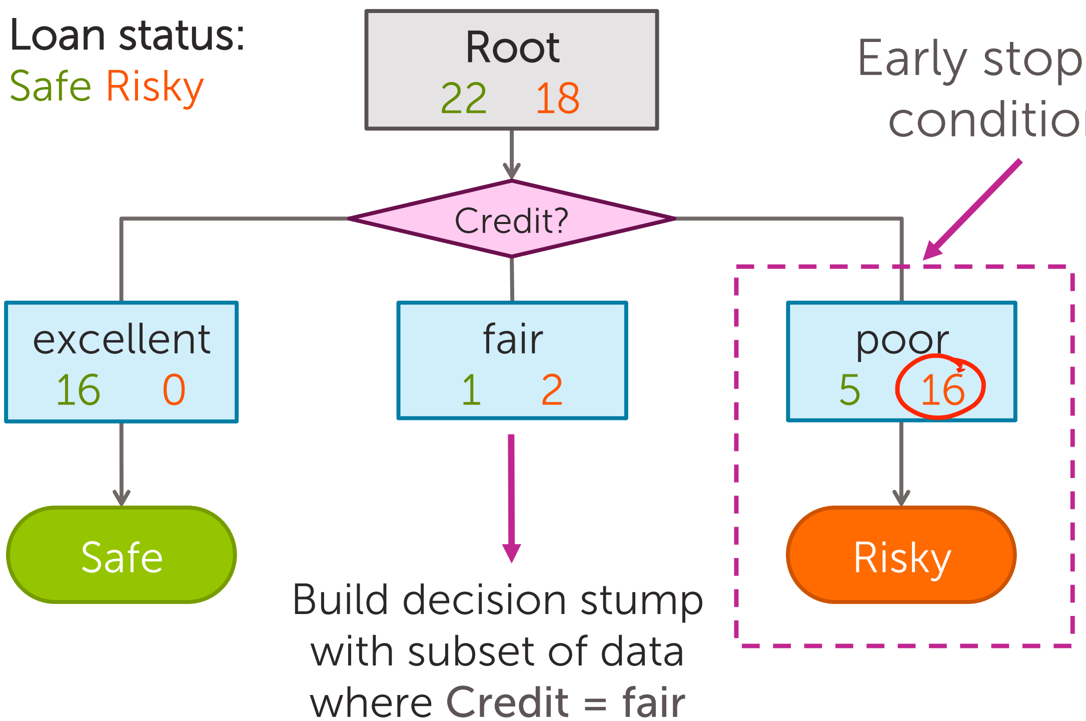
Split selection for credit=poor



No split improves classification error
➔ Stop!

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

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

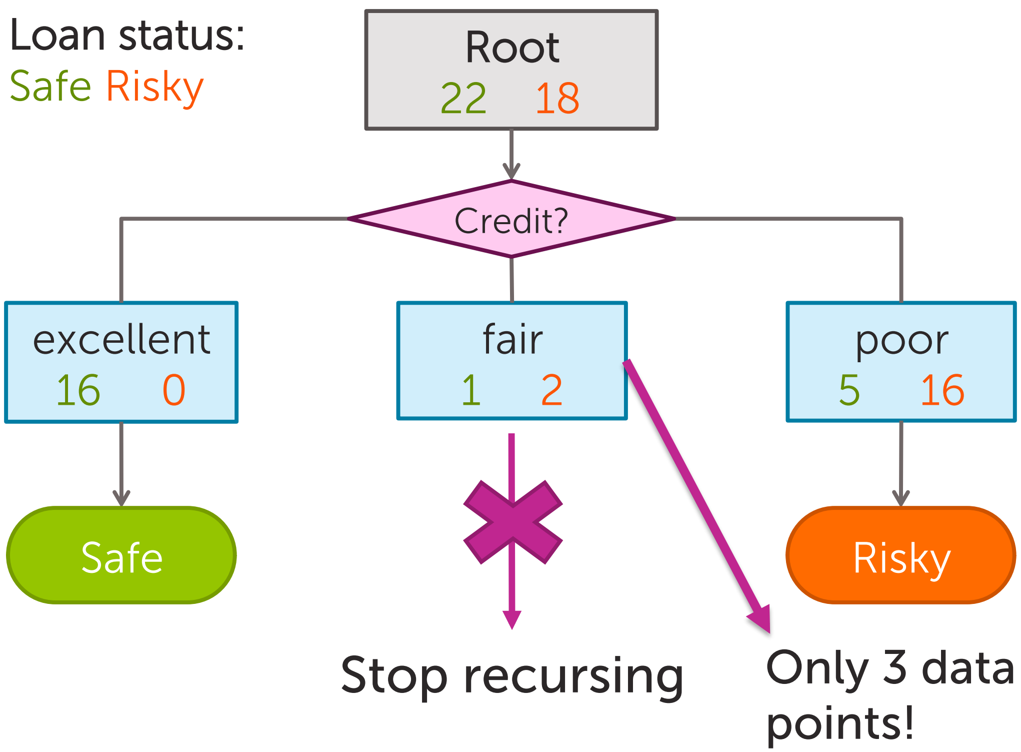
1. Typically, add magic parameter **ε**
   – Stop if error doesn't decrease by more than **ε**

2. Some pitfalls to this rule (see pruning section)

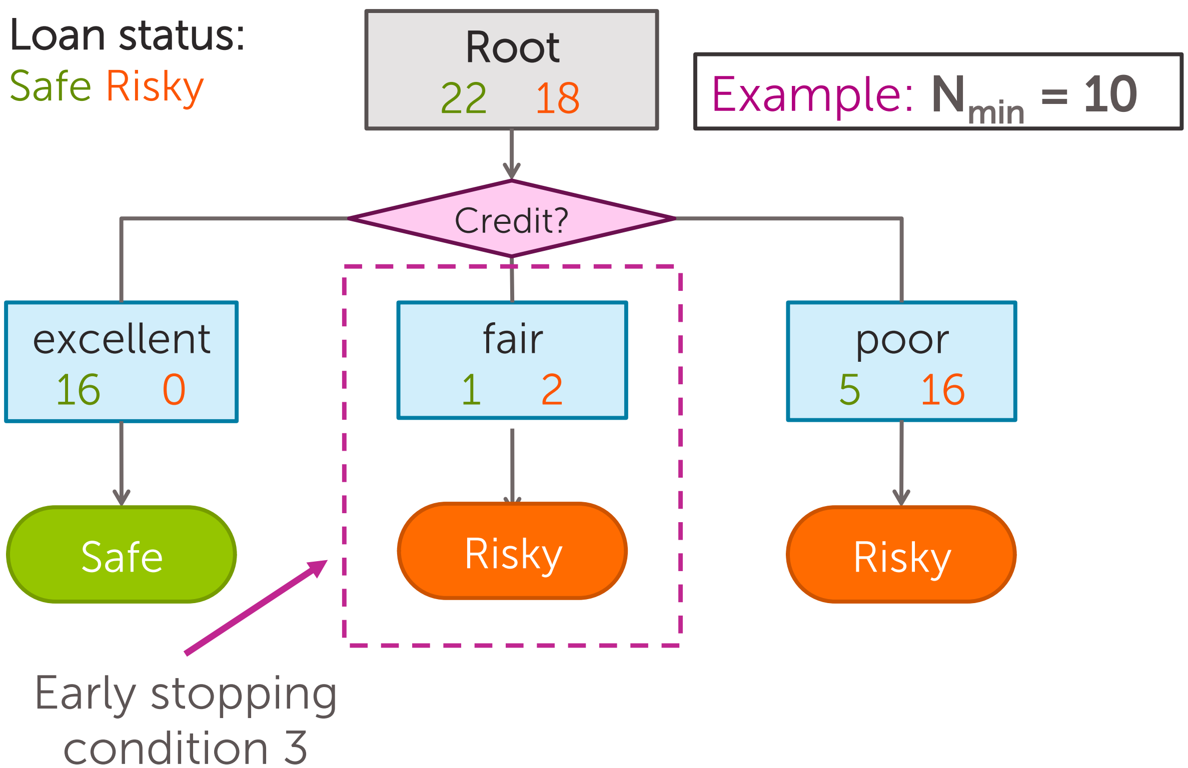
3. Very useful in practice

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 <= 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

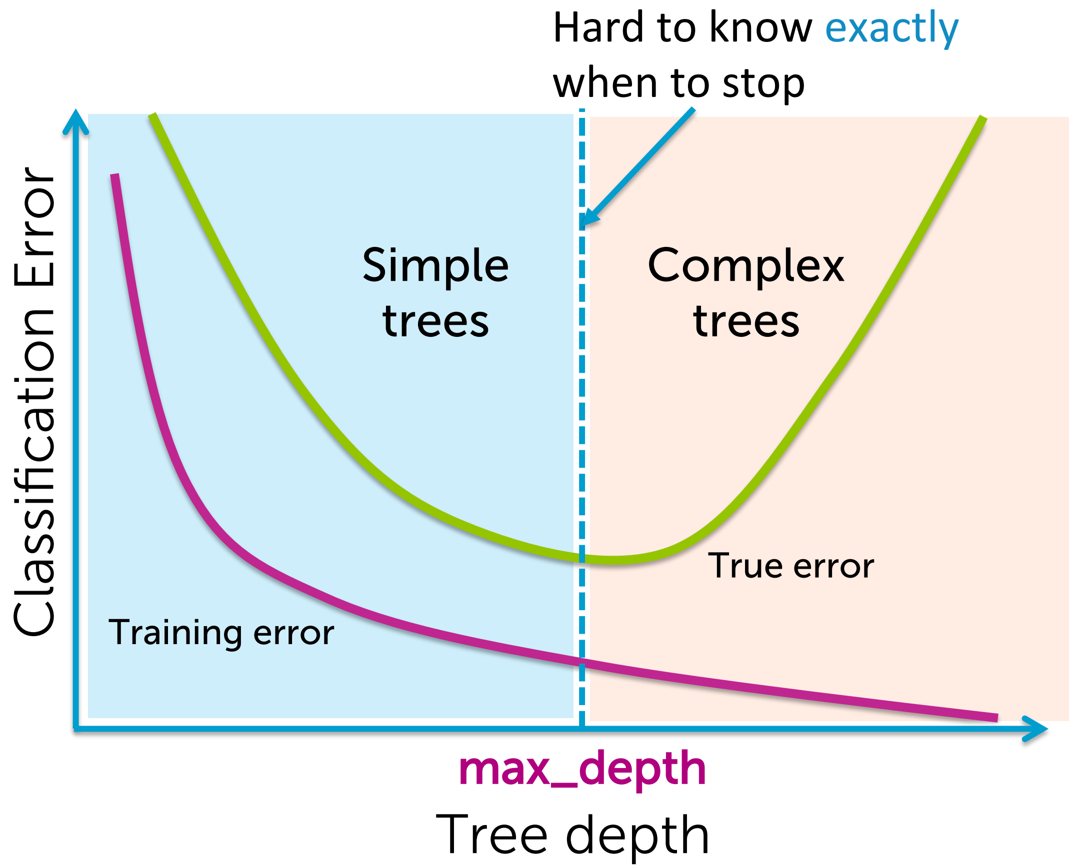
Stopping condition summary

- Stopping condition:
  1. All examples have the same target value
  2. No more features to split on

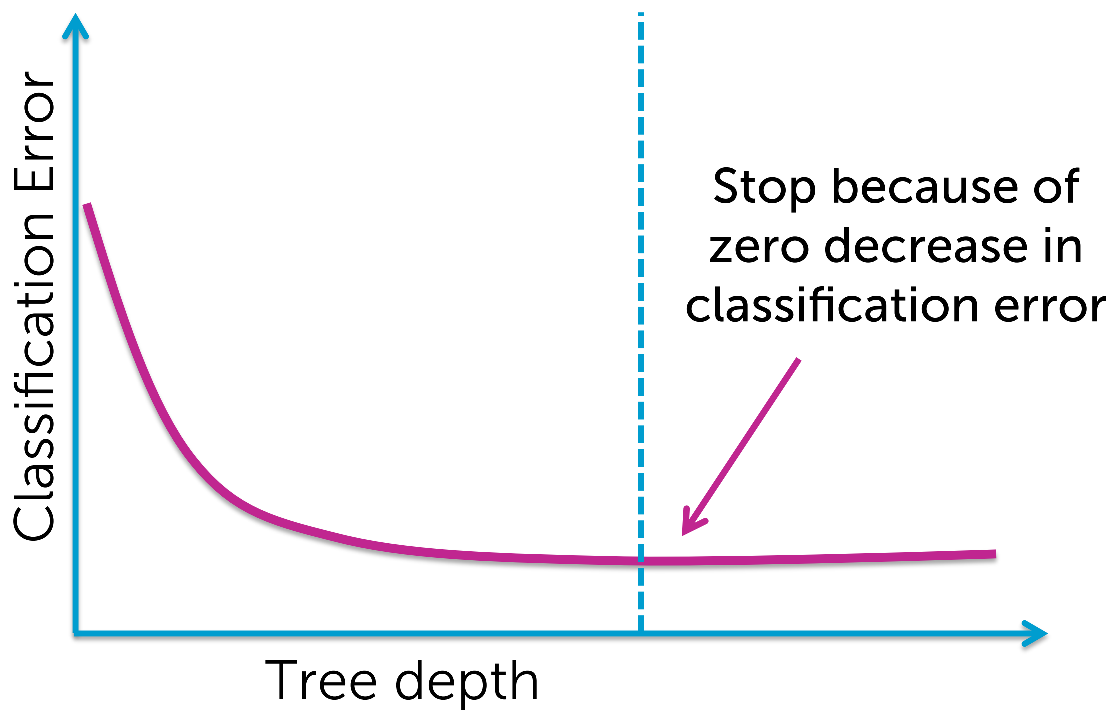
- Early stopping conditions:
  1. Limit tree depth
  2. Do not consider splits that do not cause a sufficient decrease in classification error
  3. Do not split an intermediate node which contains too few data points

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???

$y = \mathbf{x}[1]$ 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

Root
2 2

+1

mistakes

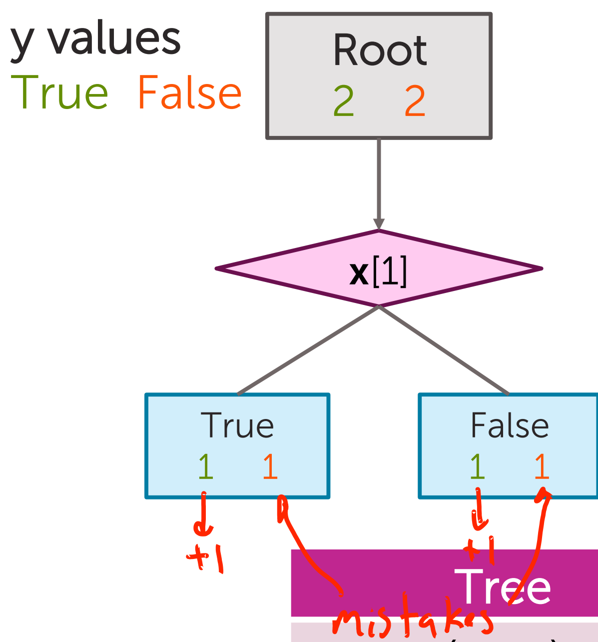
$$\text{Error} = \frac{2}{4}$$
$$= 0.5$$

Tree	Classification error
(root)	0.5

Consider split on **x**[1]

y = **x**[1] xor **x**[2]

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



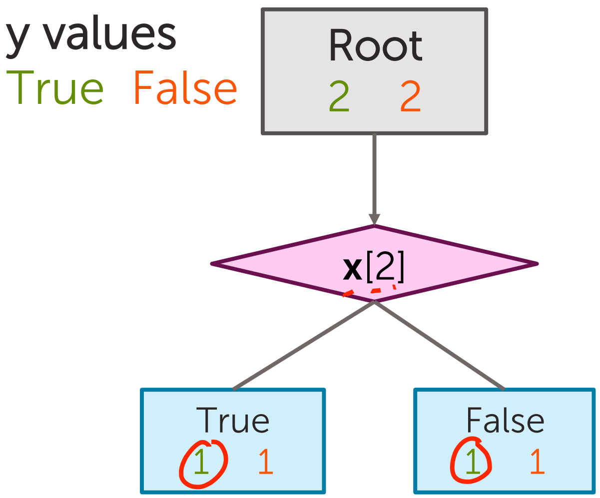
$$\text{Error} = \frac{1+1}{4}$$
$$= 0.5$$

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

Consider split on x[2]

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

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

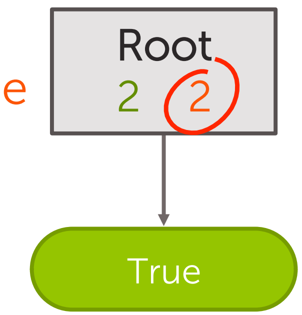
Same error

Final tree with early stopping condition 2

y = **x**[1] xor **x**[2]

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

y values
True False

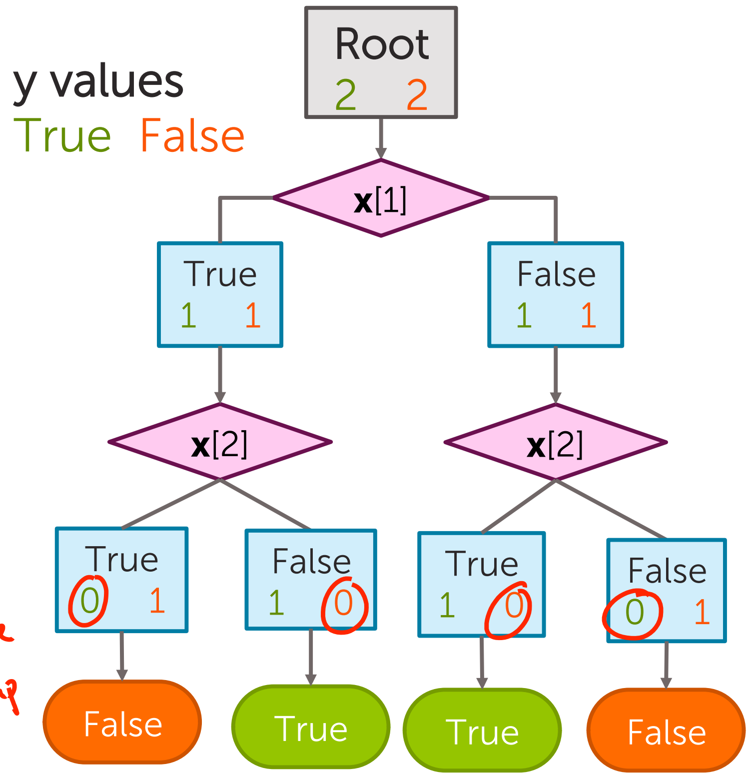


Tree	Classification error
with early stopping condition 2	0.5

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	0.0

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

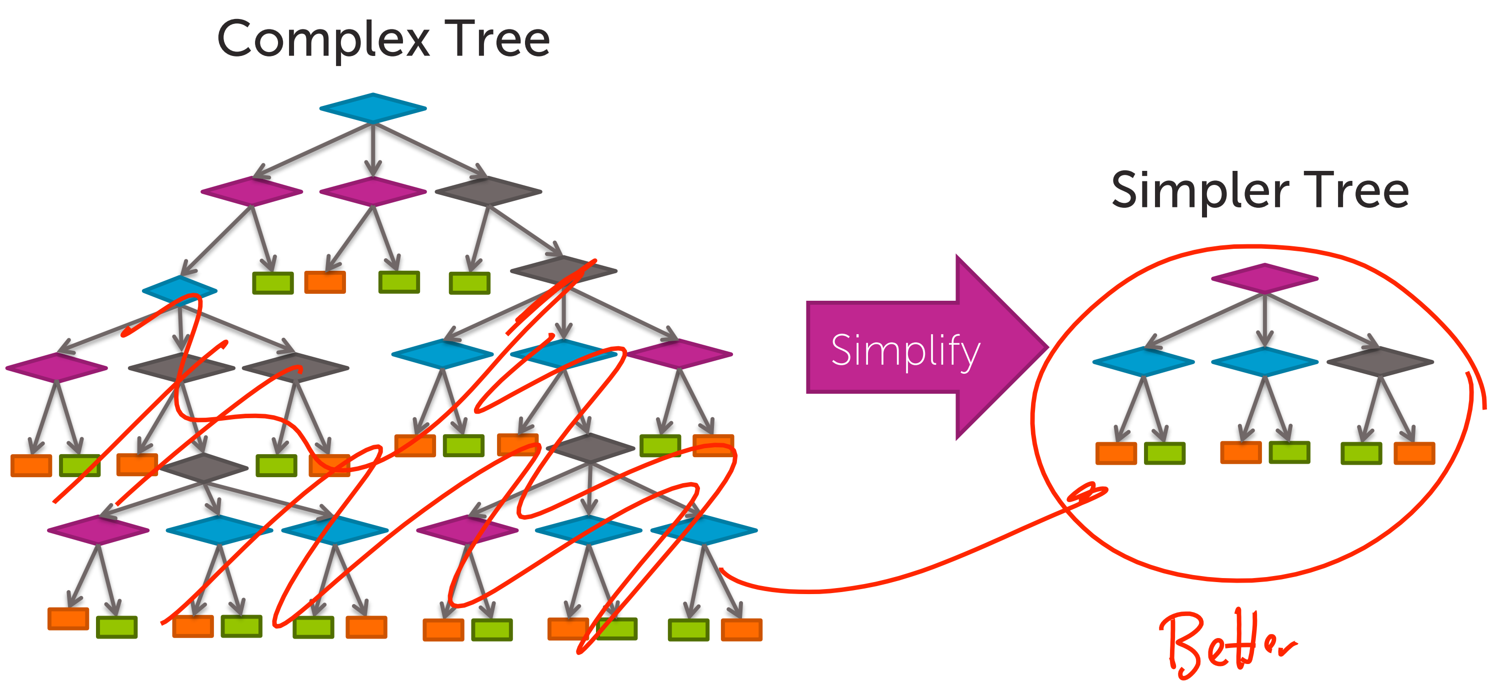
1. Early Stopping: Stop the learning algorithm **before** the tree becomes too complex

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

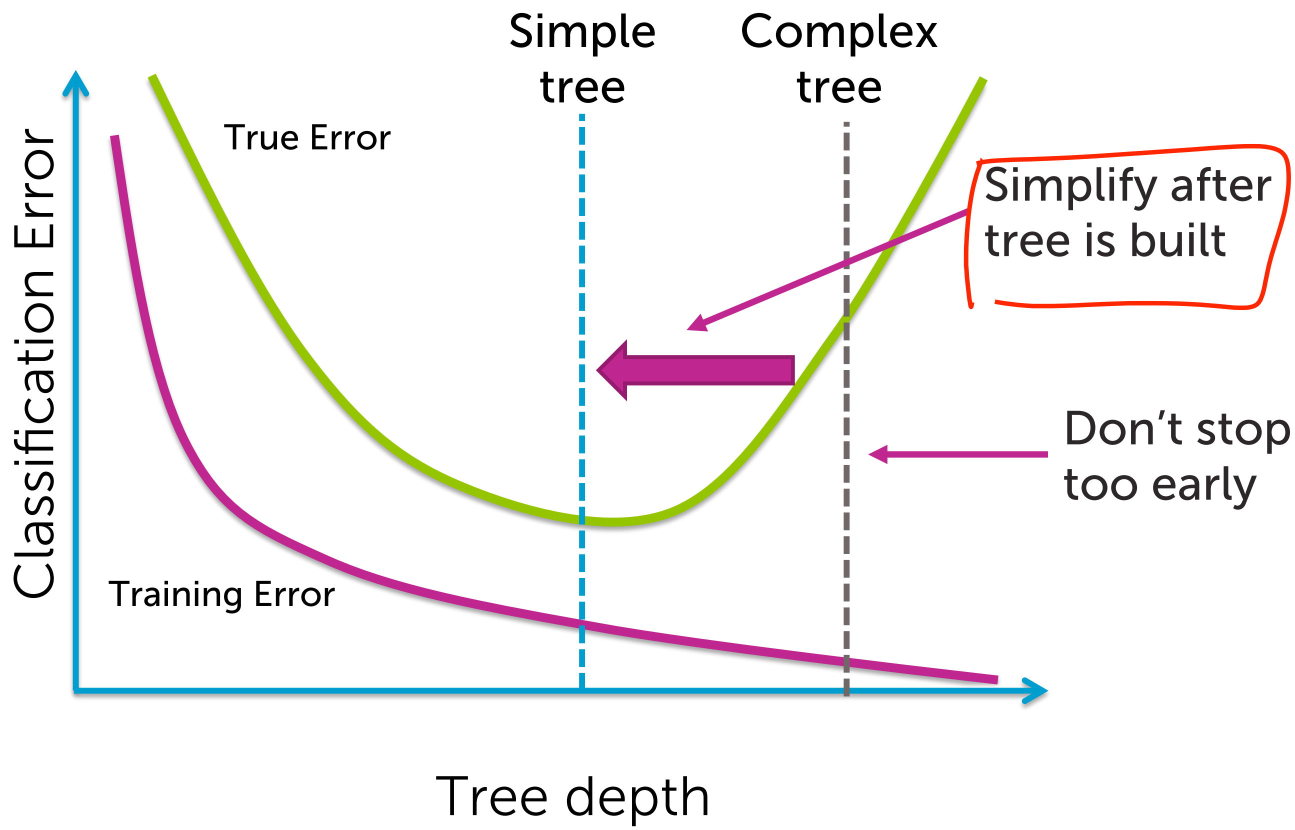
Complements early stopping

Pruning: *Intuition*

Train a complex tree, simplify later

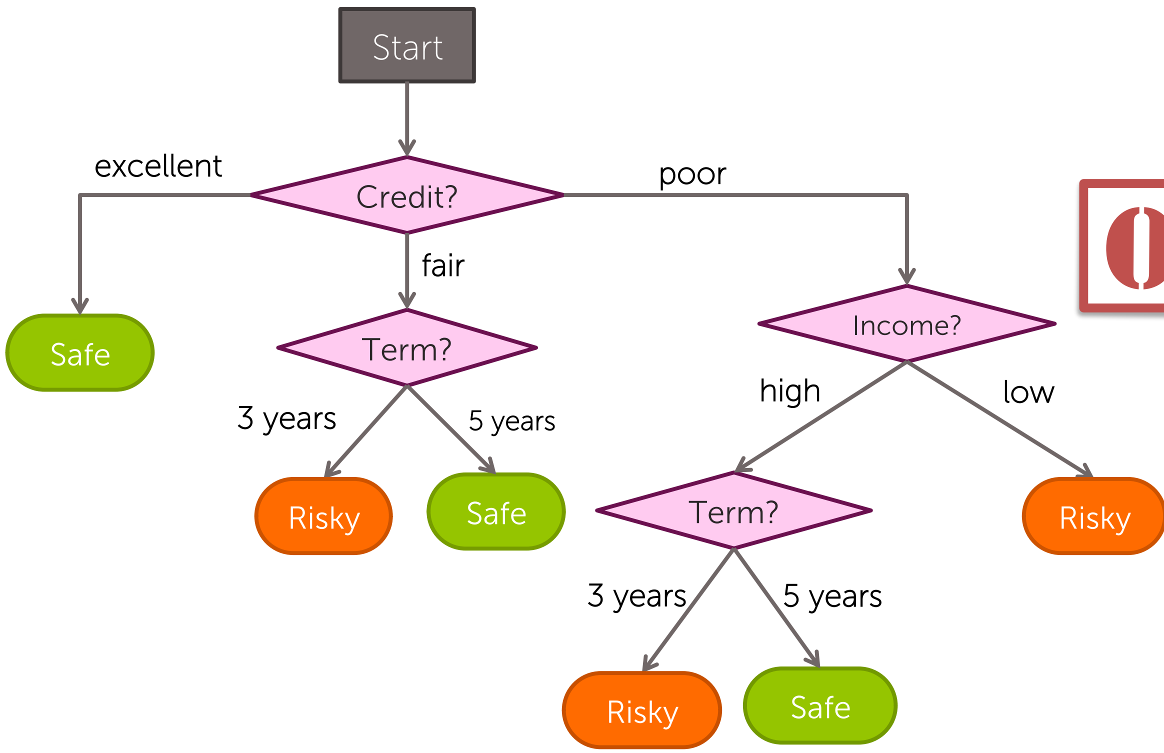


Pruning motivation

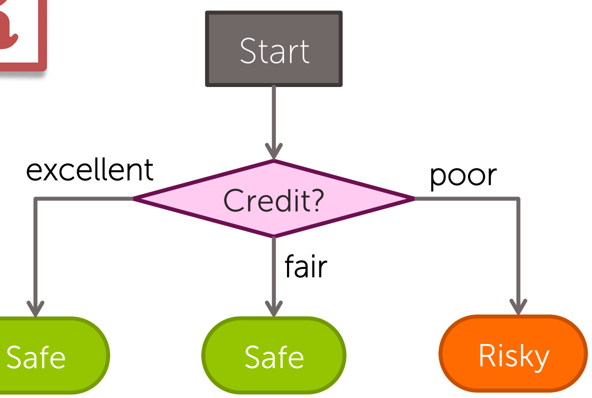


Example 1: Which tree is simpler?

Depth



OR

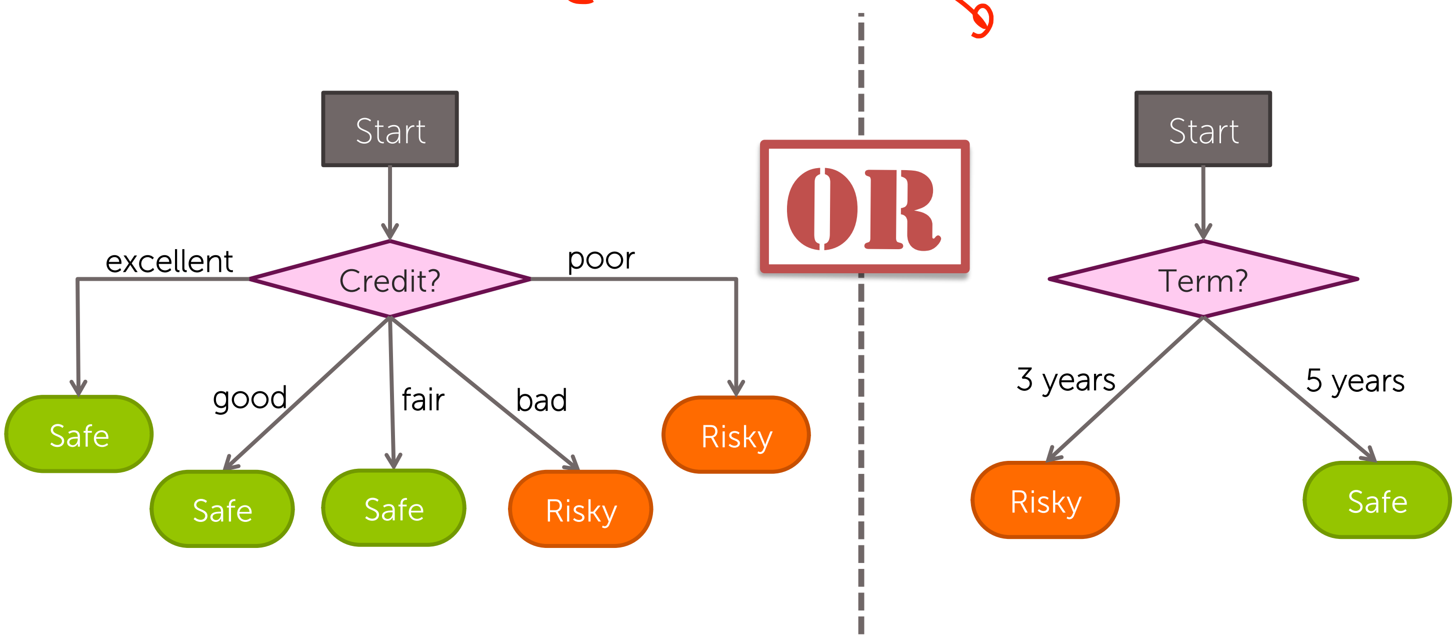


No brainer !! :)

SIMPLER

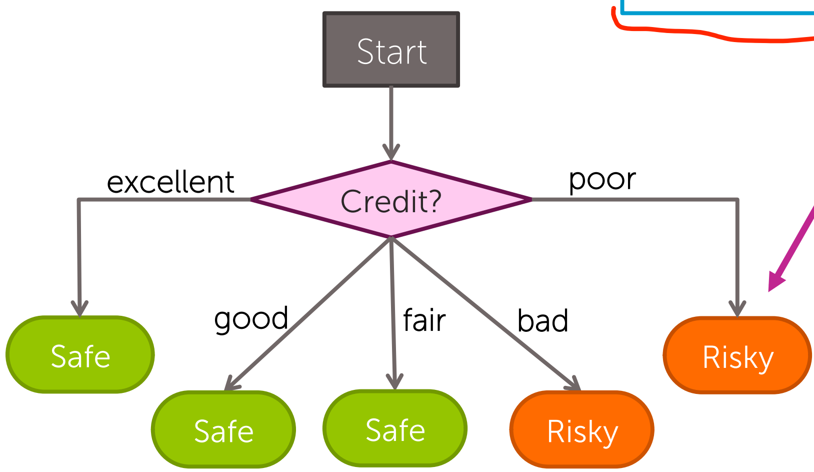
Example 2: Which tree is simpler???

Same Depth:
Simpler?

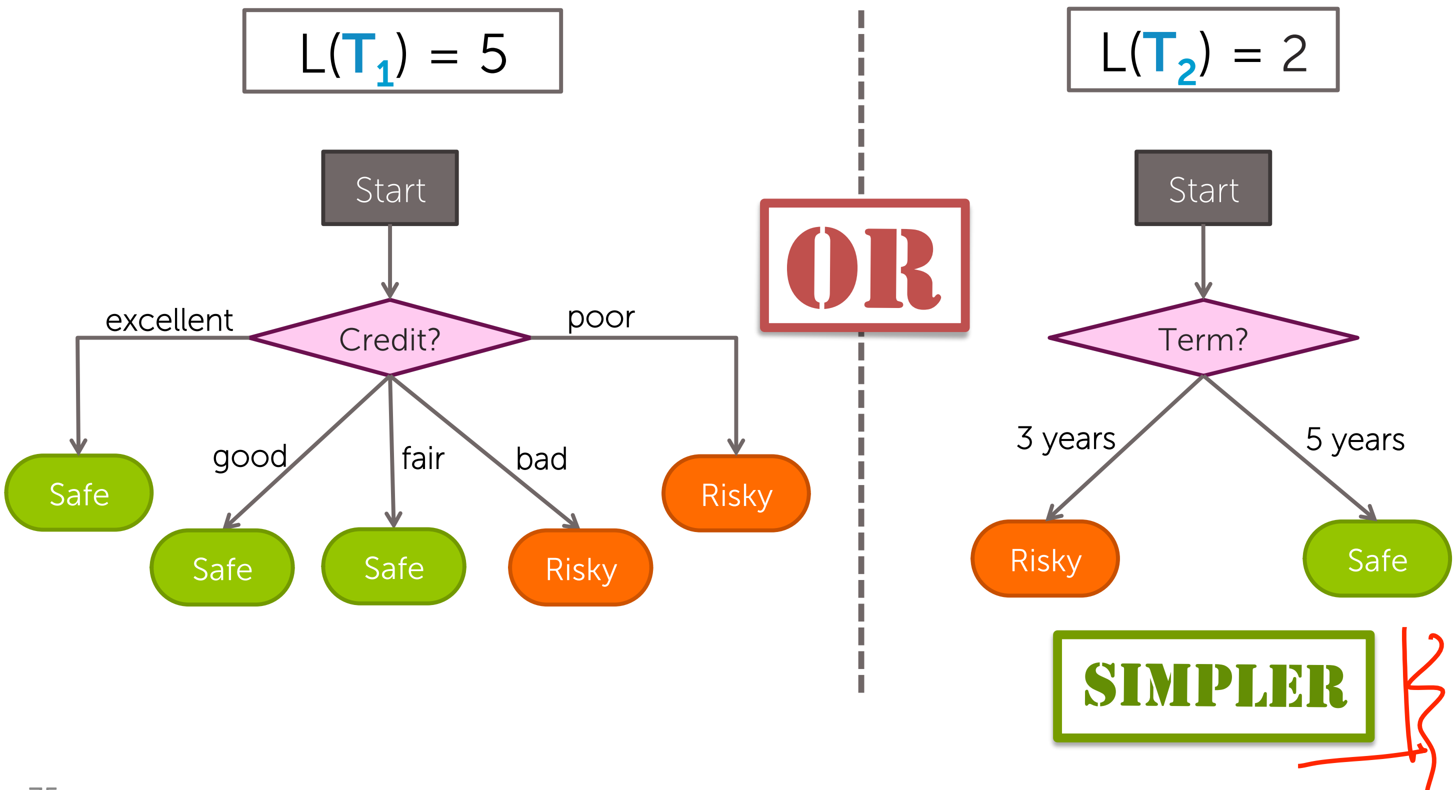


Simple measure of complexity of tree

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



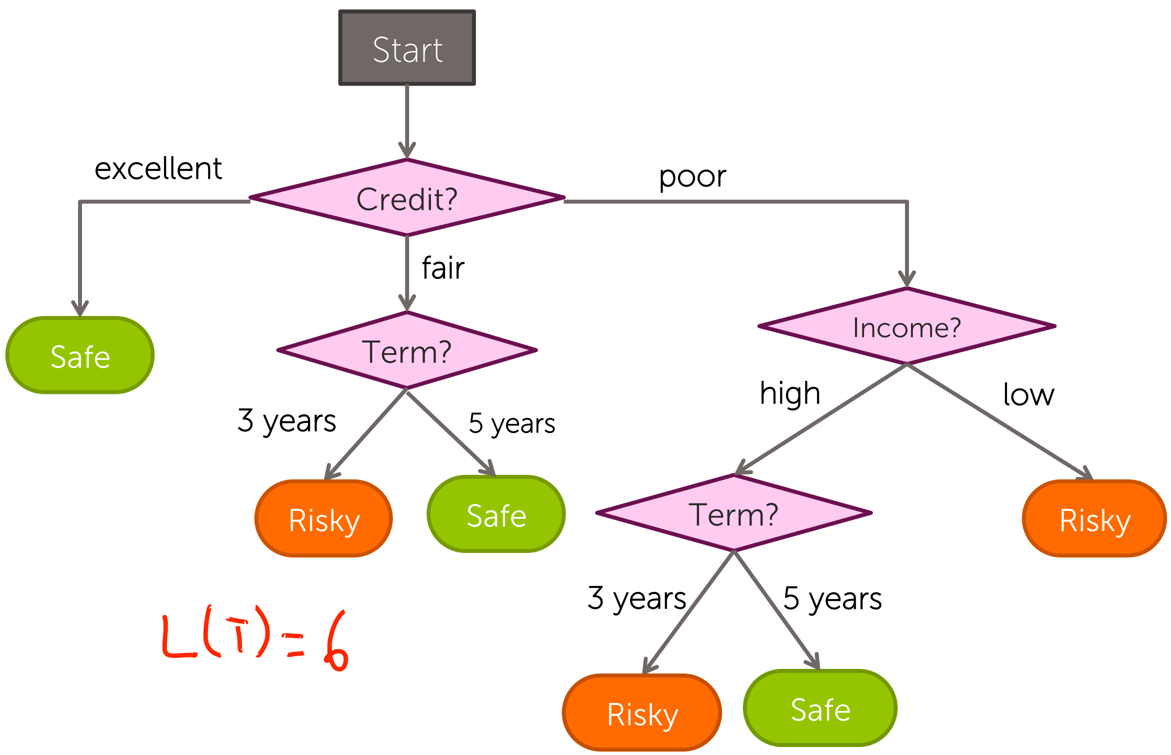
Which tree has lower L(T)?



Balance simplicity & predictive power

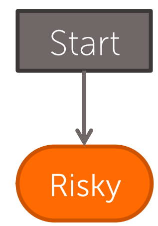
solution in between

Too complex, risk of overfitting



$L(T) = 6$

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

want to balance

Total cost =

measure of fit + measure of complexity

(classification error)
Large # = bad fit to training data

Large # = likely to overfit

Consider specific total cost

Total cost =

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

Balancing fit and complexity

Total cost C(**T**) = Error(**T**) + λ L(**T**)

tuning parameter

If λ=0:

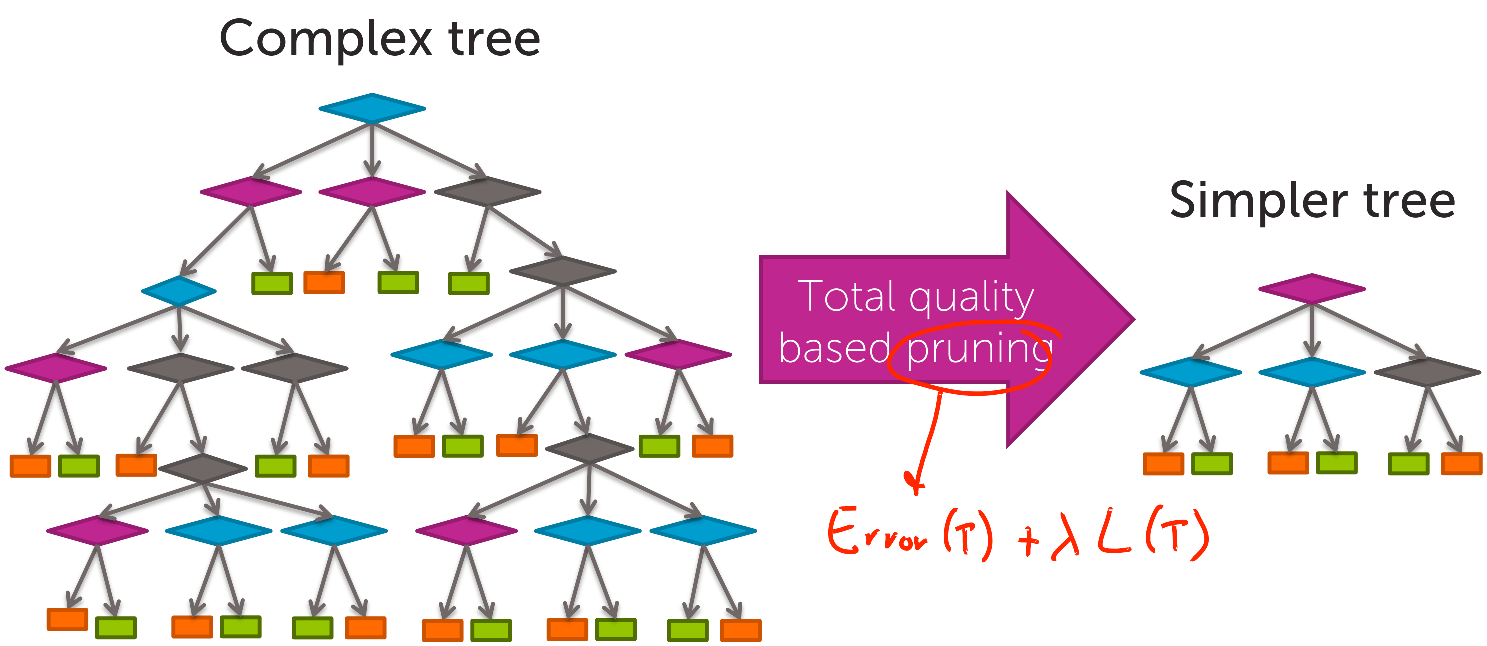
Standard decision tree learning

If λ=∞:

∞ penalty → $\boxed{\text{Root}}$ → $\hat{y}$ = Majority class

If λ in between: Balance fit & complexity

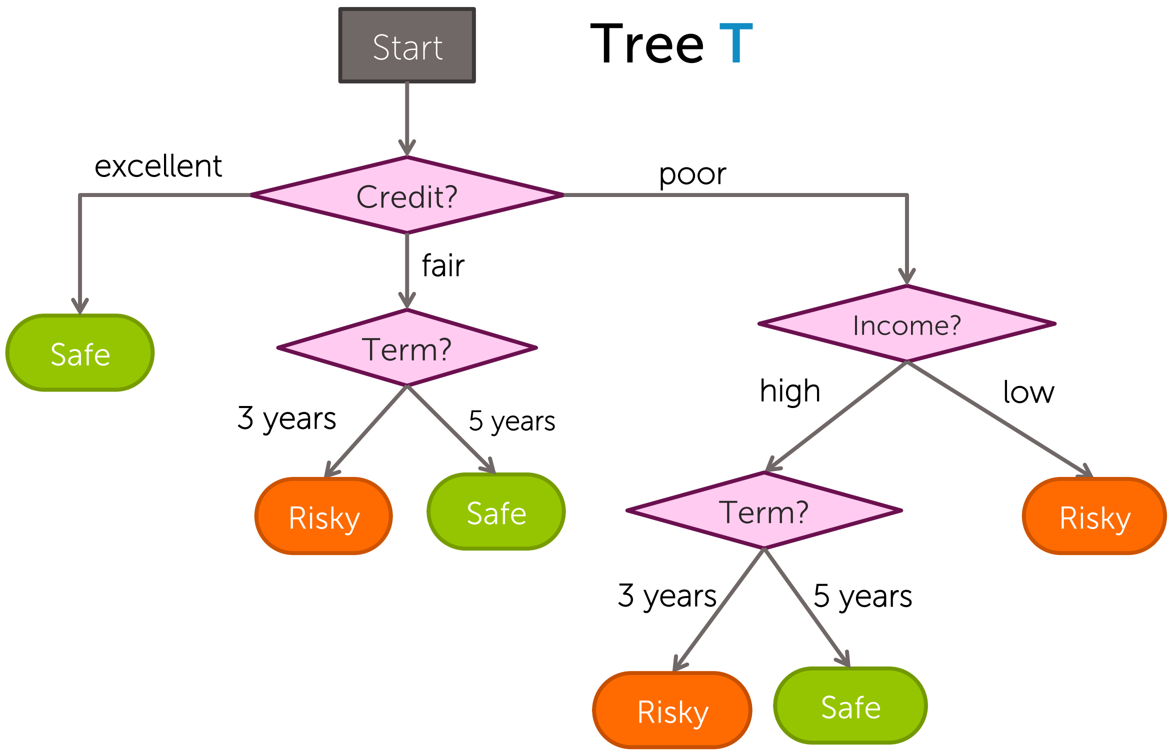
Use total cost to simplify trees



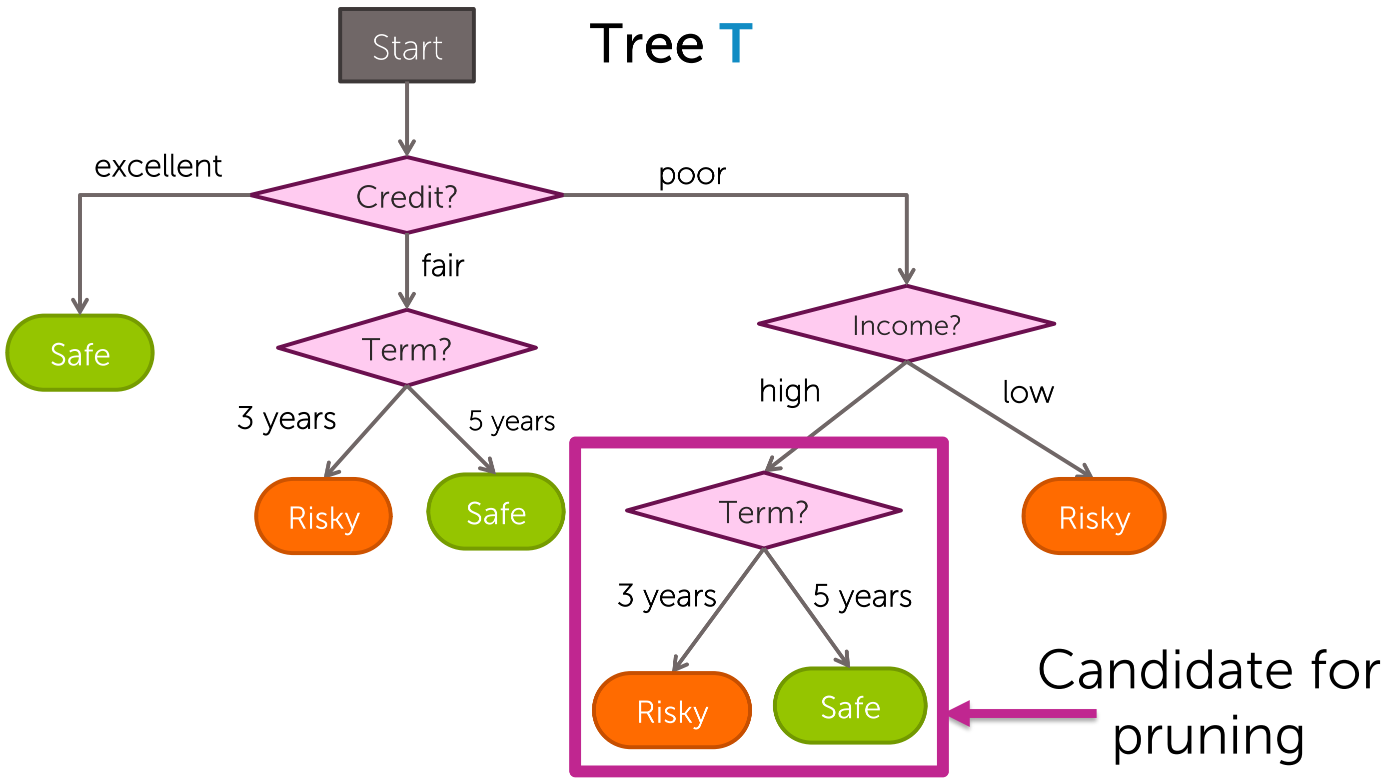
$\text{Error}(T) + \lambda L(T)$

Tree pruning algorithm

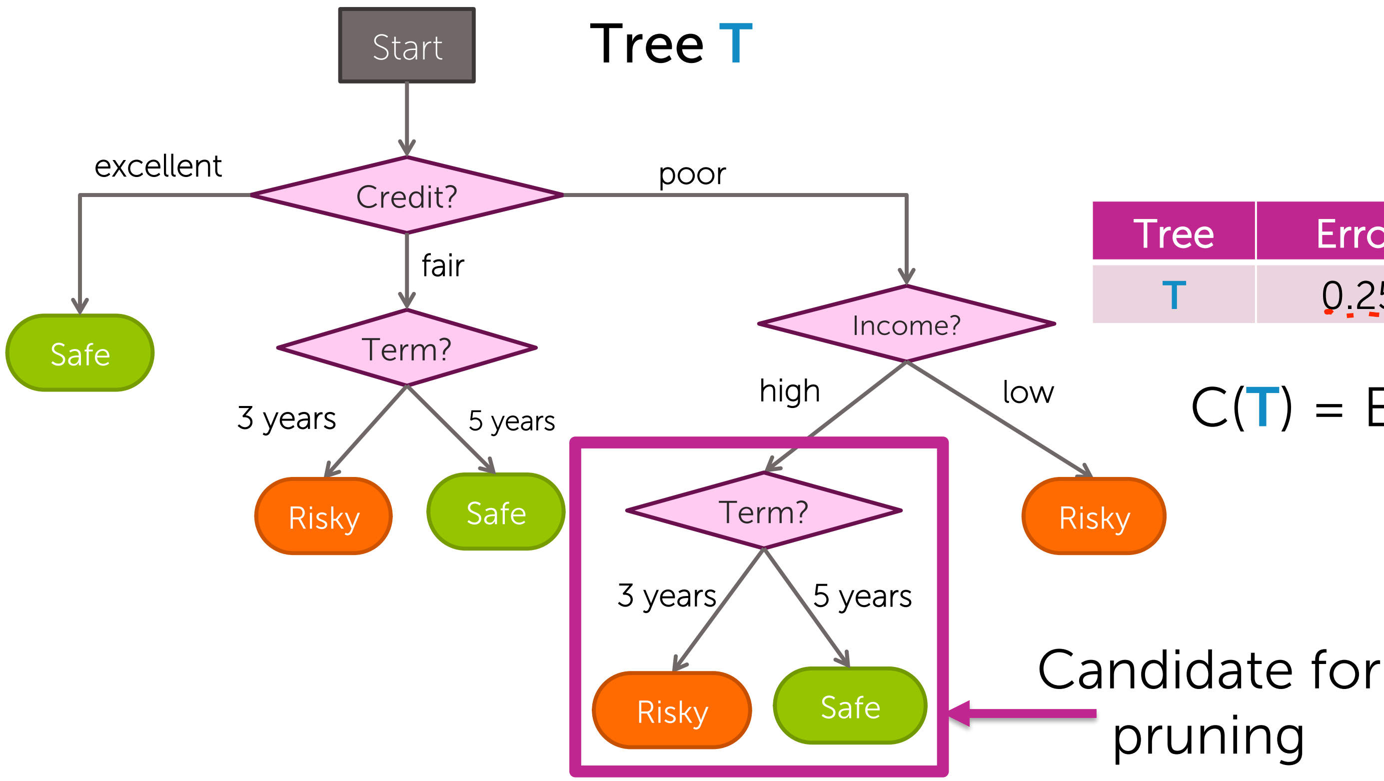
Pruning Intuition



Step 1: Consider a split



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

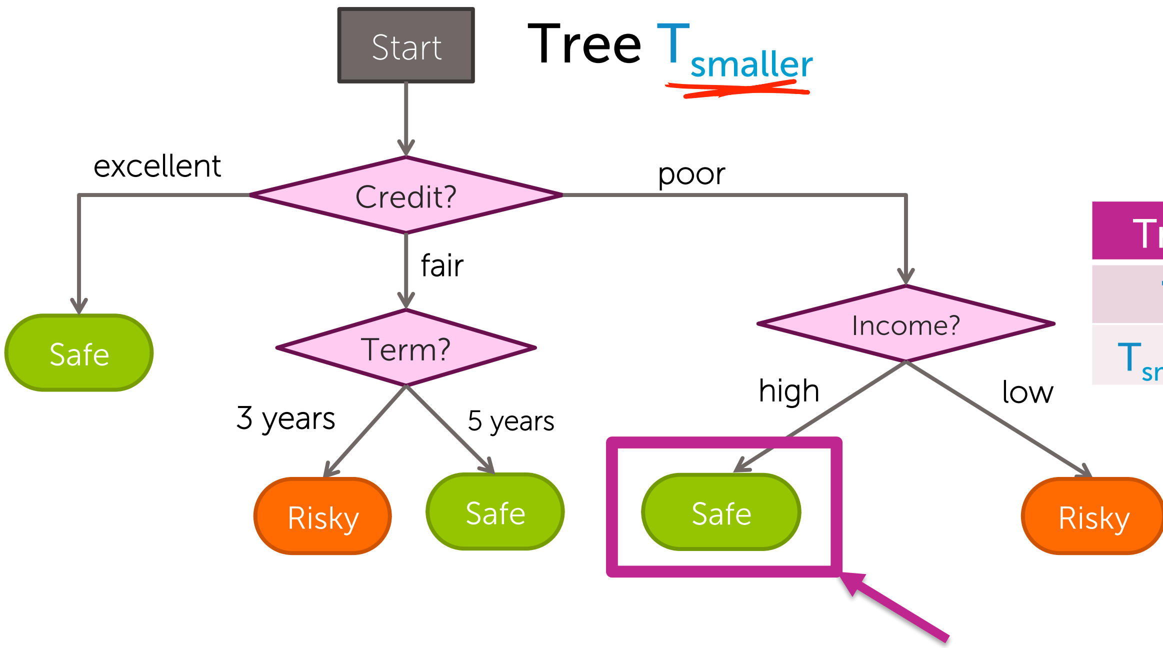


$\lambda = 0.3$

Tree	Error	#Leaves	Total
T	0.25	6	0.43

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

Step 2: "Undo" the splits on $T_{smaller}$



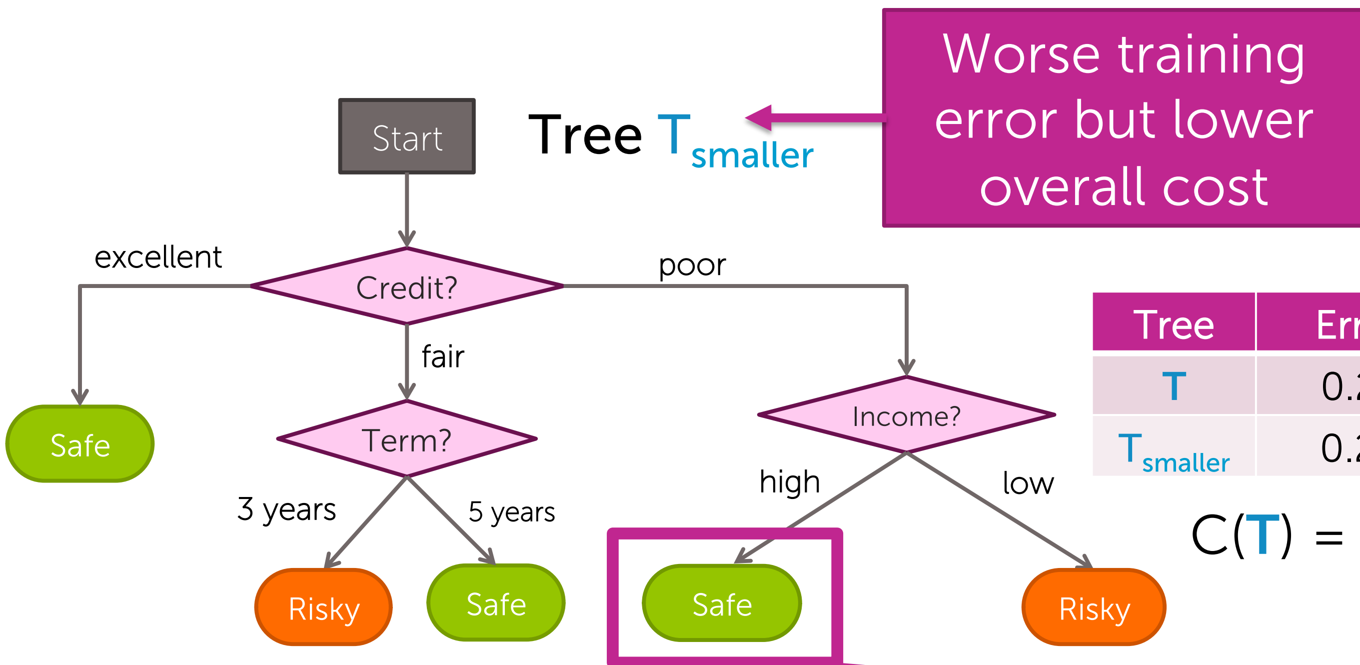
Replace split by leaf node?

$\lambda = 0.3$

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

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

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



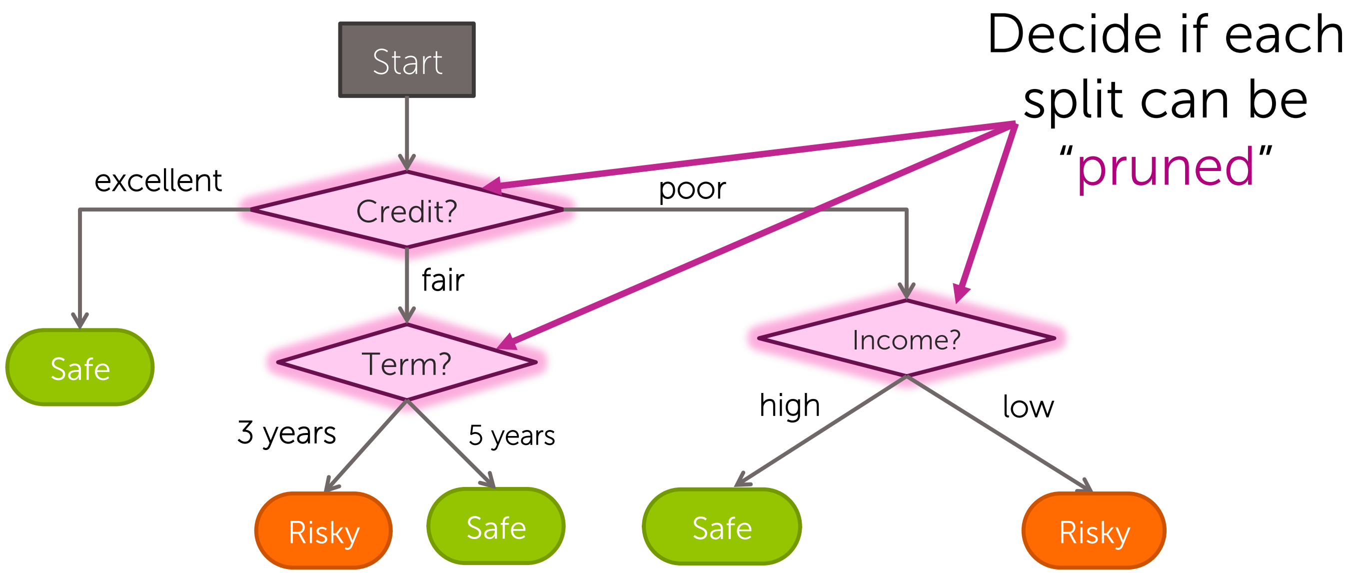
$\lambda = 0.3$

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

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

Replace split by leaf node? ← YES!

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 $T_{smaller}$
     $C(T_{smaller}) = \text{Error}(T_{smaller}) + \lambda\, L(T_{smaller})$
  4. If $C(T_{smaller}) < C(T)$, 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.