

Tree pruning and bagging

STAT 4710

October 31, 2023

Where we are

- ✓ **Unit 1:** R for data mining
- ✓ **Unit 2:** Prediction fundamentals
- ✓ **Unit 3:** Regression-based methods
- Unit 4:** Tree-based methods
- Unit 5:** Deep learning

Lecture 1: Growing decision trees

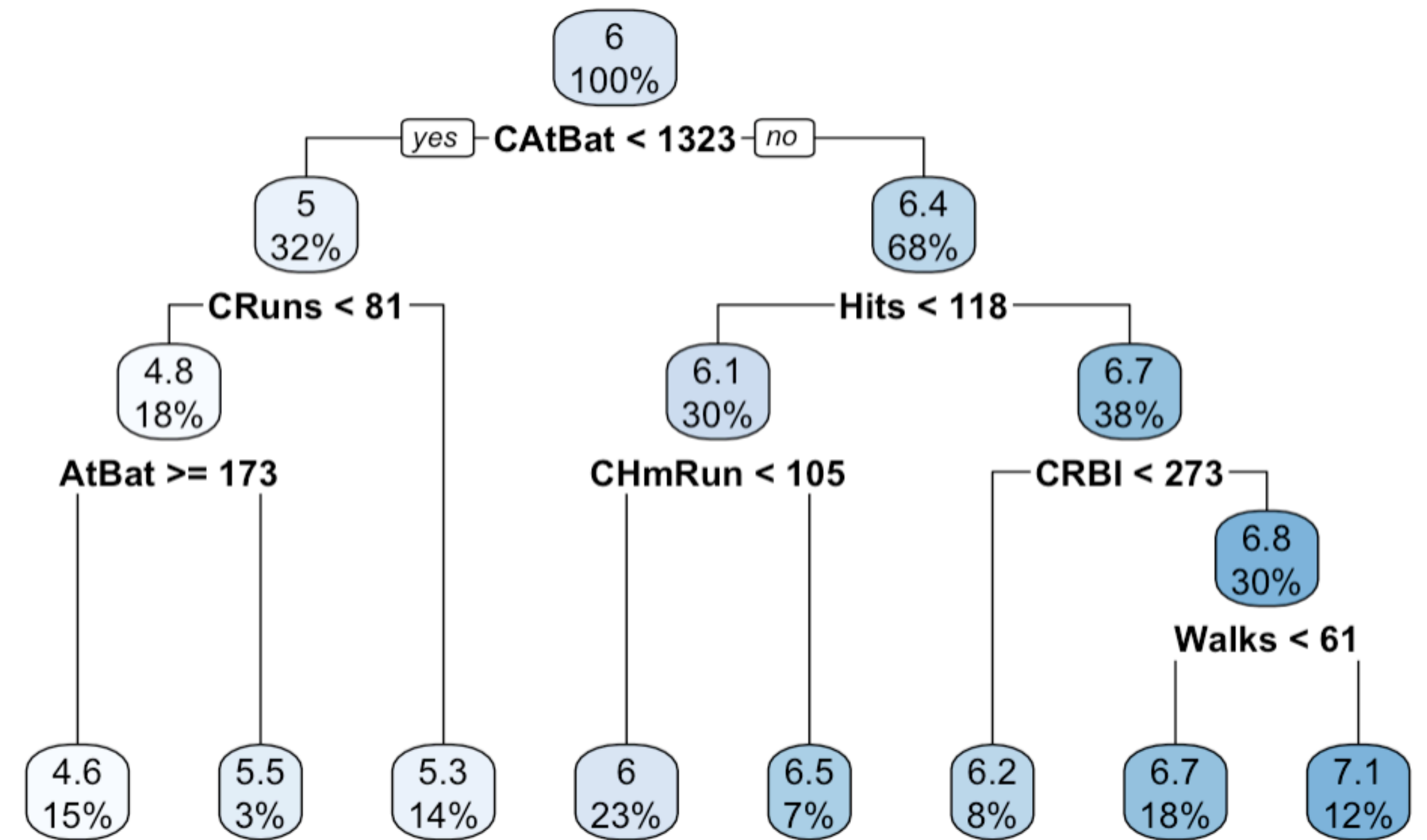
Lecture 2: Tree pruning and bagging

Lecture 3: Random forests

Lecture 4: Boosting

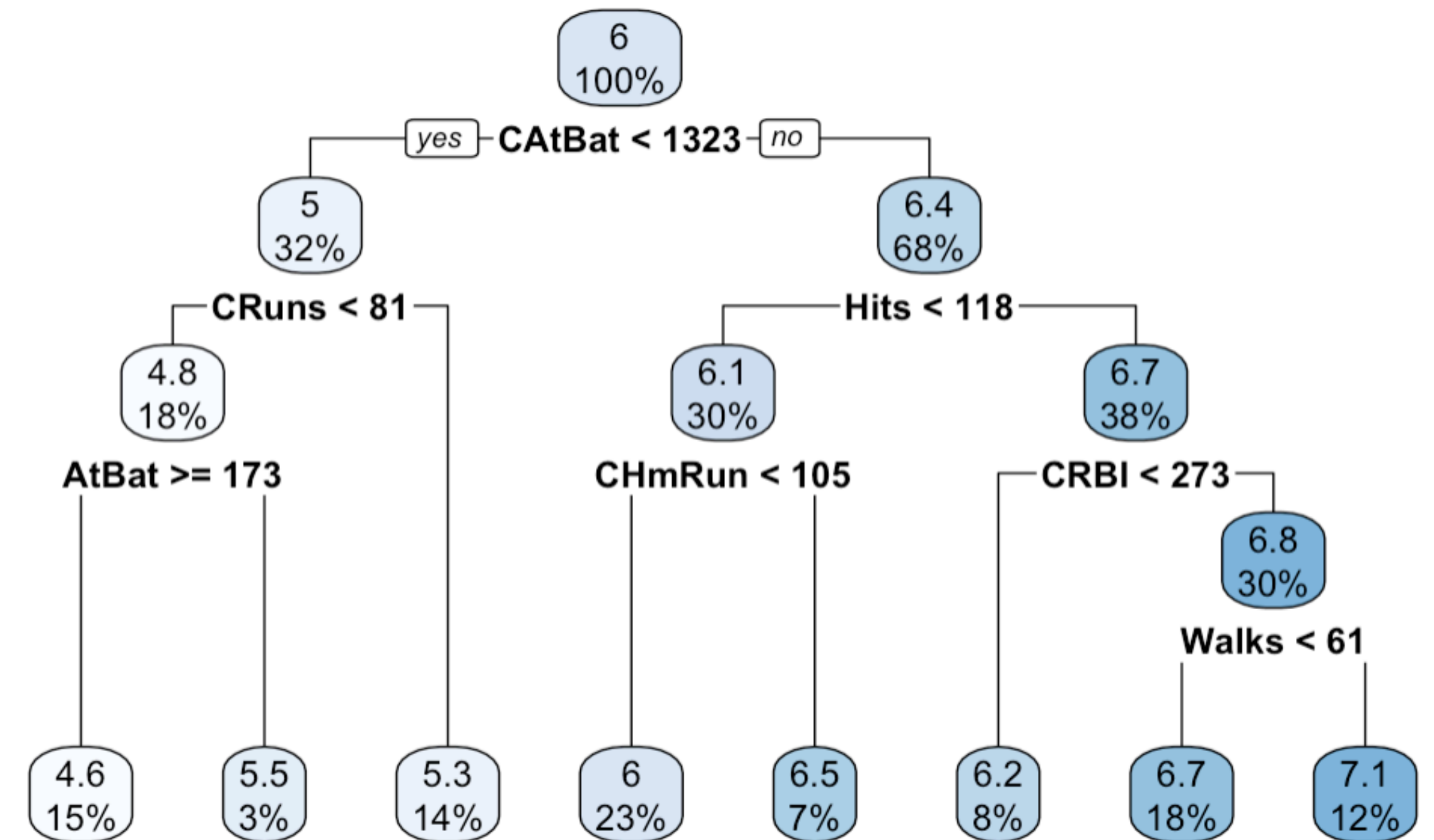
Lecture 5: Unit review and quiz in class

Recall: Decision trees



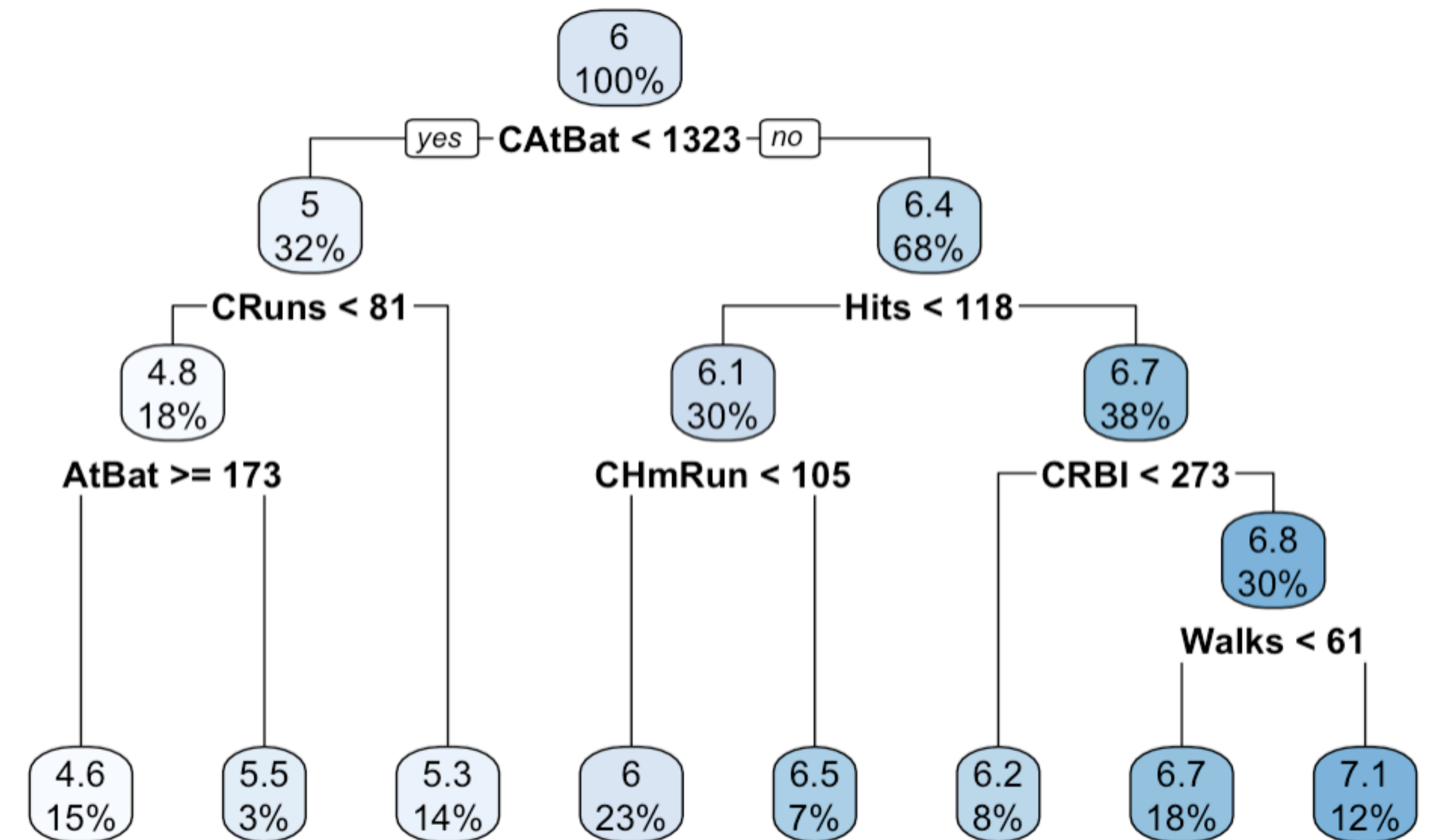
Recall: Decision trees

- Create a partition of feature space by recursively splitting on different features



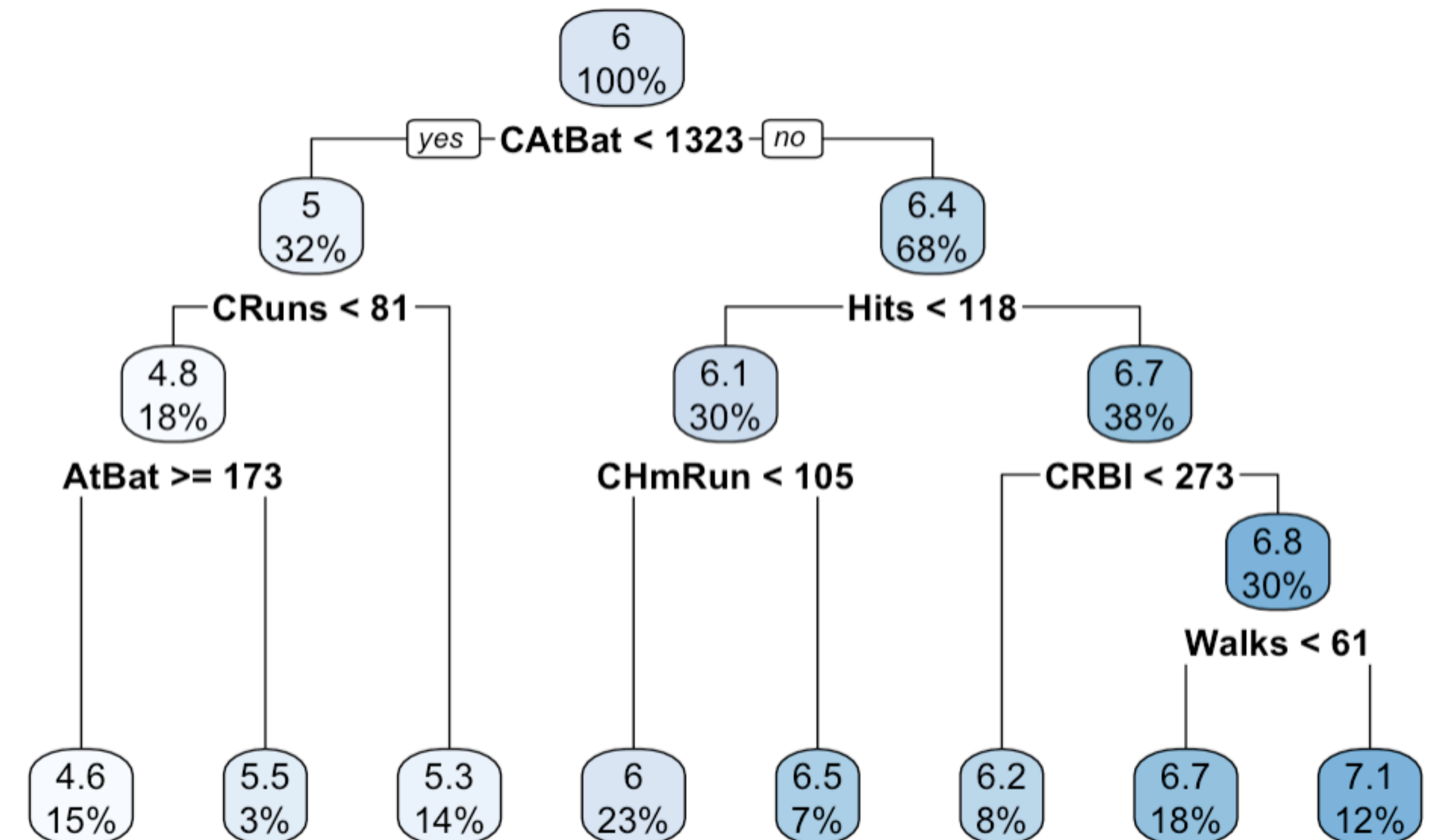
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- Regression and classification trees



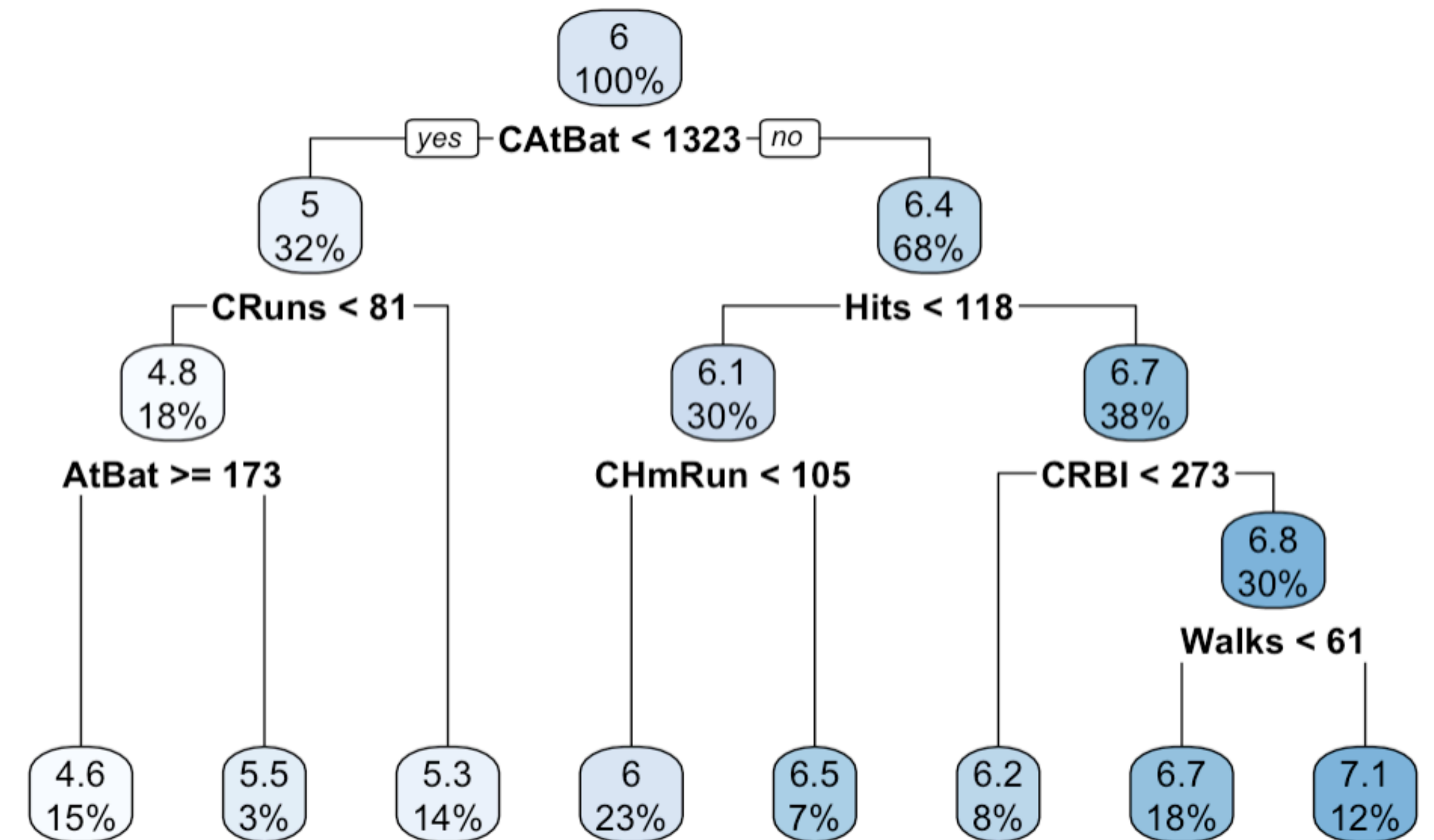
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Recall: Decision trees

- Create a partition of feature space by recursively splitting on different features
- Regression and classification trees
- Terminal nodes in the tree correspond to the rectangles in the partition
- Predict a single number (category) for each terminal node in a regression (classification) tree



Complexity of a decision tree

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The more terminal nodes (regions), the more flexibly the tree fits training data:

- if there are as many terminal nodes as training points, training error = 0
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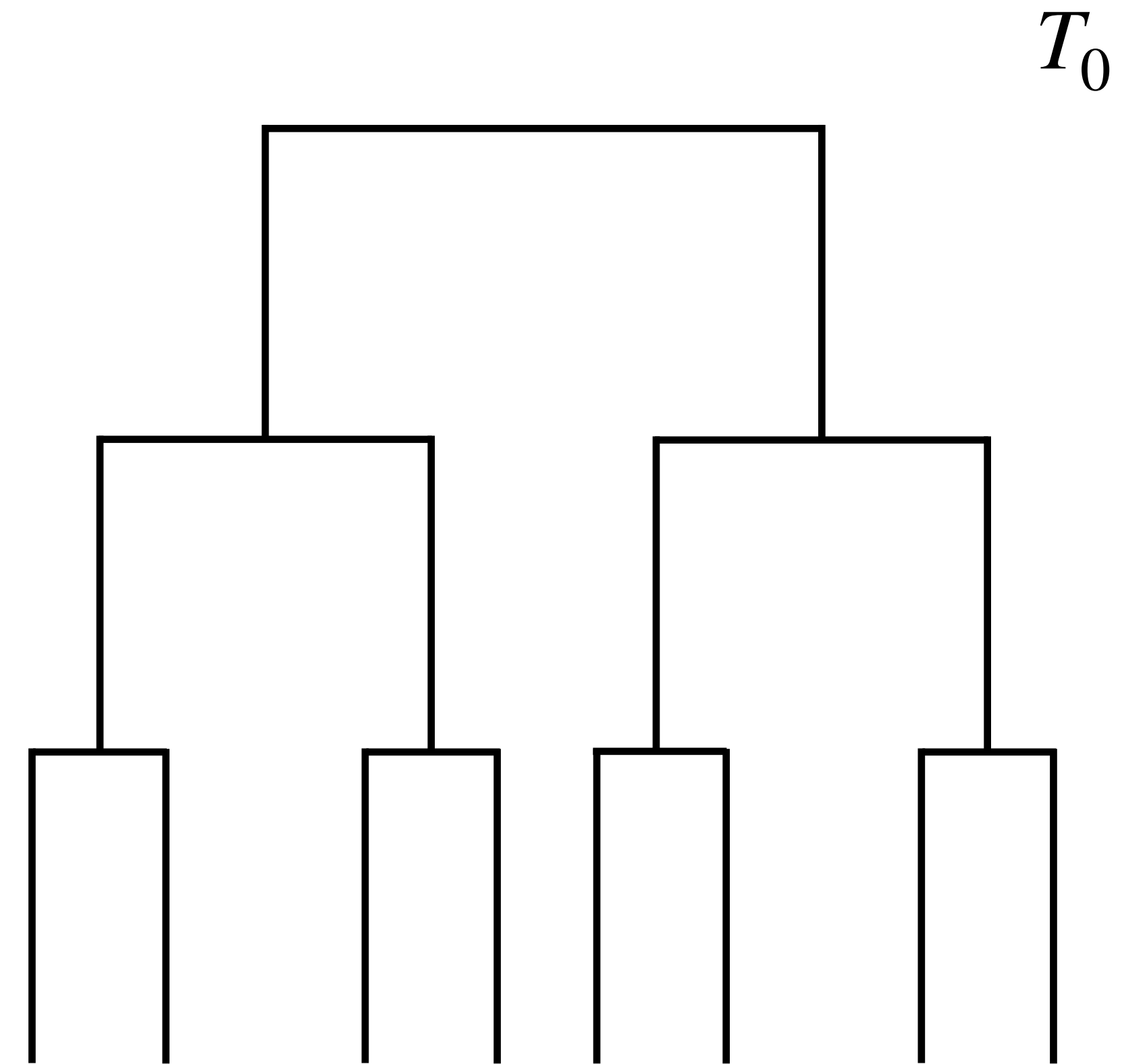
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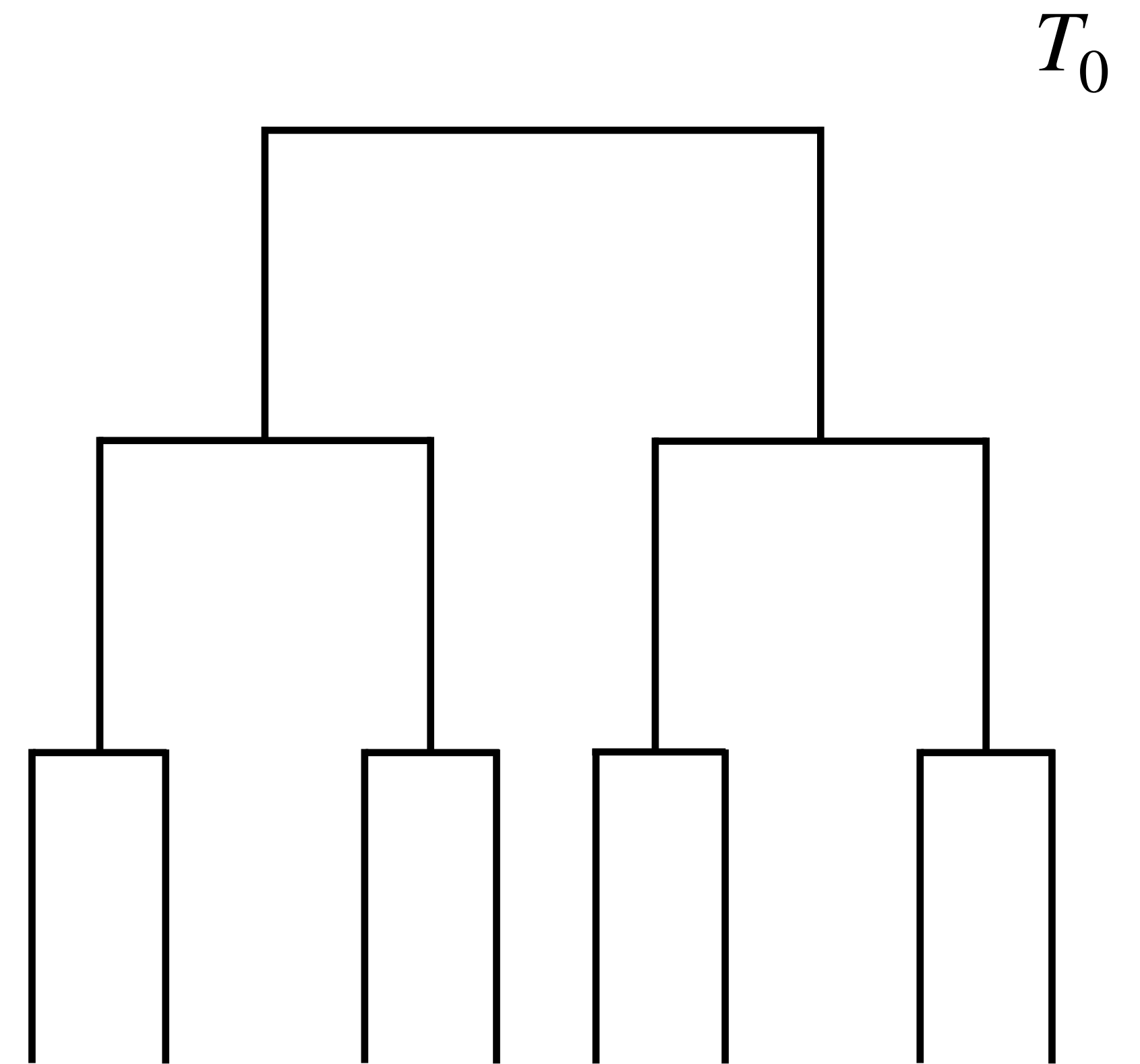
How to choose the best model complexity? [Cross-validation.](#)

A family of decision trees of varying complexity



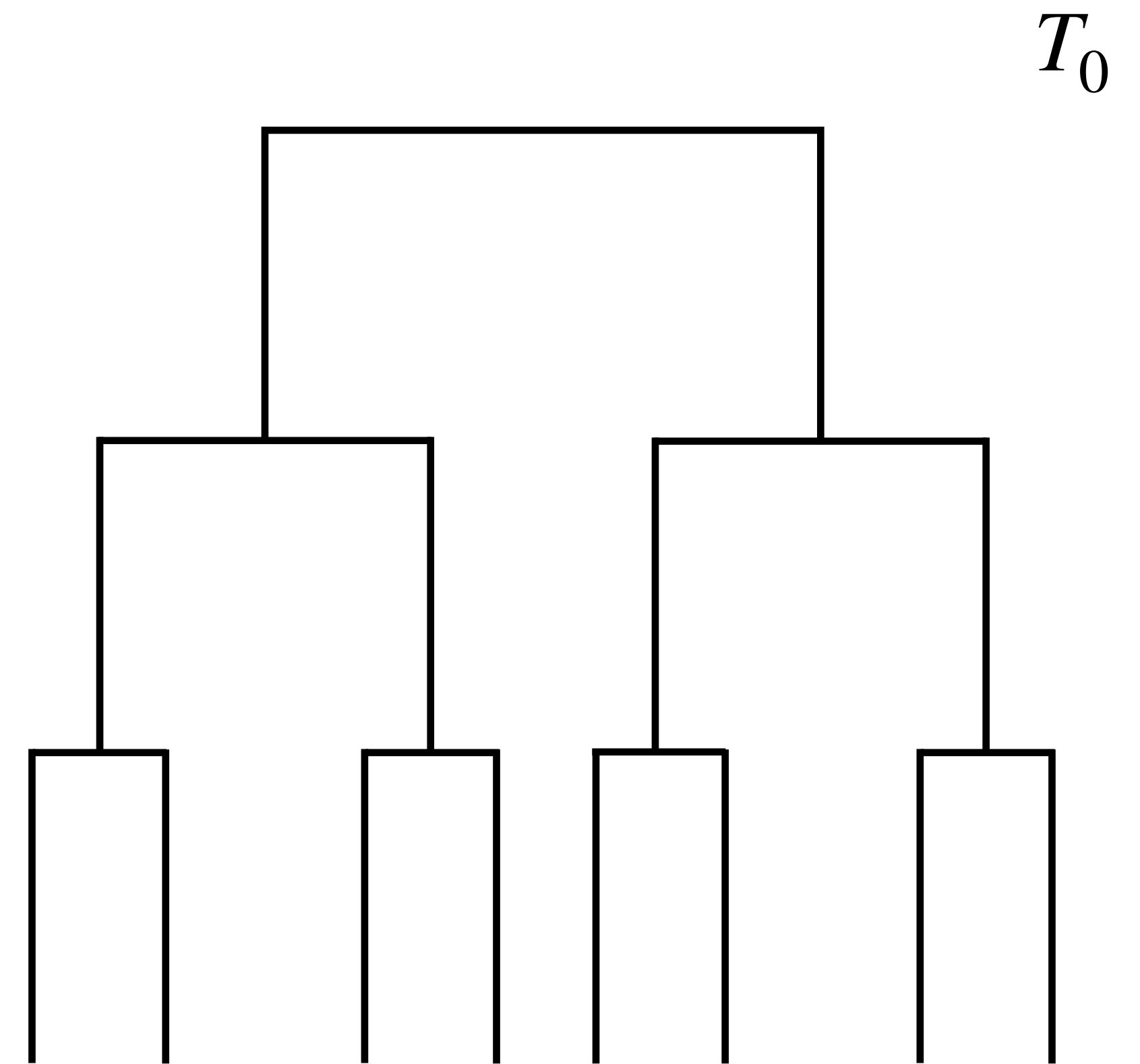
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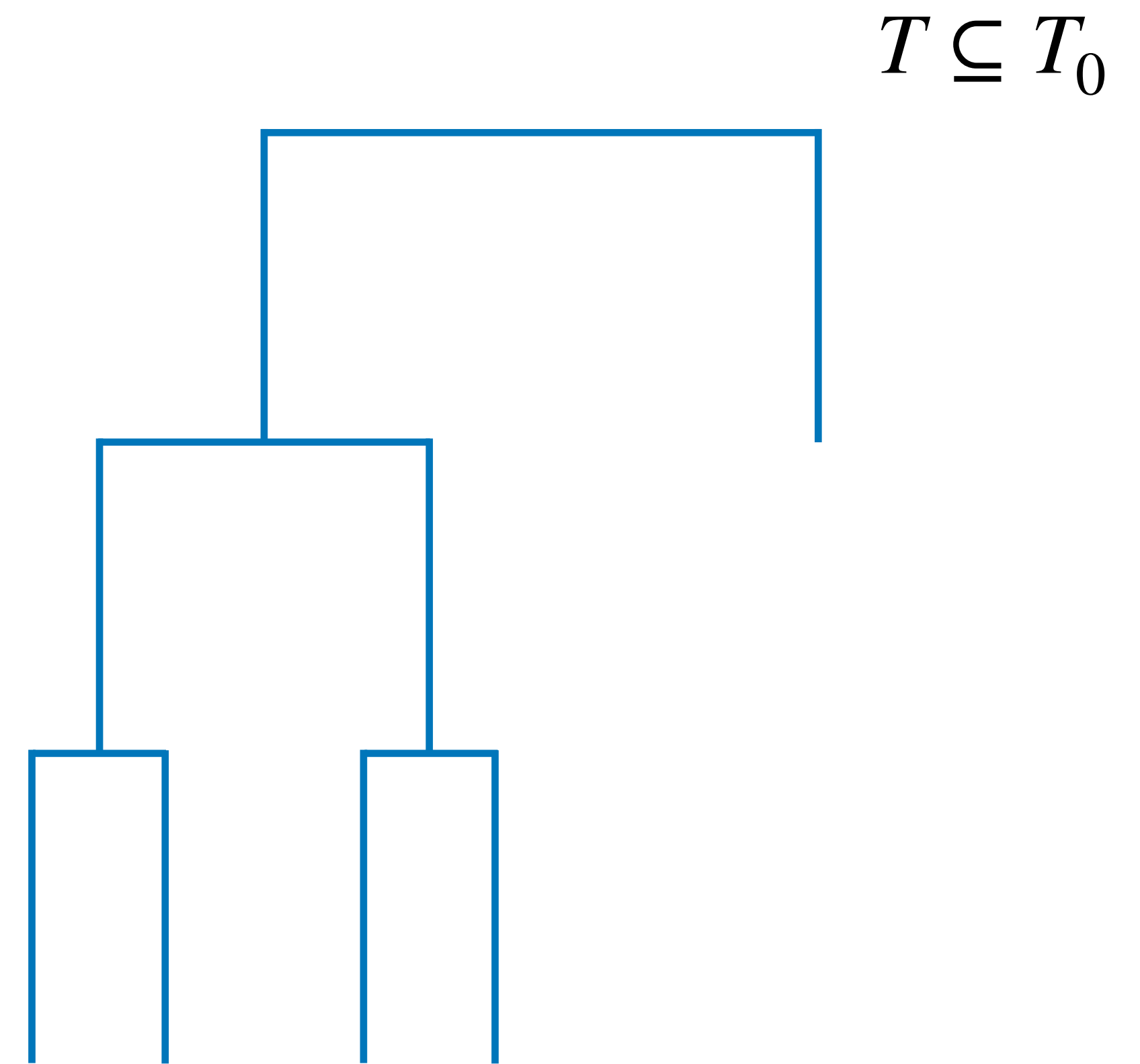
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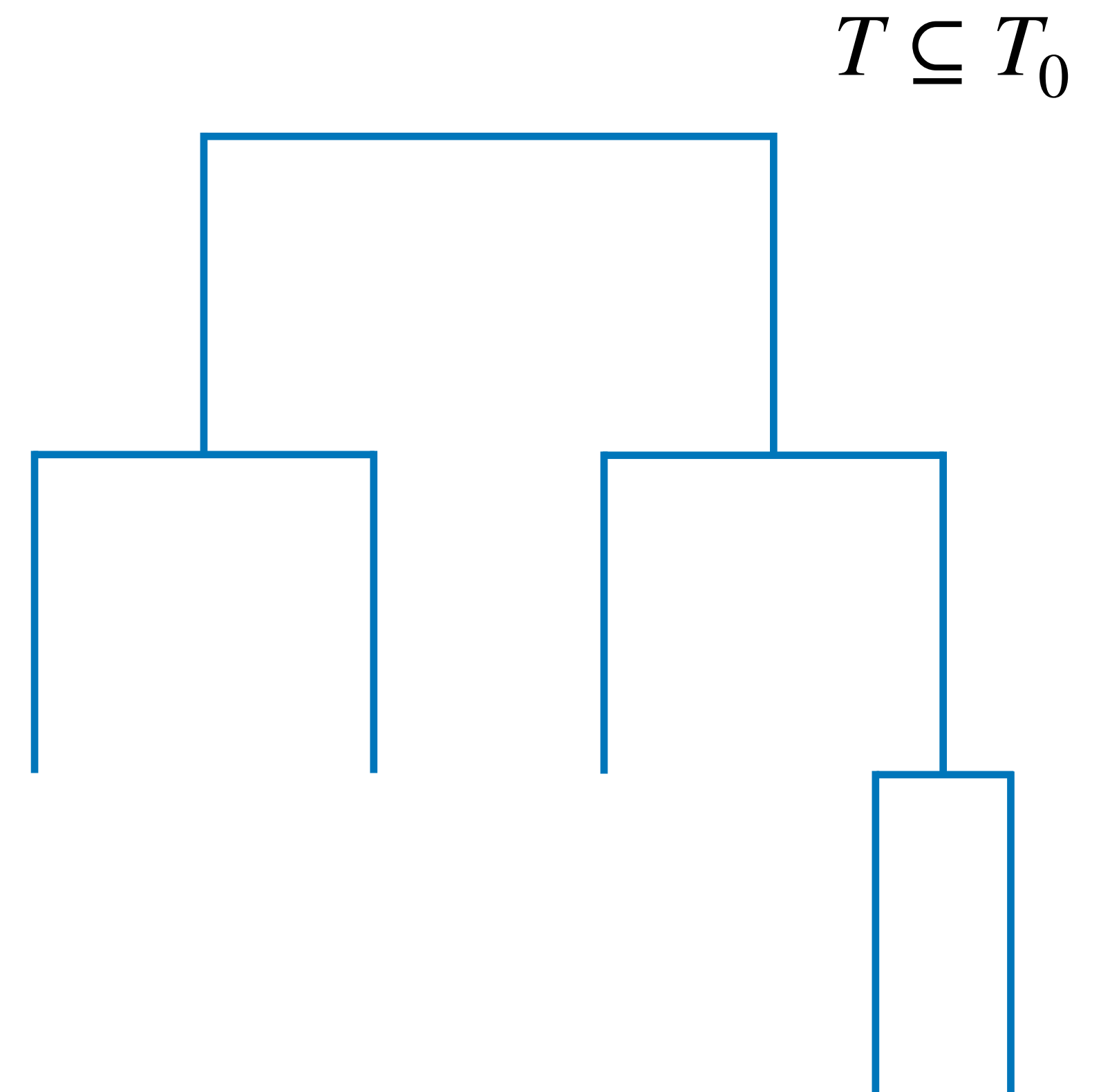
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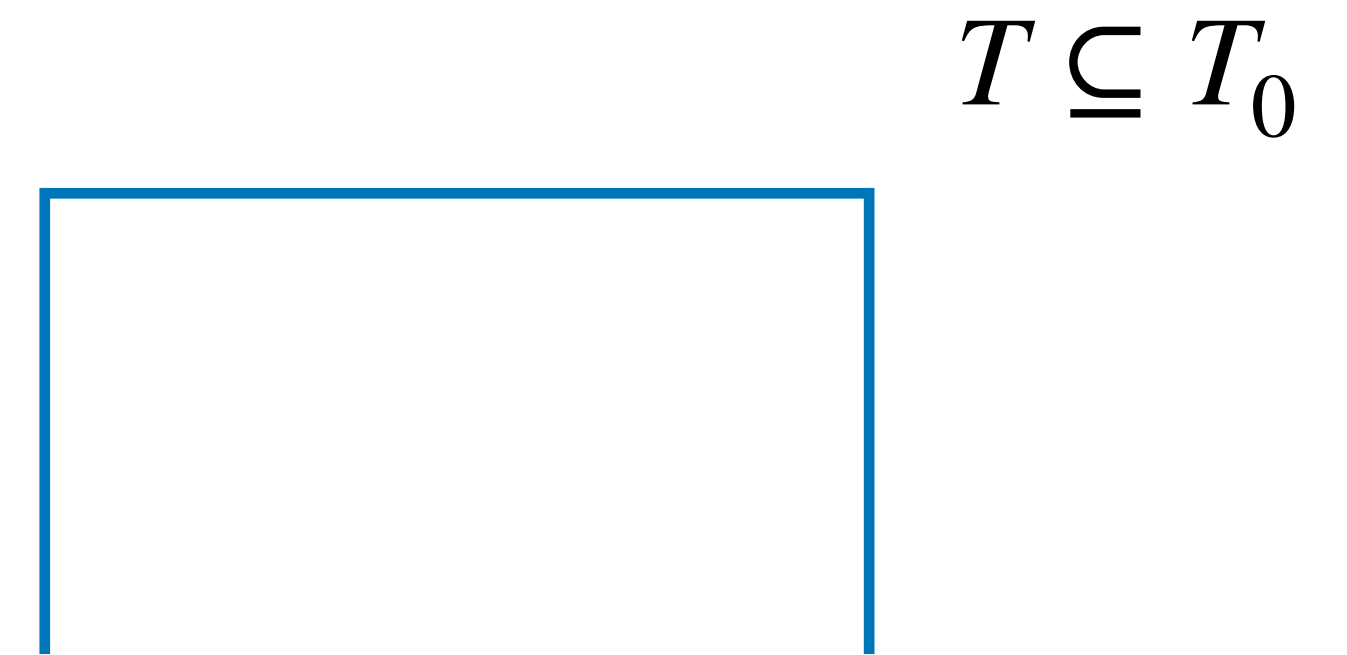
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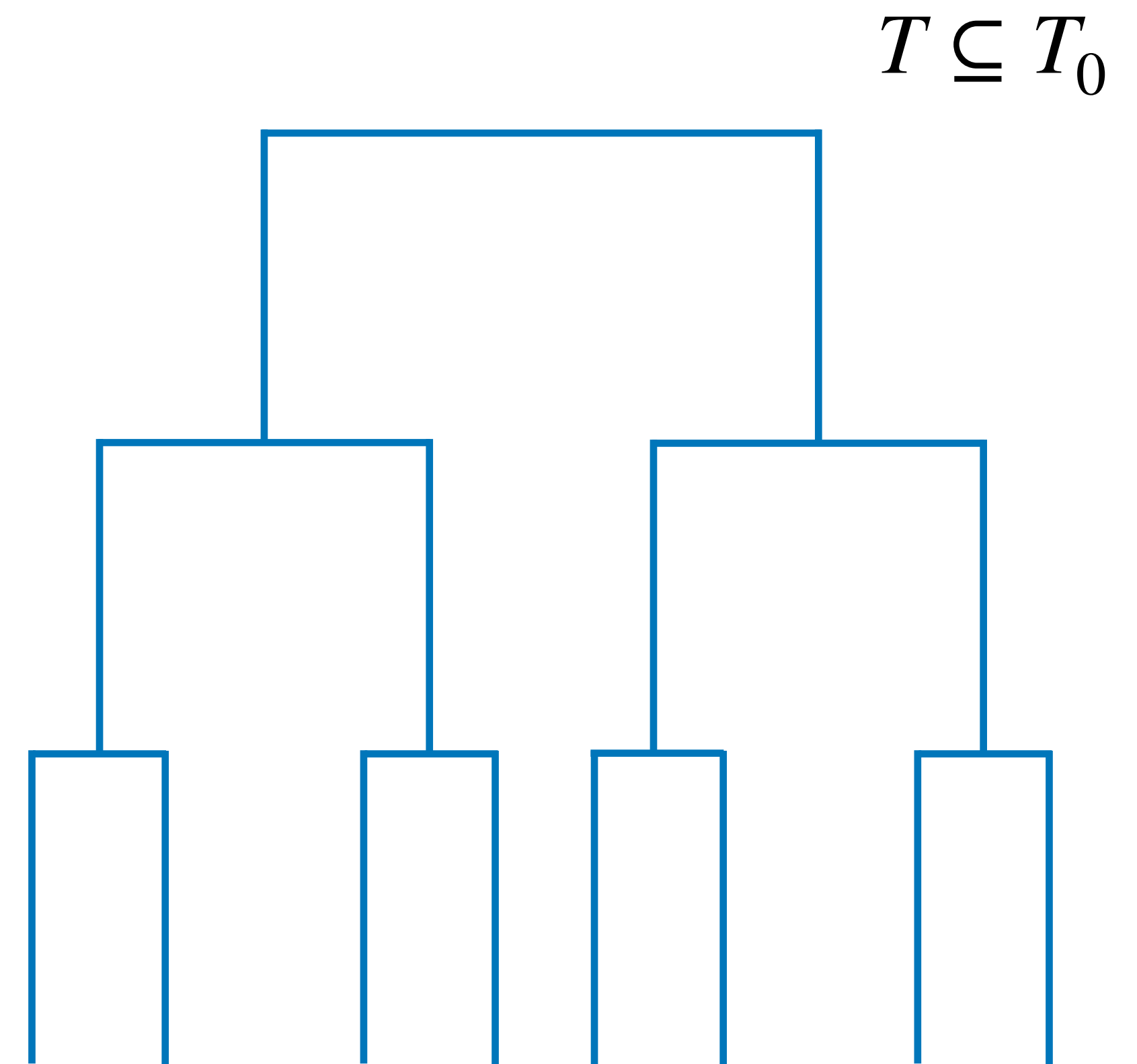
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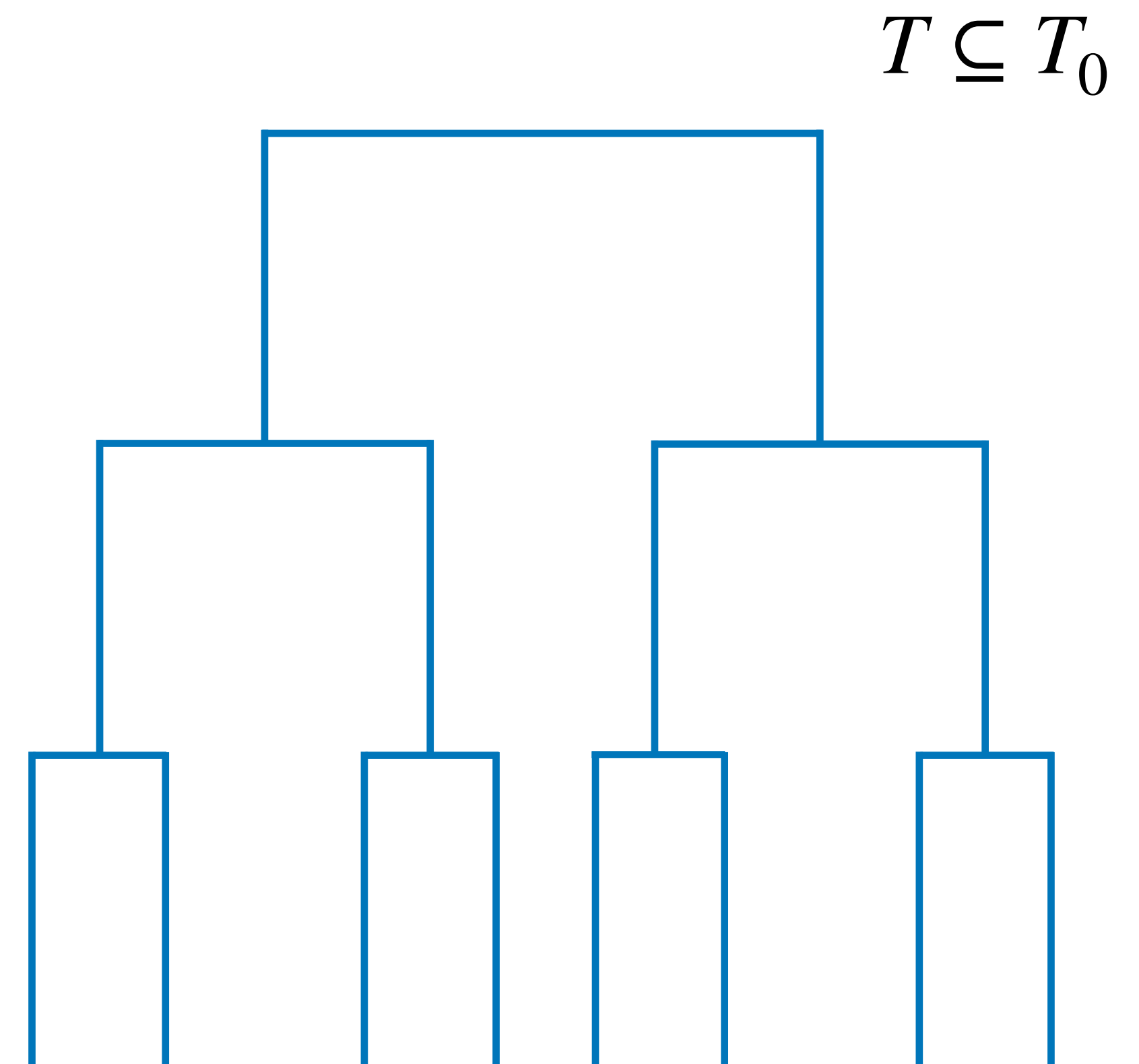
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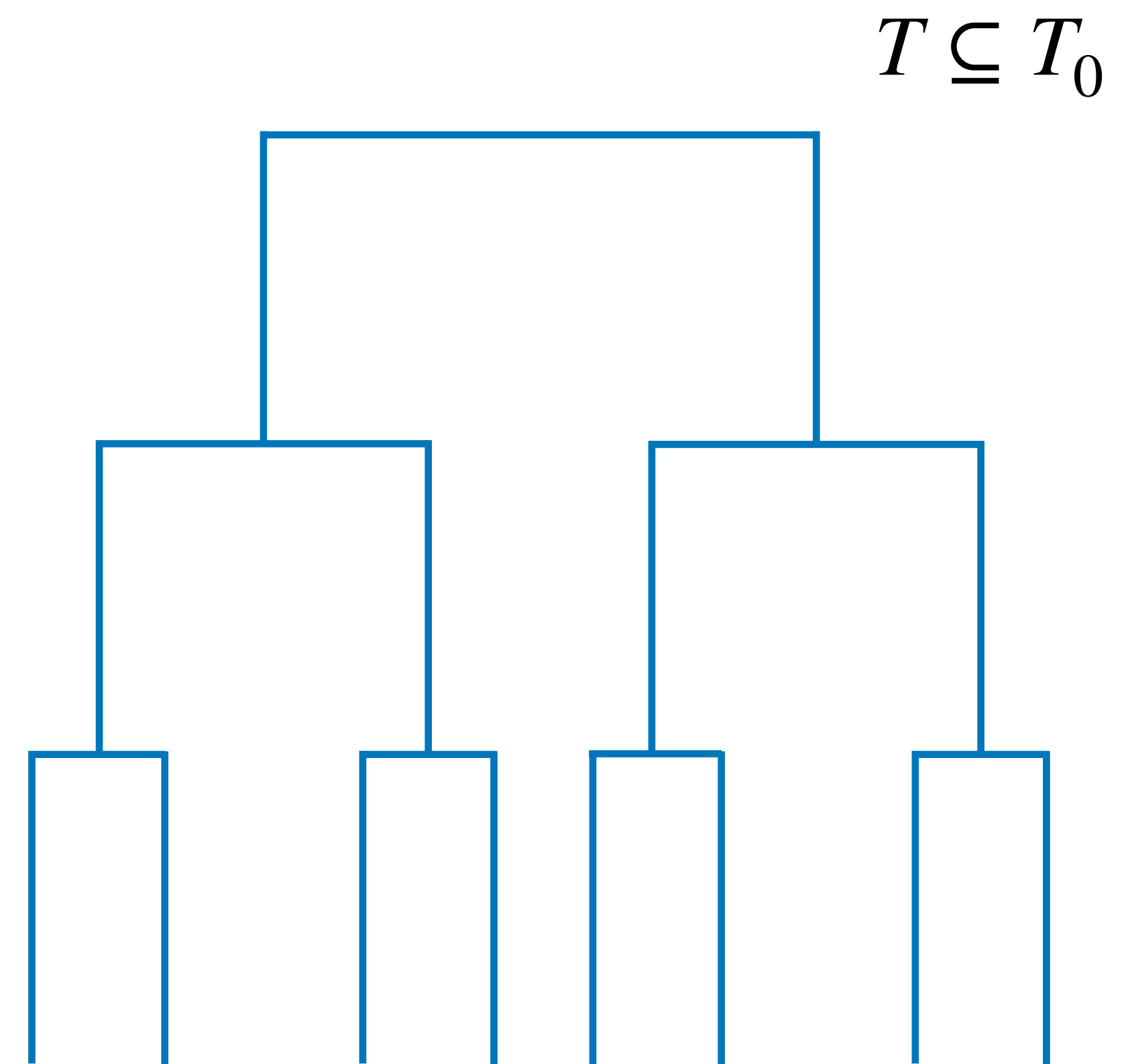


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In other model selection scenarios, we have just had one model for each complexity.



Finding a sequence of trees of increasing complexity

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Let $|T|$ be number of terminal nodes in tree T . Fixing some $\alpha \geq 0$, consider

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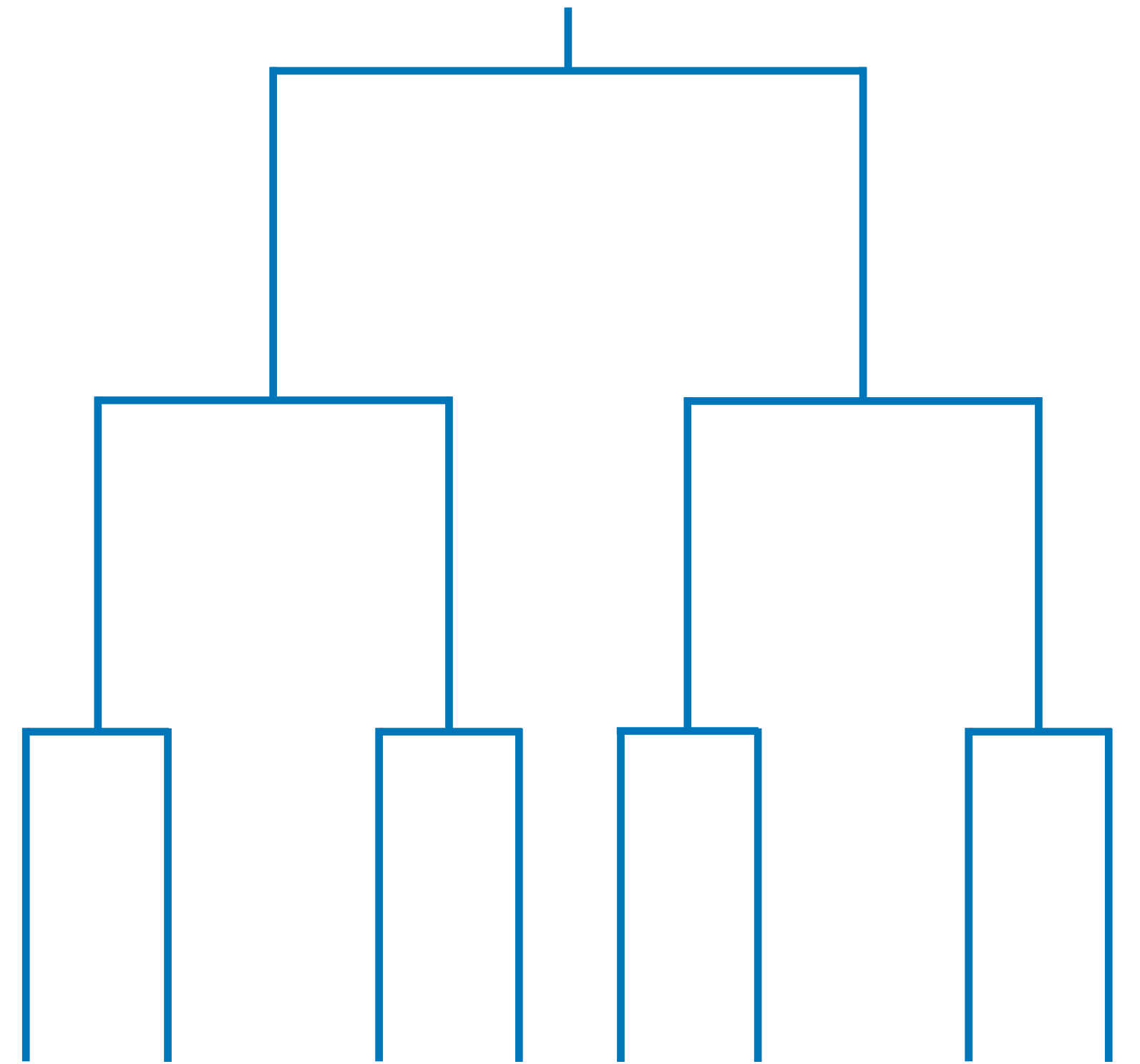
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Unlike lasso, discrete set of α values gives all possible solutions as α varies.

Cost complexity pruning

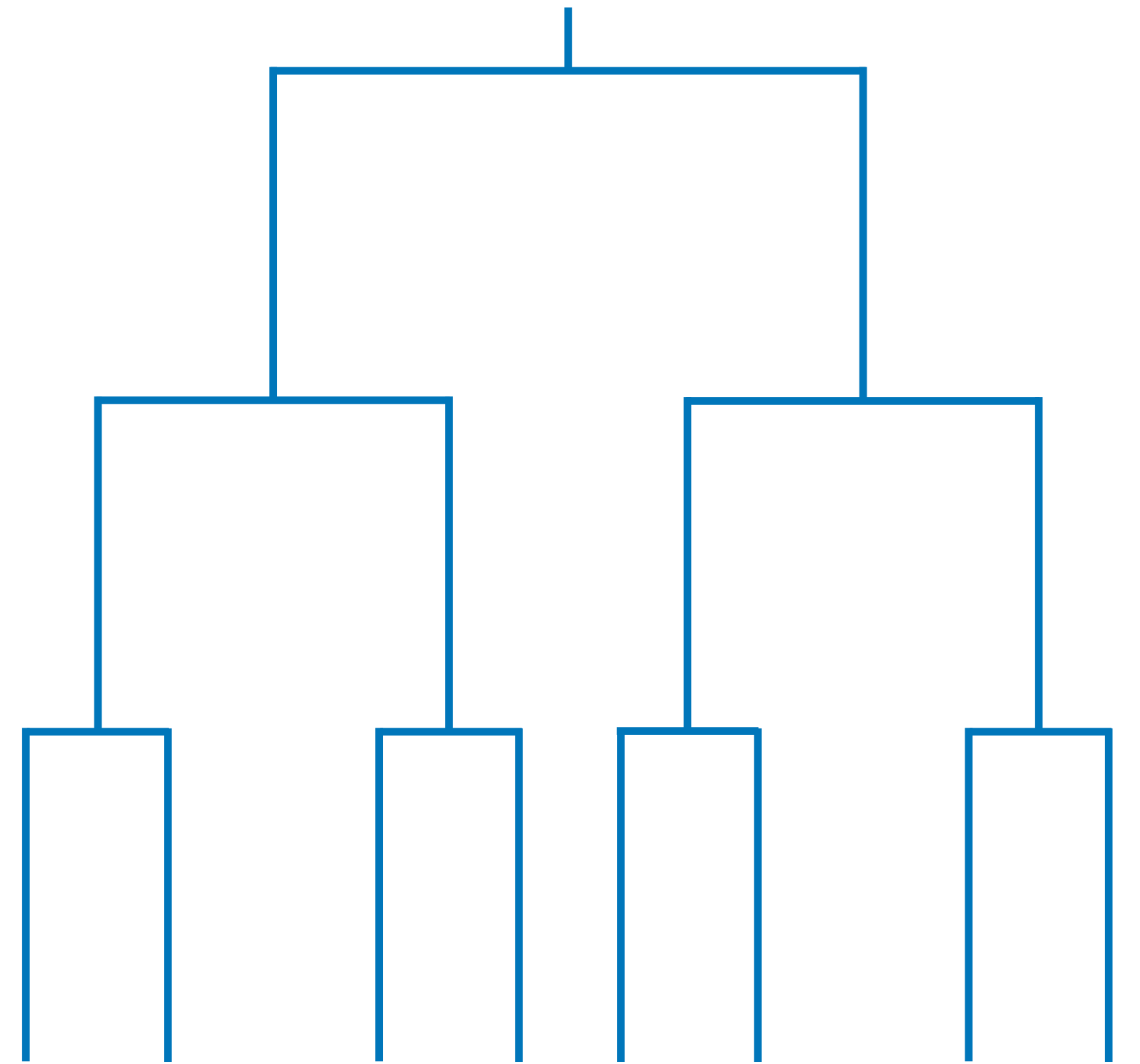
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Cost complexity pruning

Finding the sequence of trees T_α

Given a fully grown tree T_0 , **cost complexity pruning** is an algorithm that finds optimal sequence T_α , which turns out to be nested.

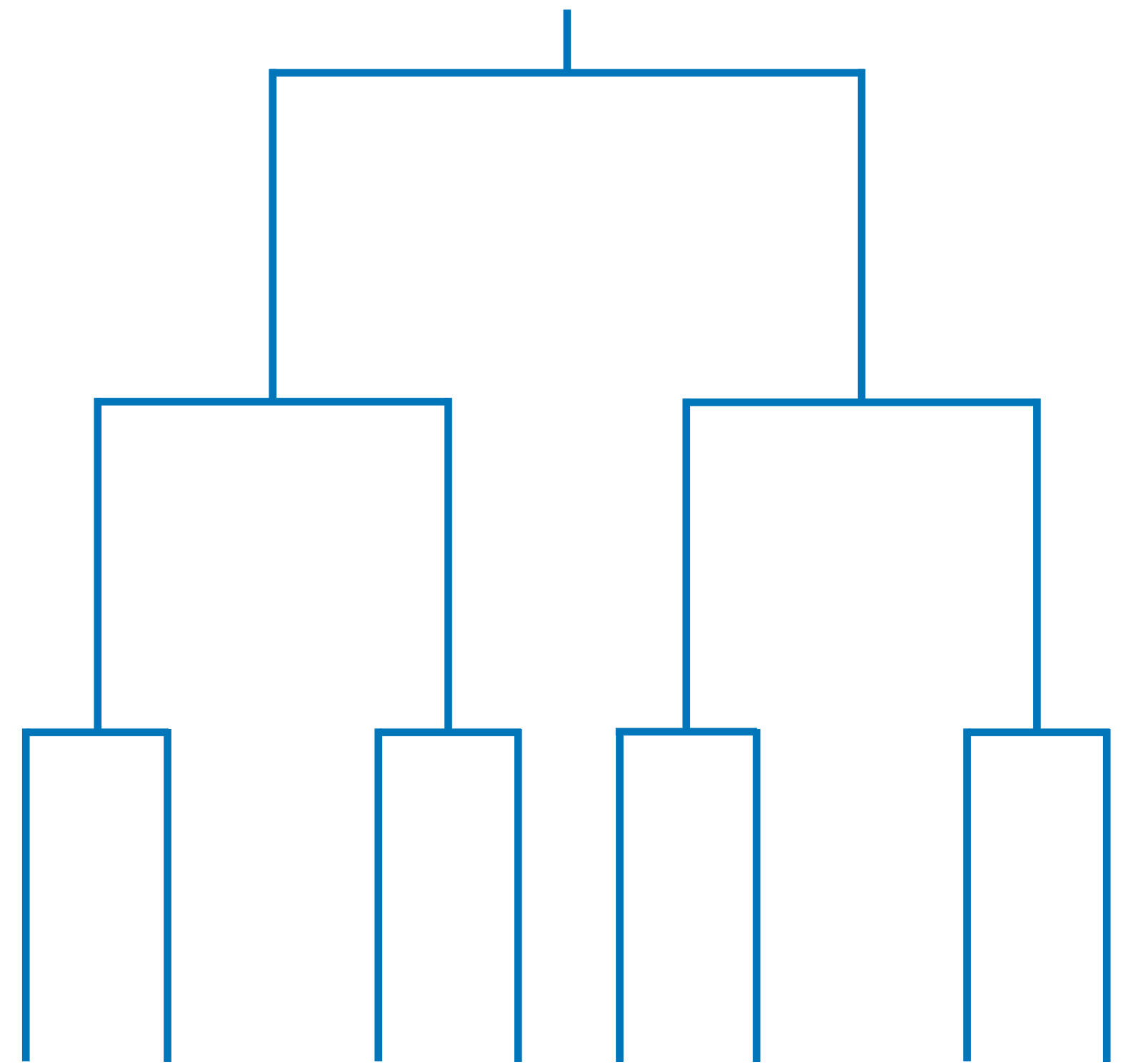


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Idea: Recursively prune “weakest link” splits.

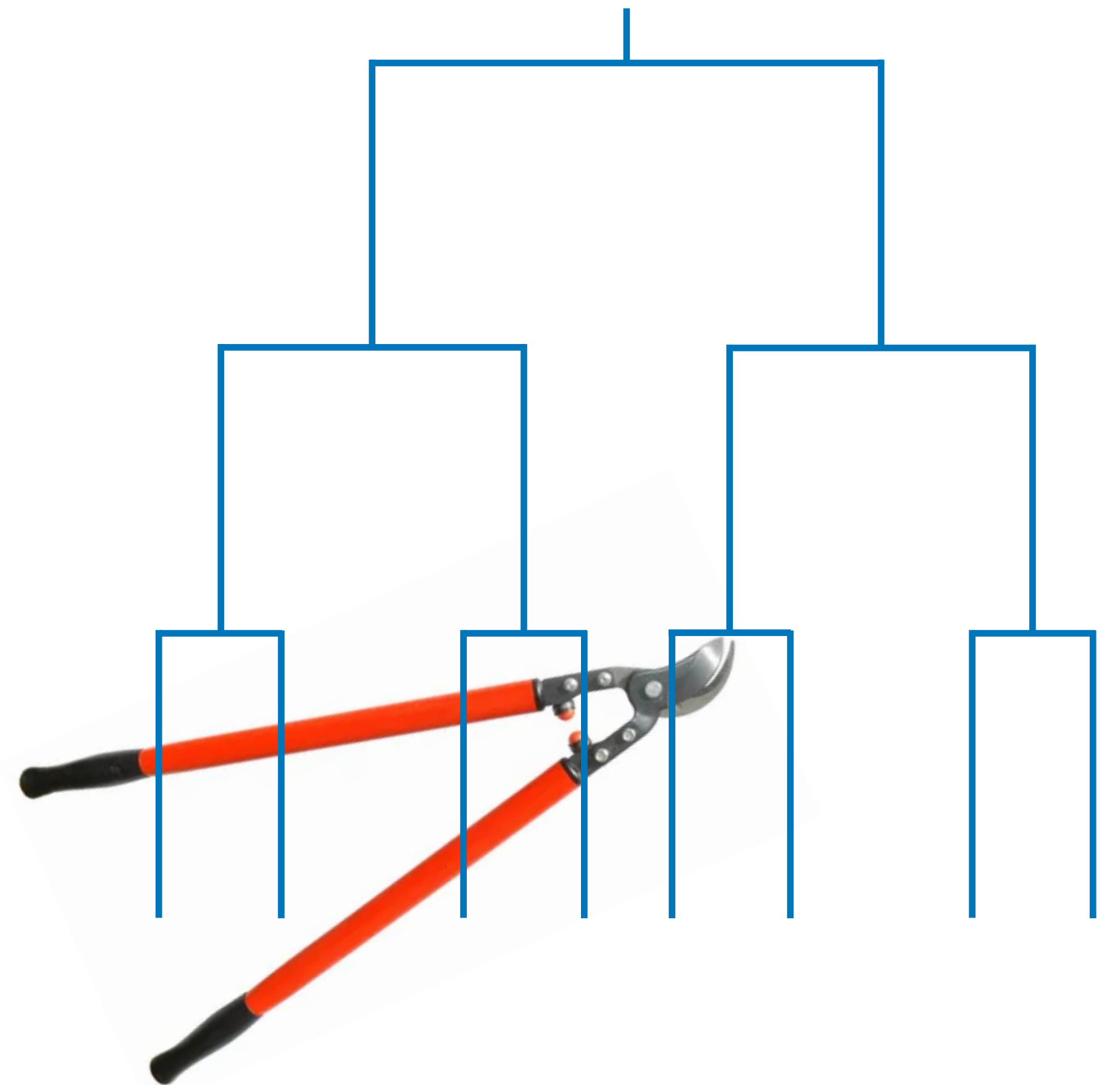


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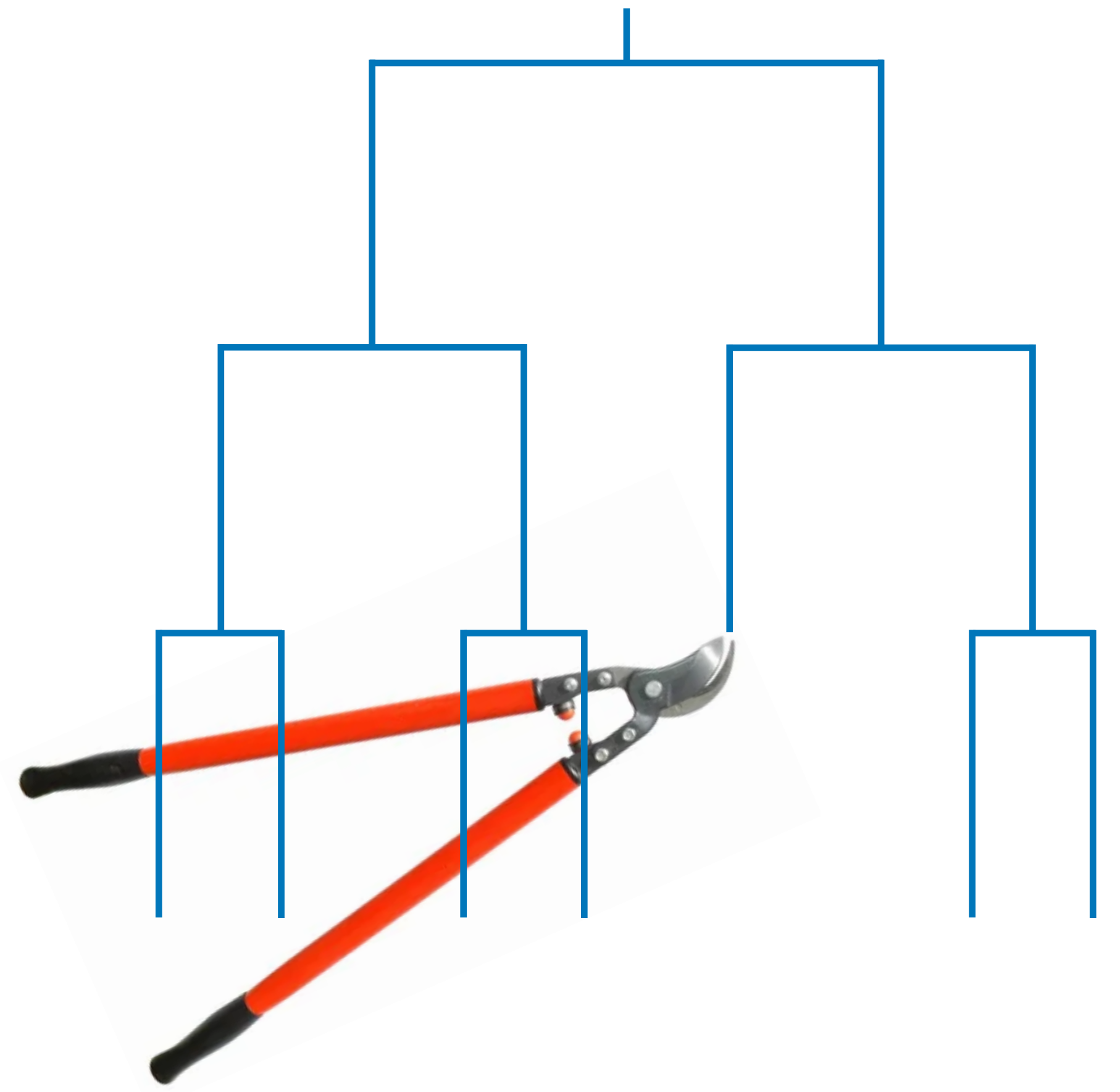


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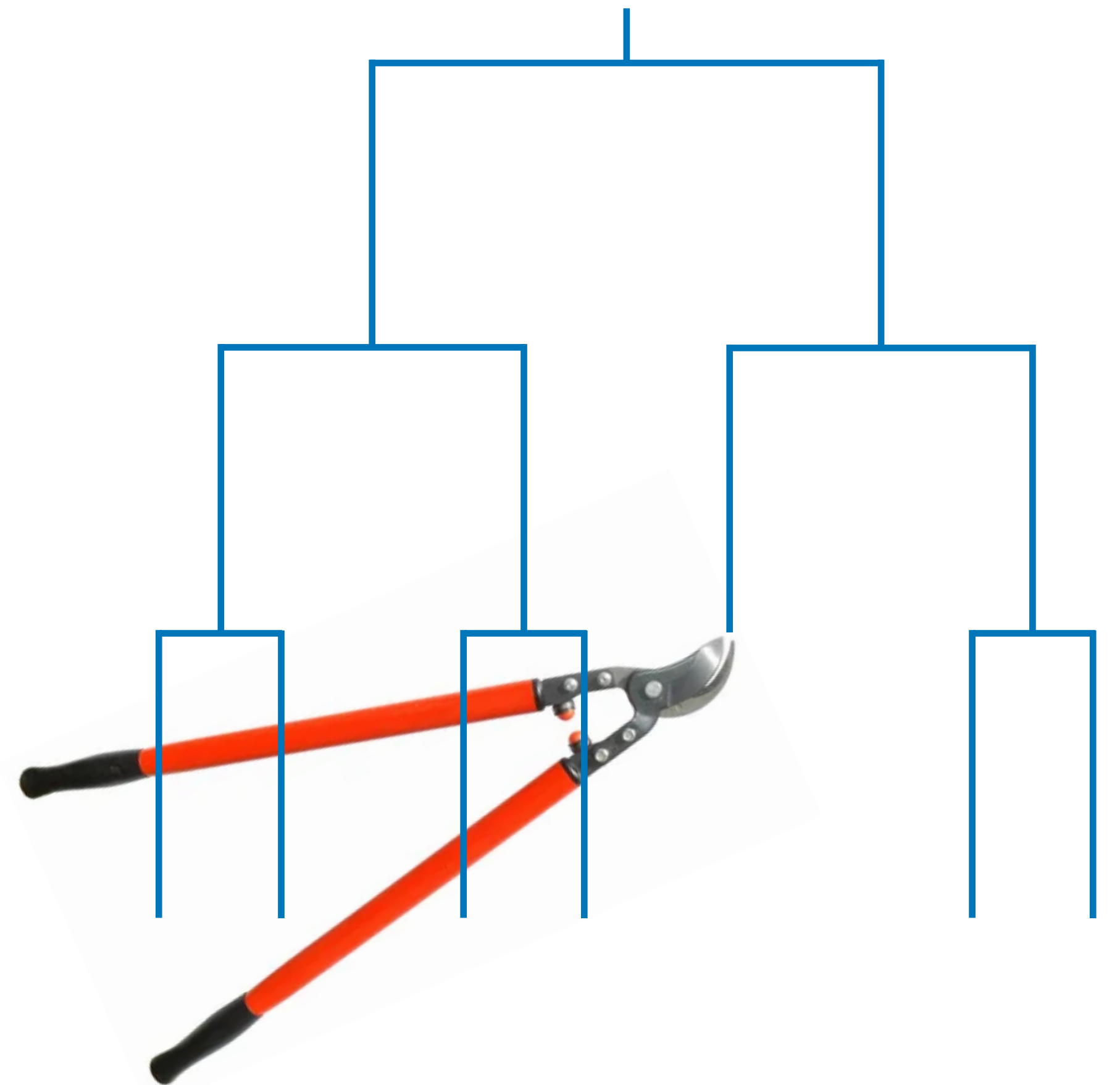
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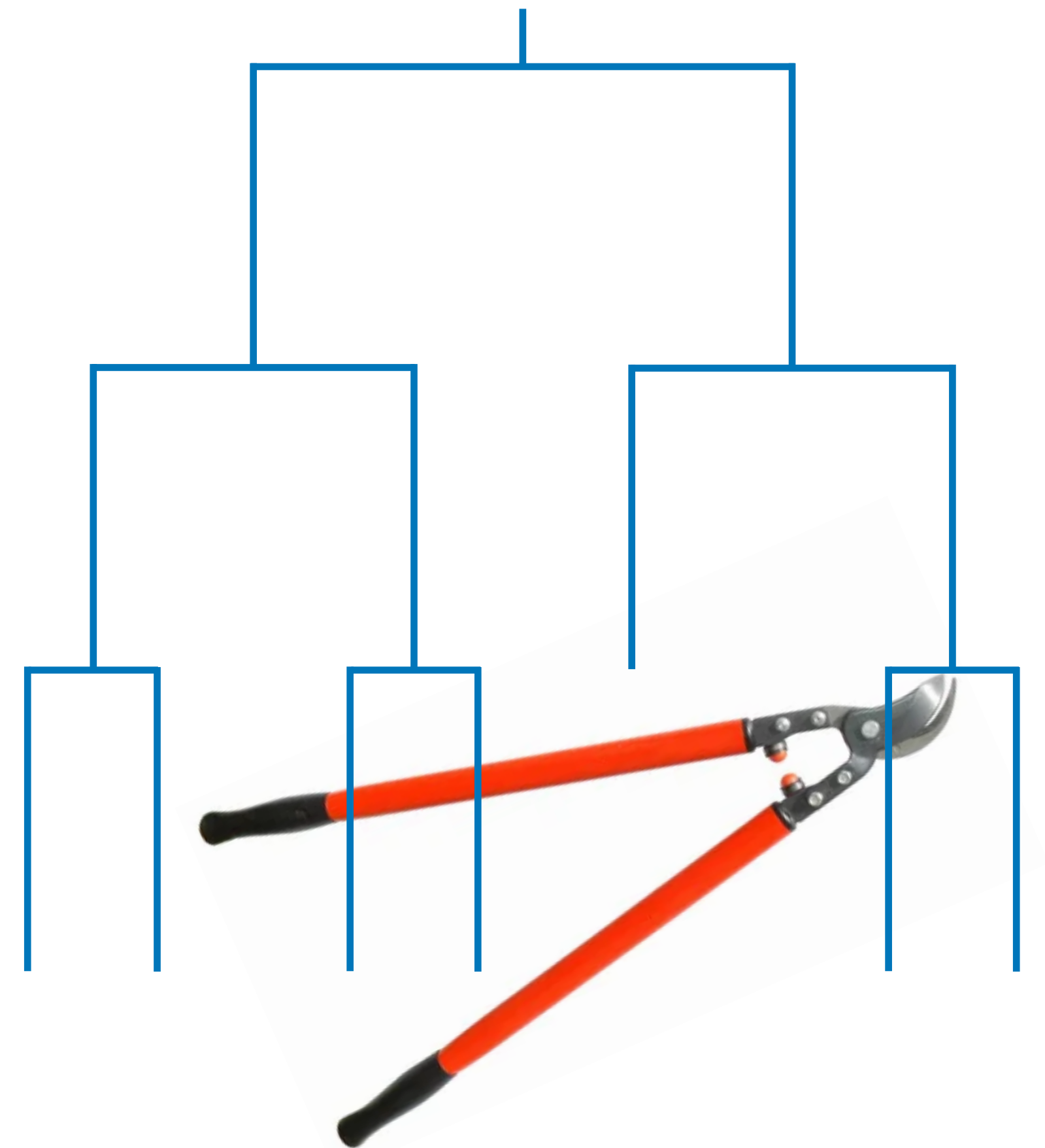
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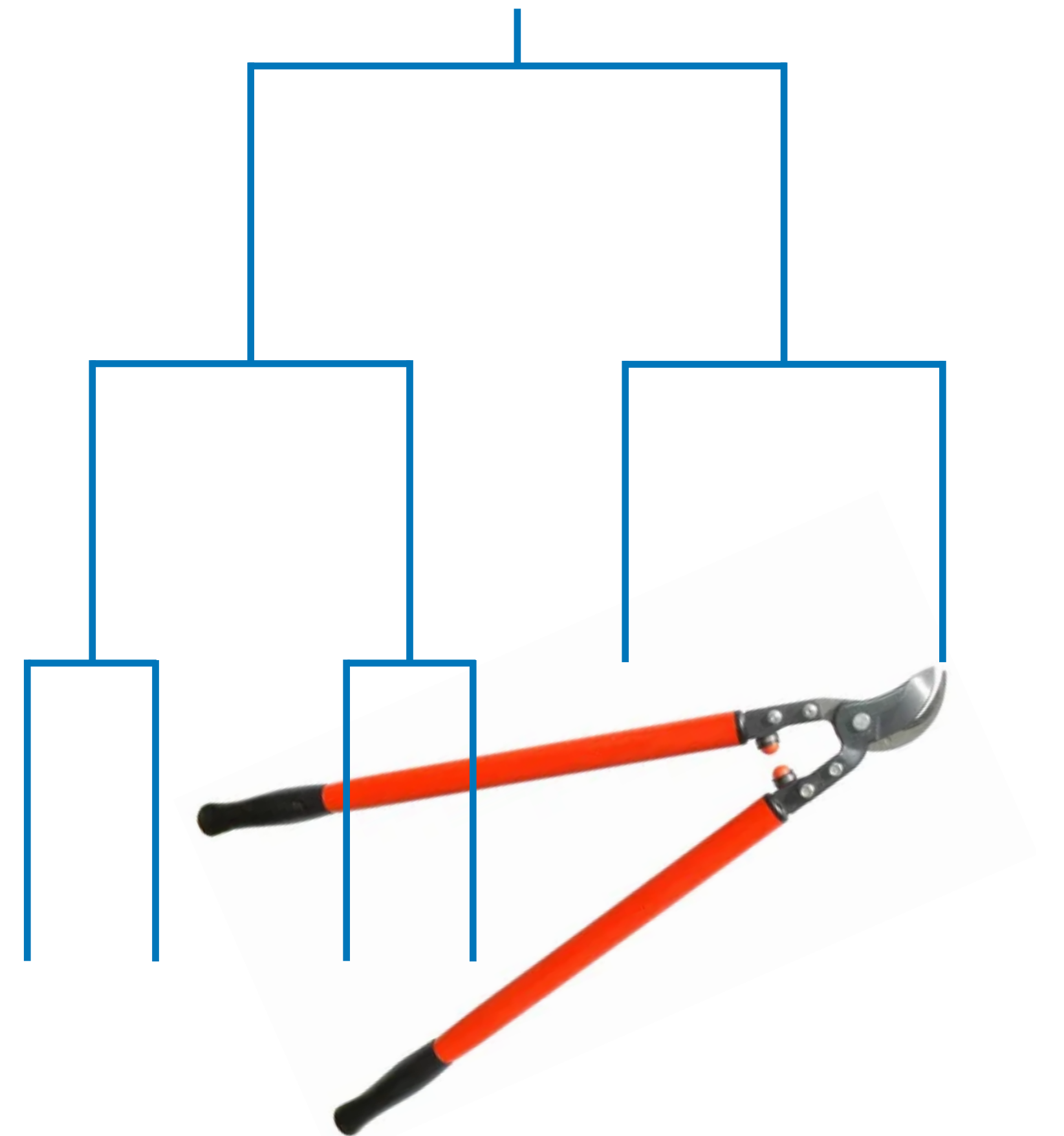
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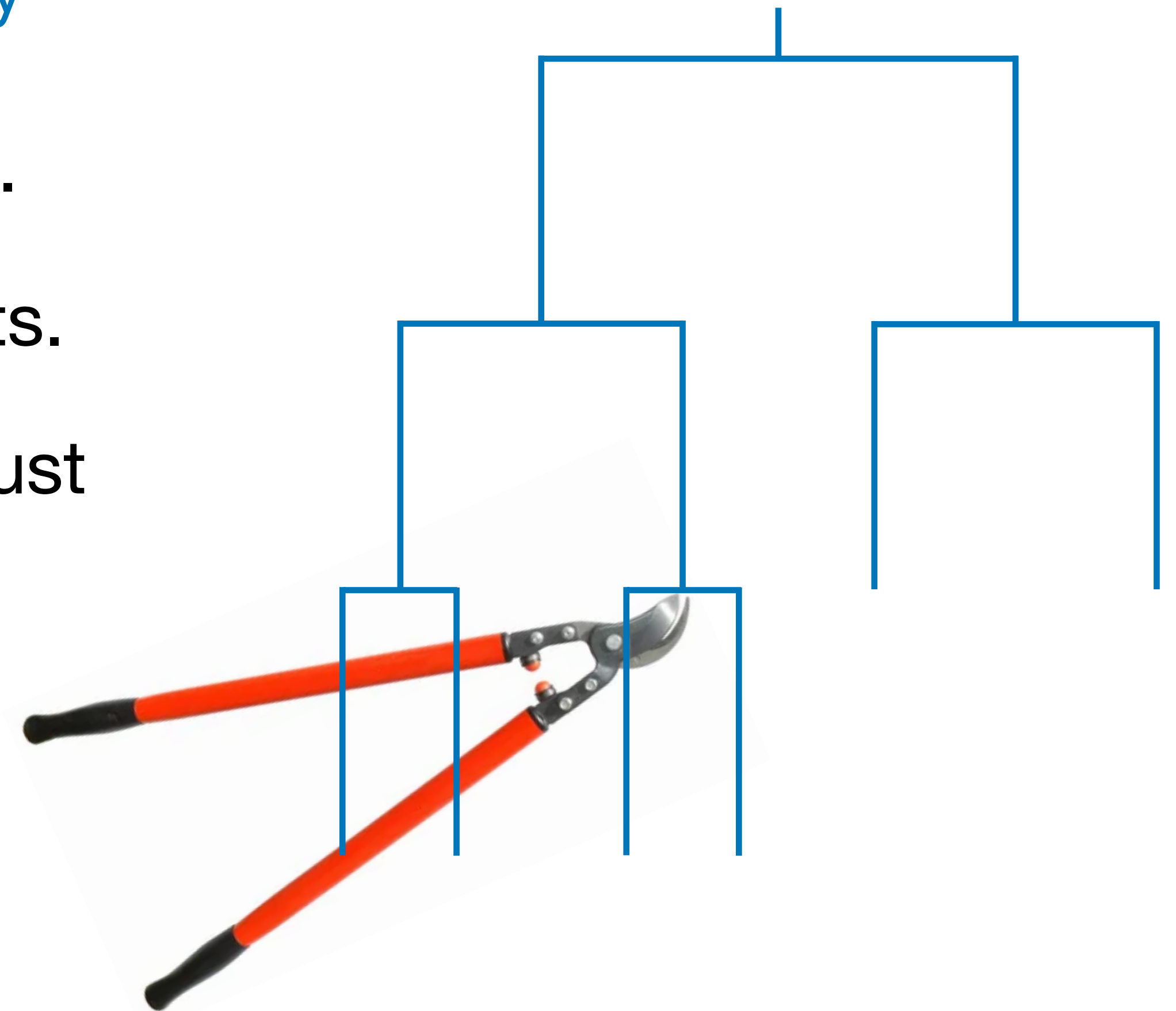
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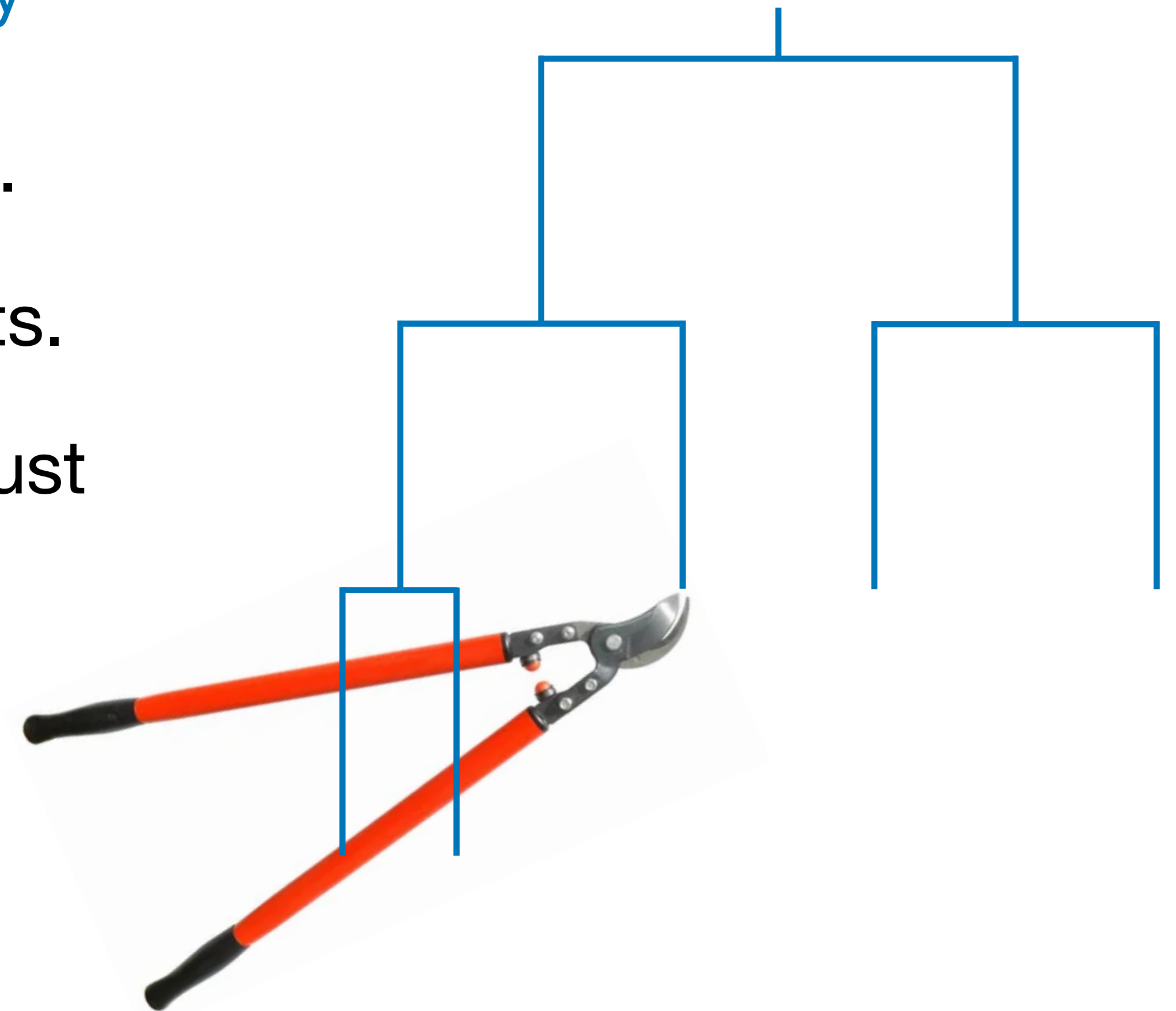
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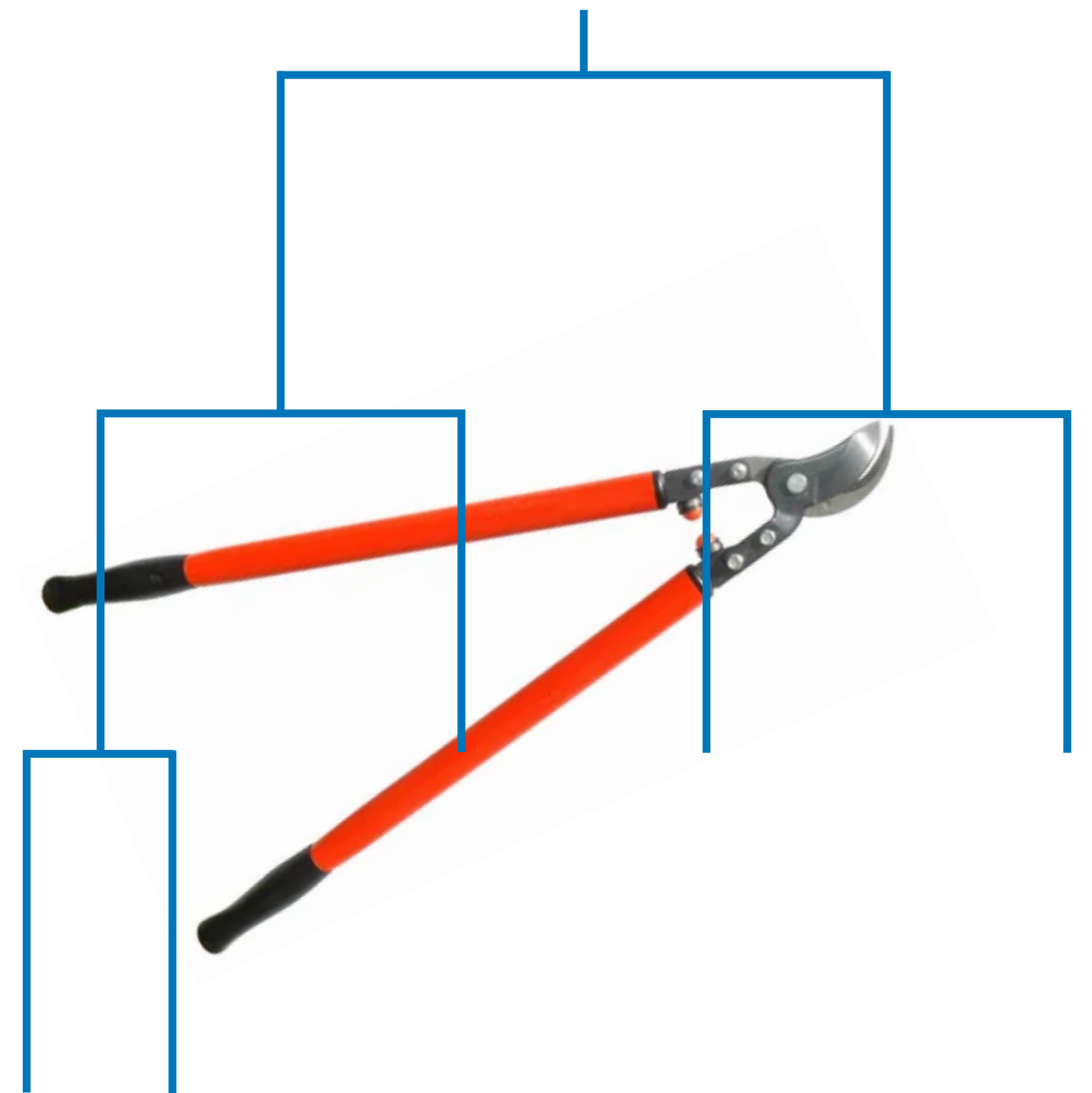
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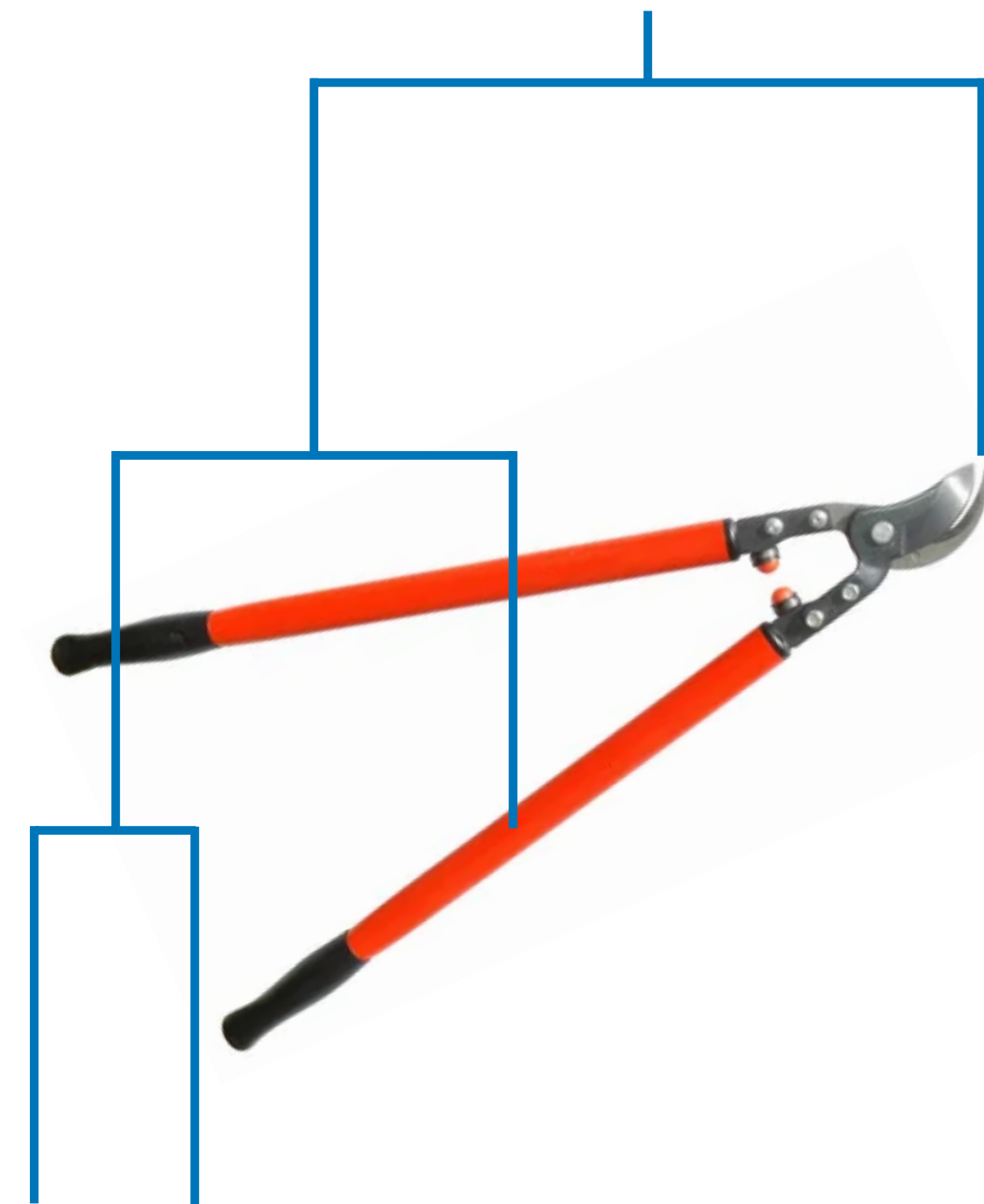
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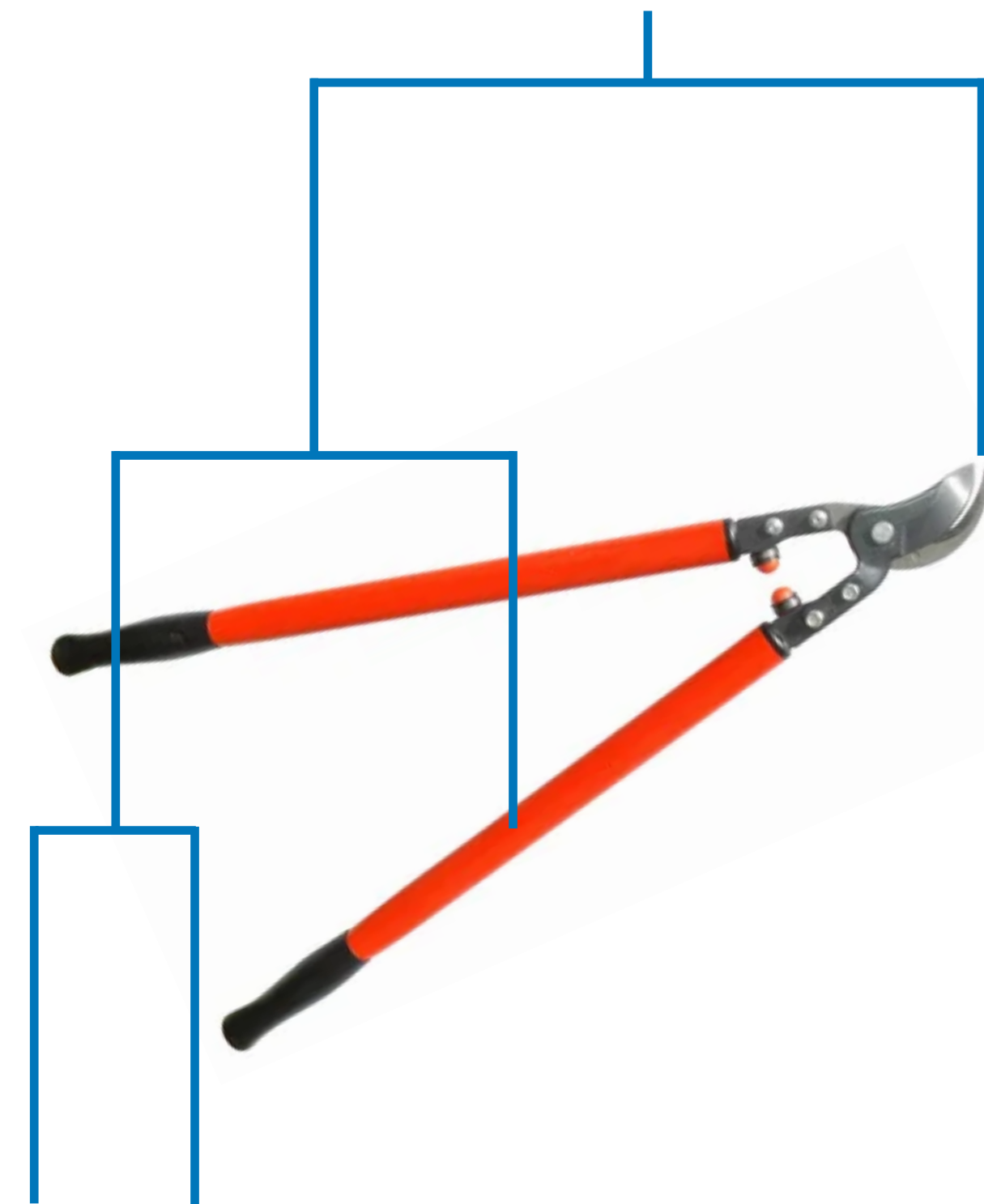
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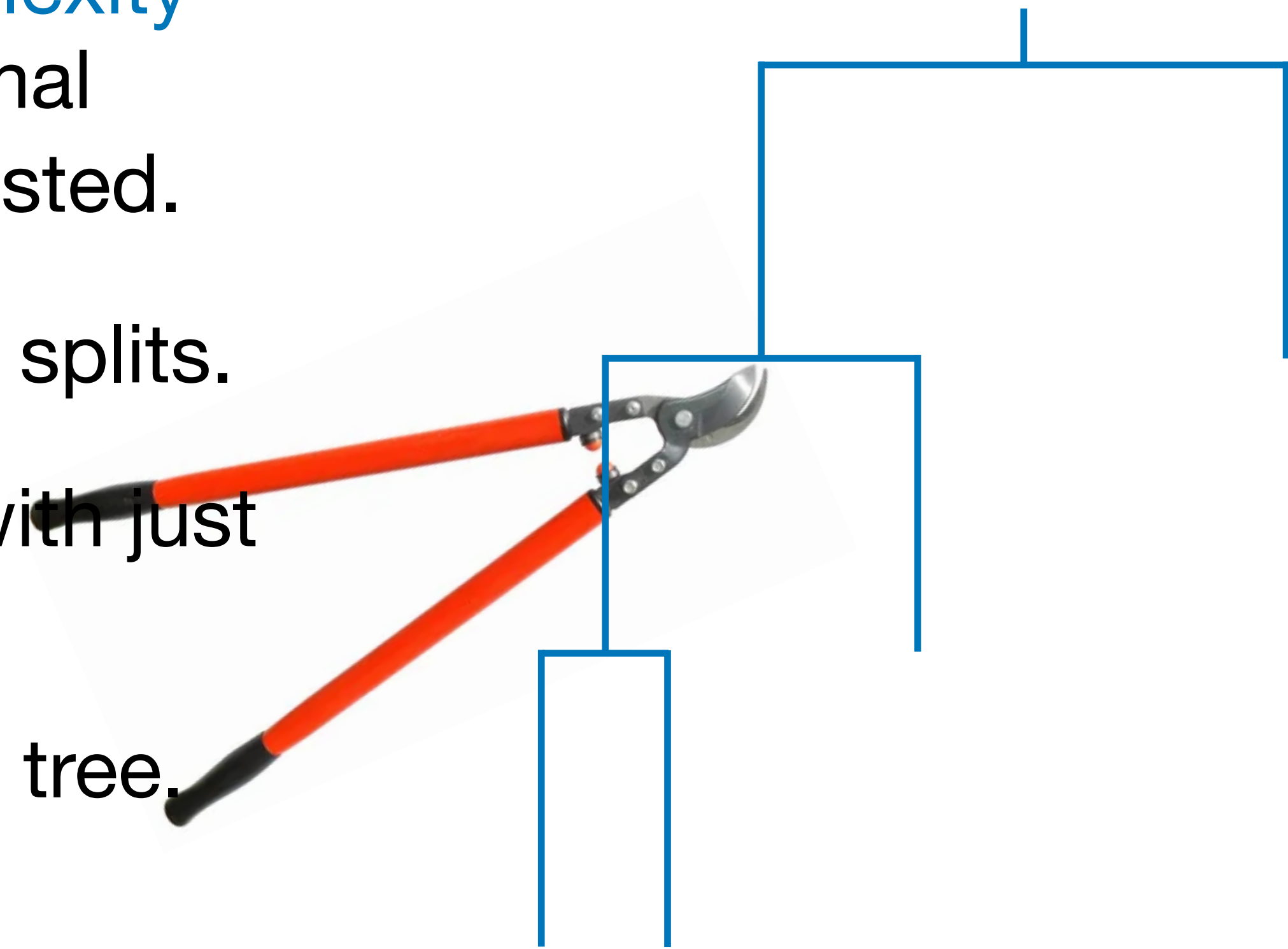
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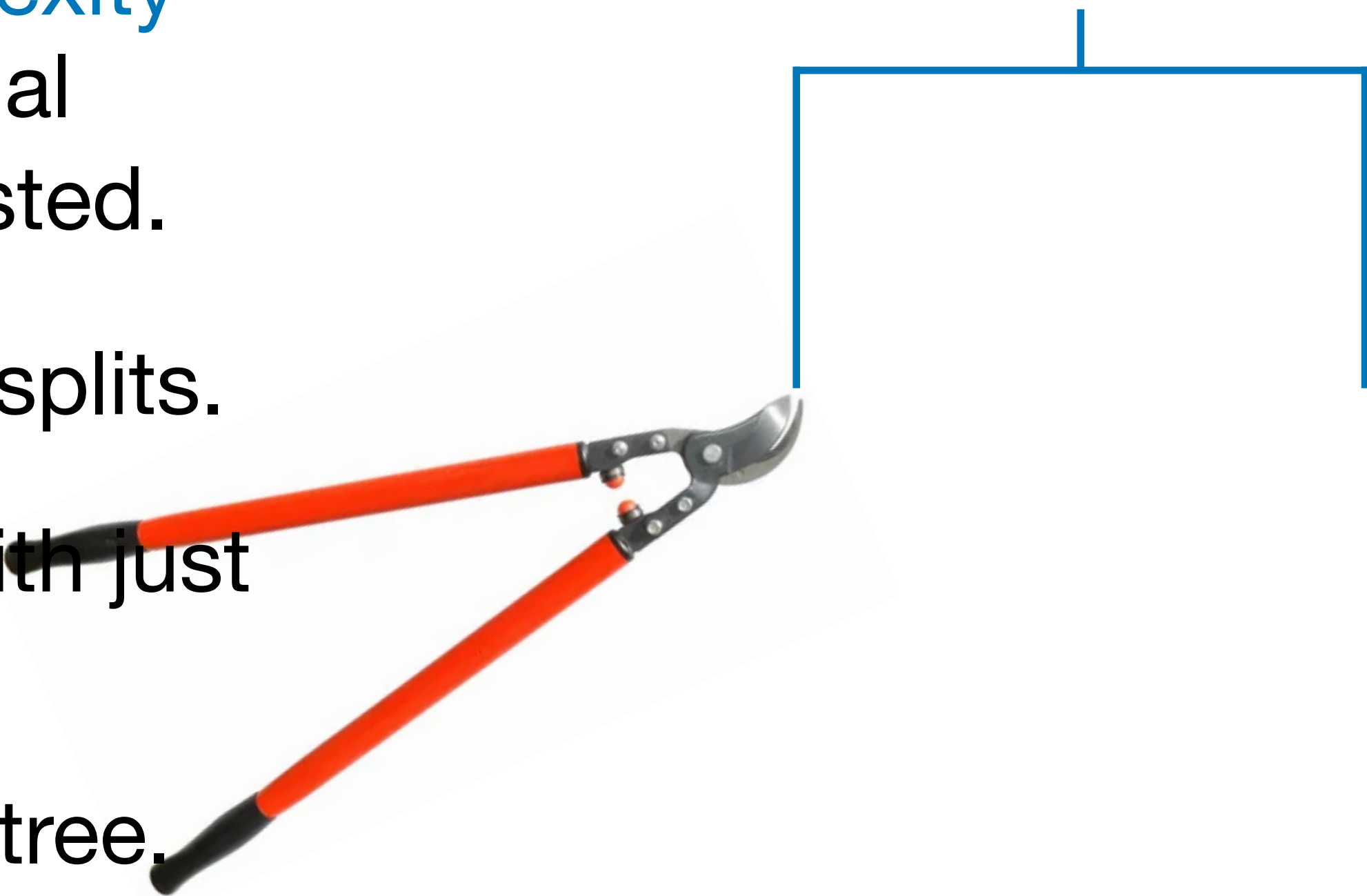
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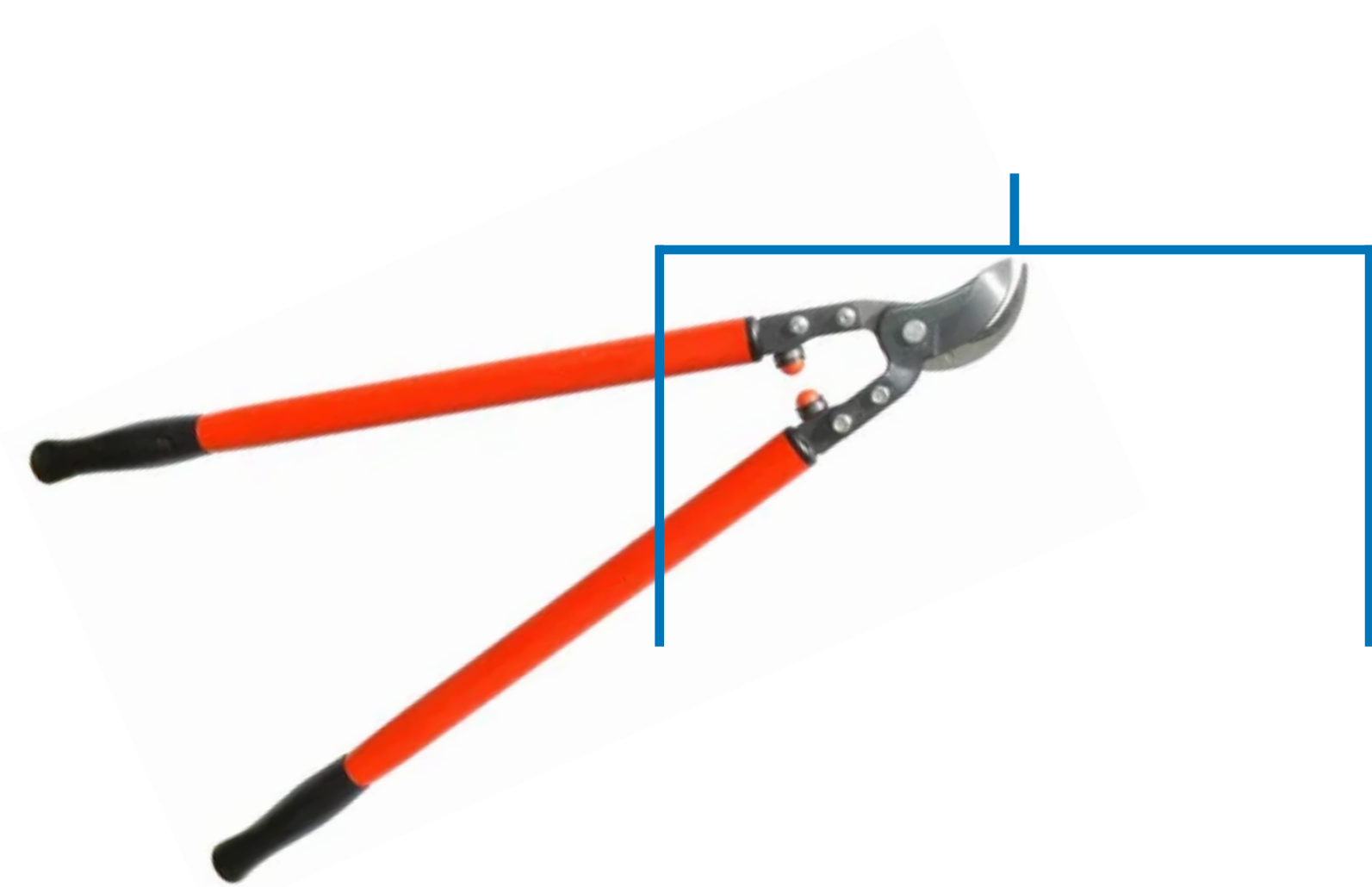
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 - Analogy with lasso: The variables selected for the same λ across different CV folds might be different.
 - Fitting to entire training data happens at the beginning of the process (for trees) rather than at the end (for lasso).

Illustration: Tree growing and pruning

Step 1: Grow tree on whole training data in greedy fashion to get T_0 .

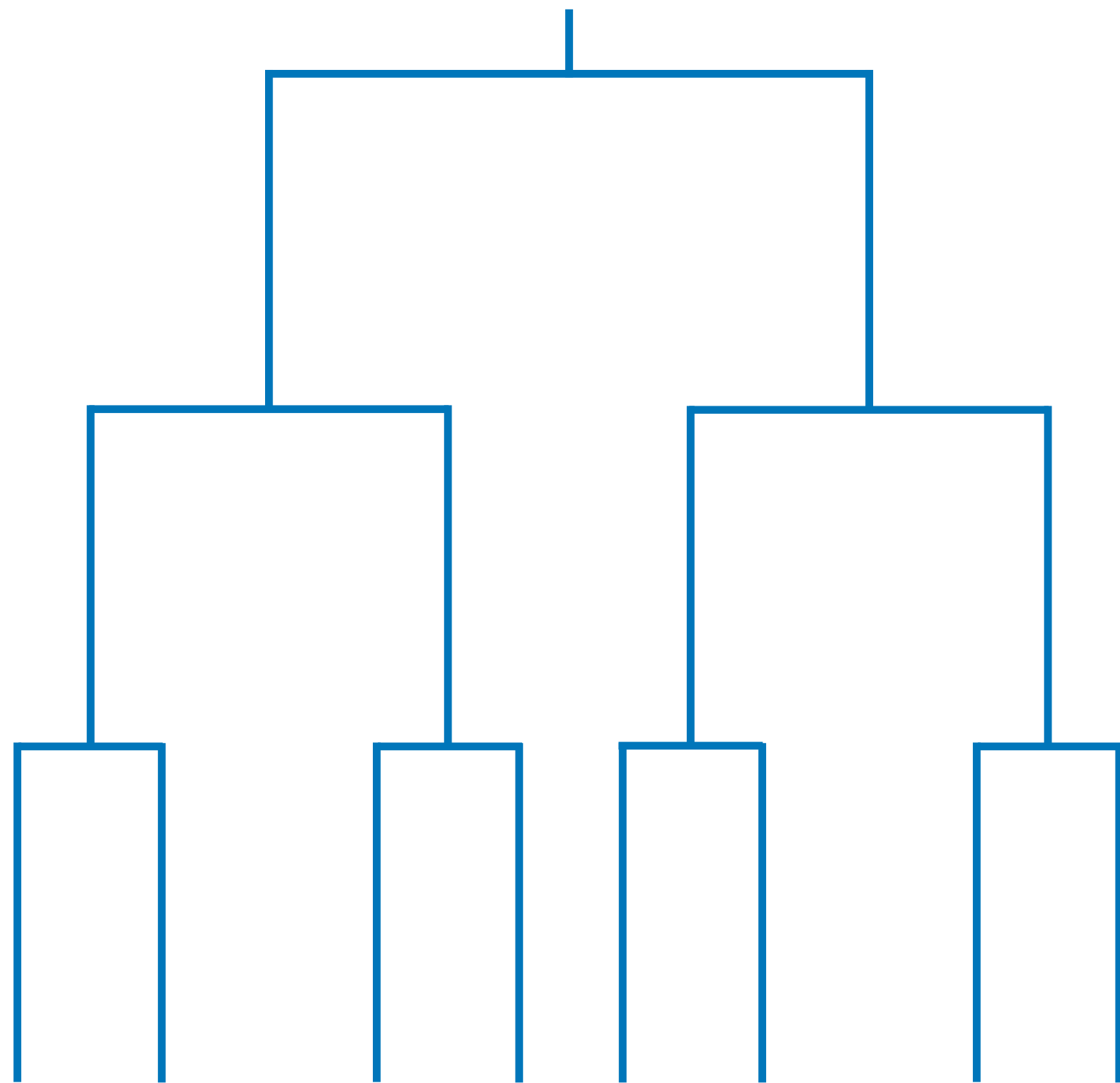
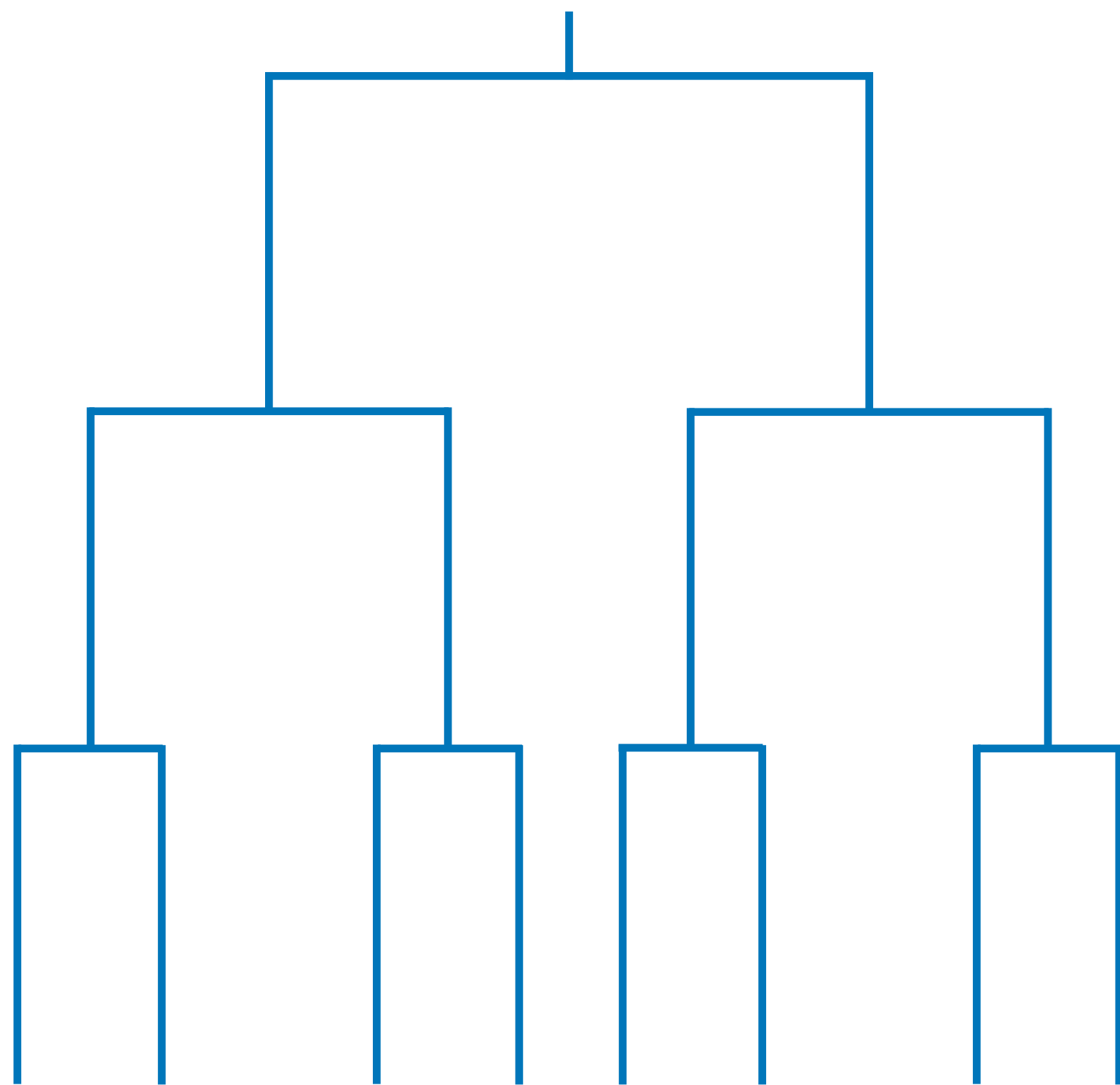


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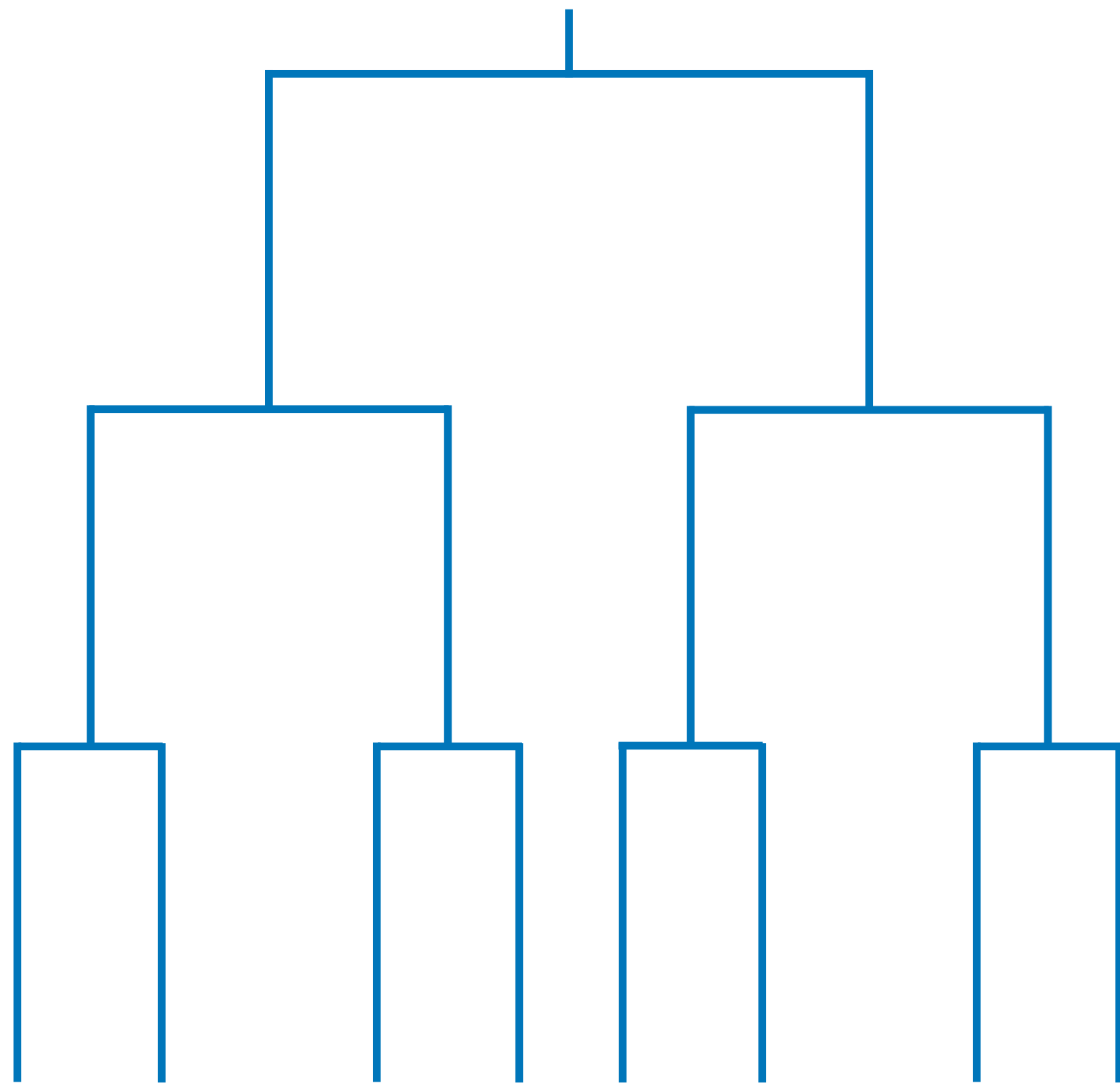
Step 2: Consider penalized objective function.



$$T_{\alpha} = \arg \min_{T \subseteq T_0} \{ \text{RSS}(T) + \alpha |T| \}$$

Illustration: Tree growing and pruning

Step 3: Sweep α from 0 to infinity, giving a nested sequence of trees.



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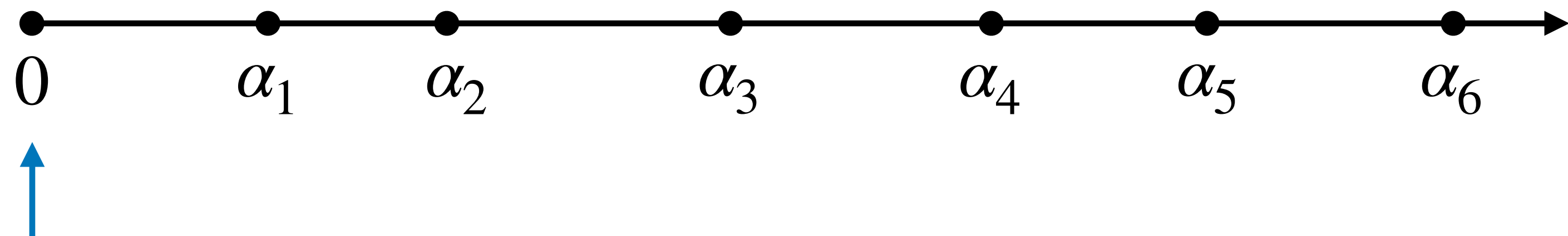


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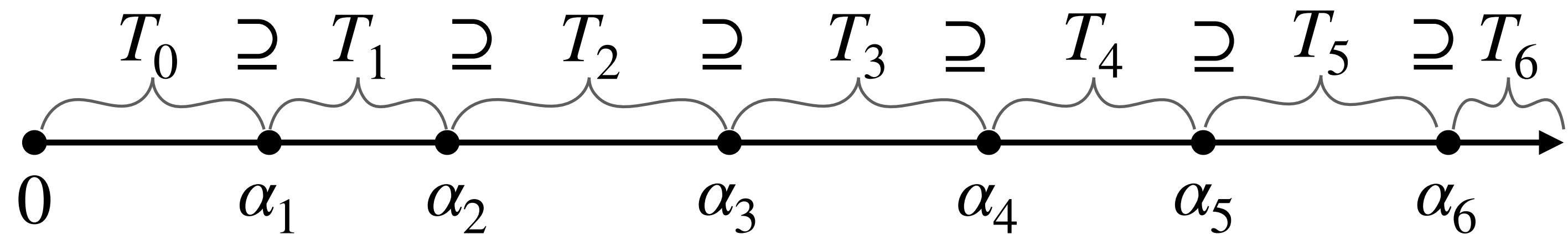


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Step 4: Choose a representative value of α for each tree.

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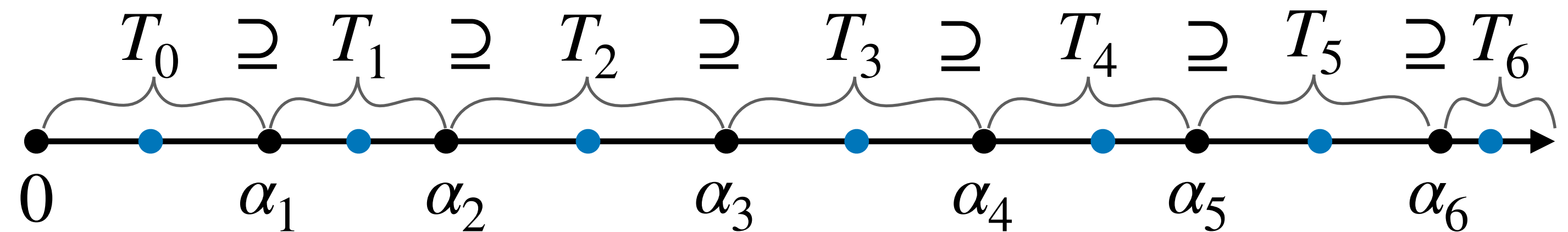
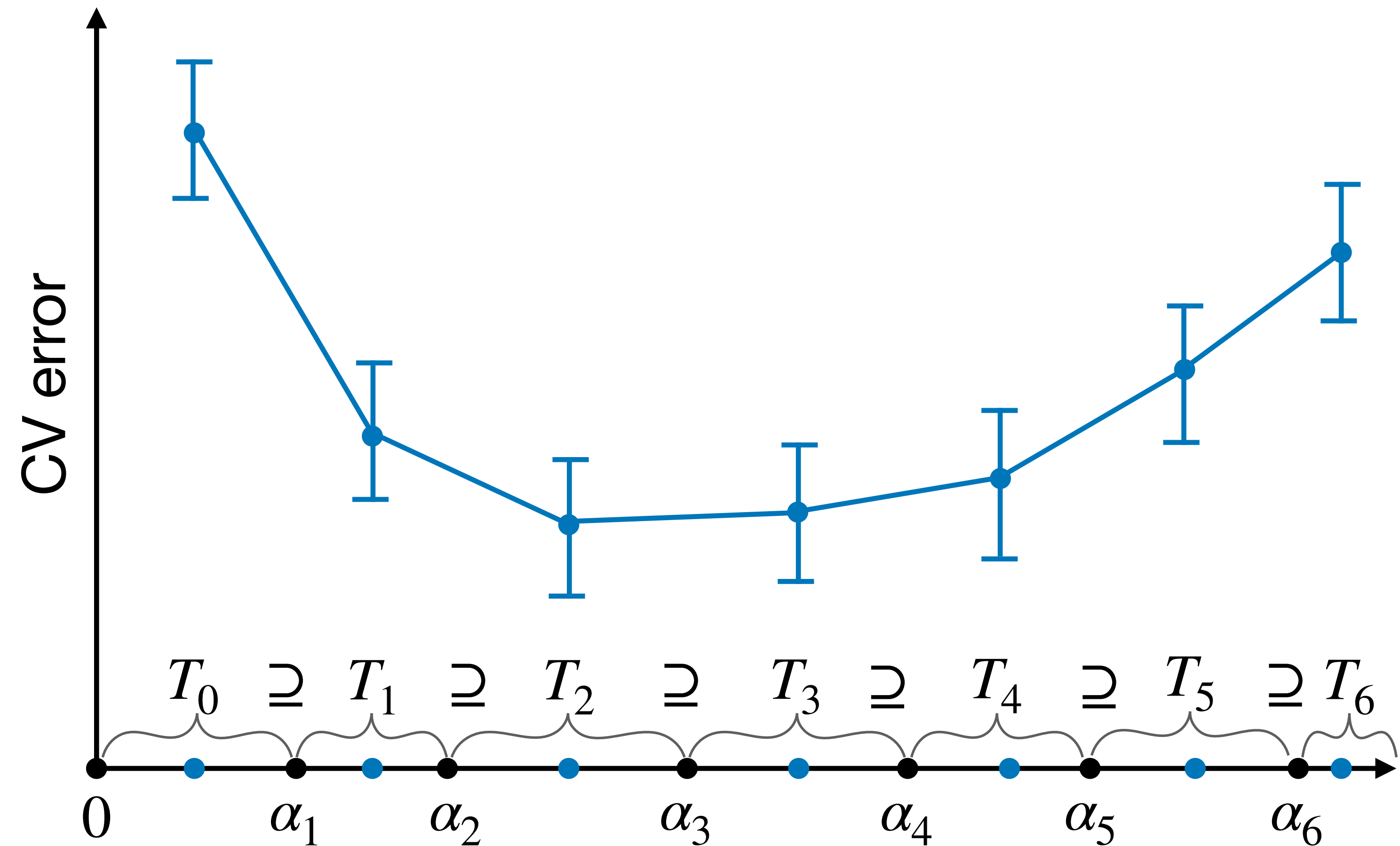


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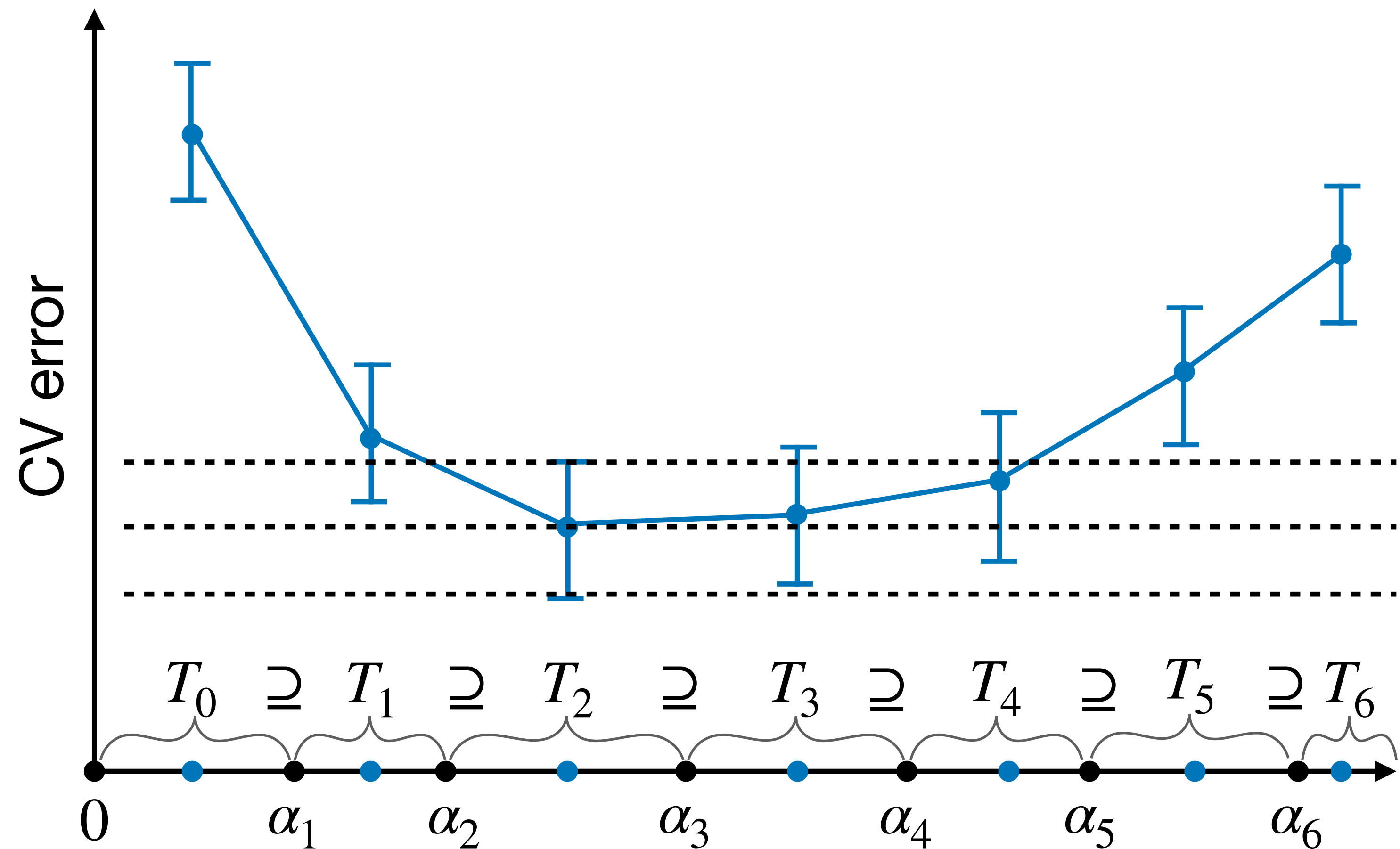
Step 5: Cross-validate over the representative values of α .



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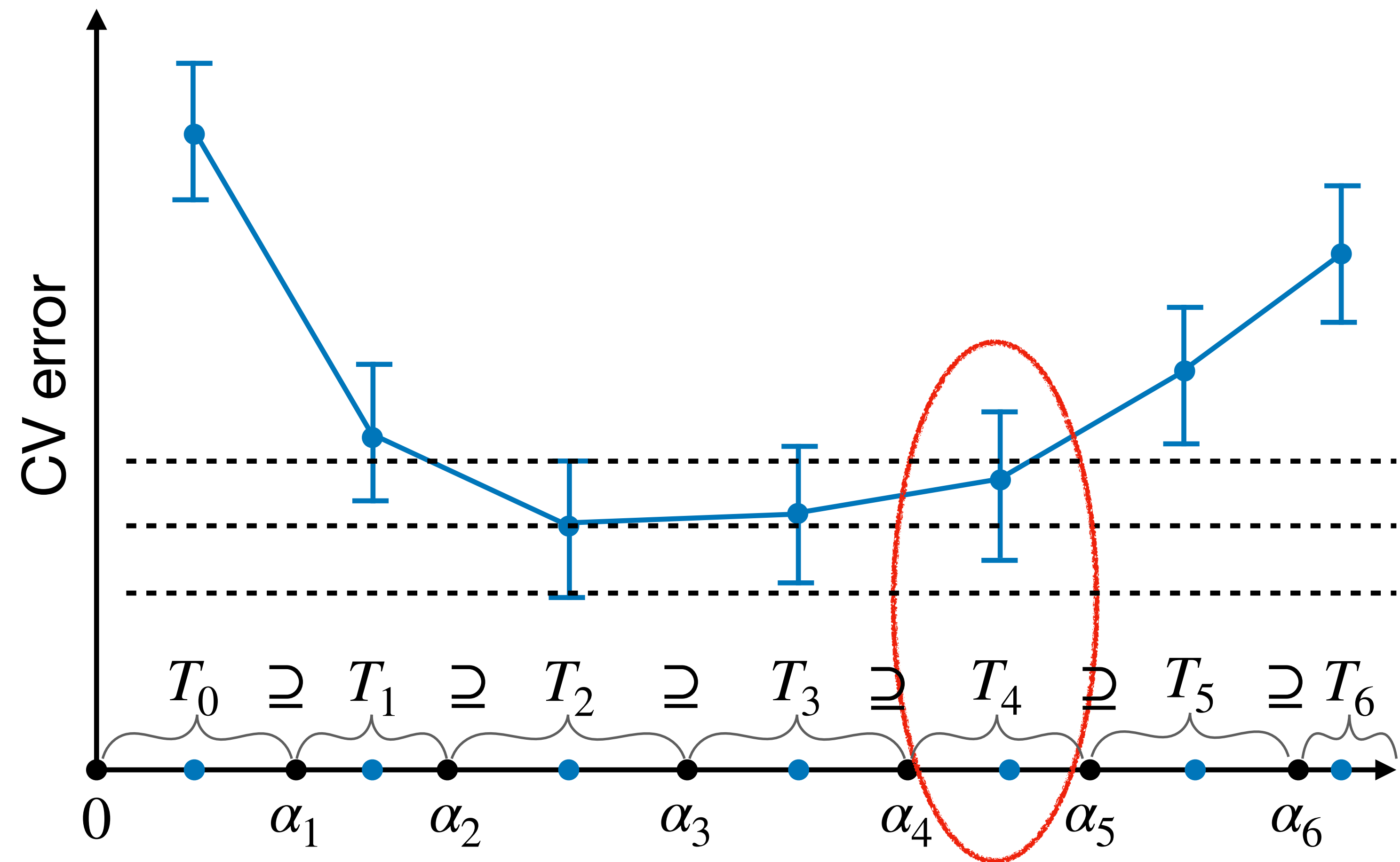
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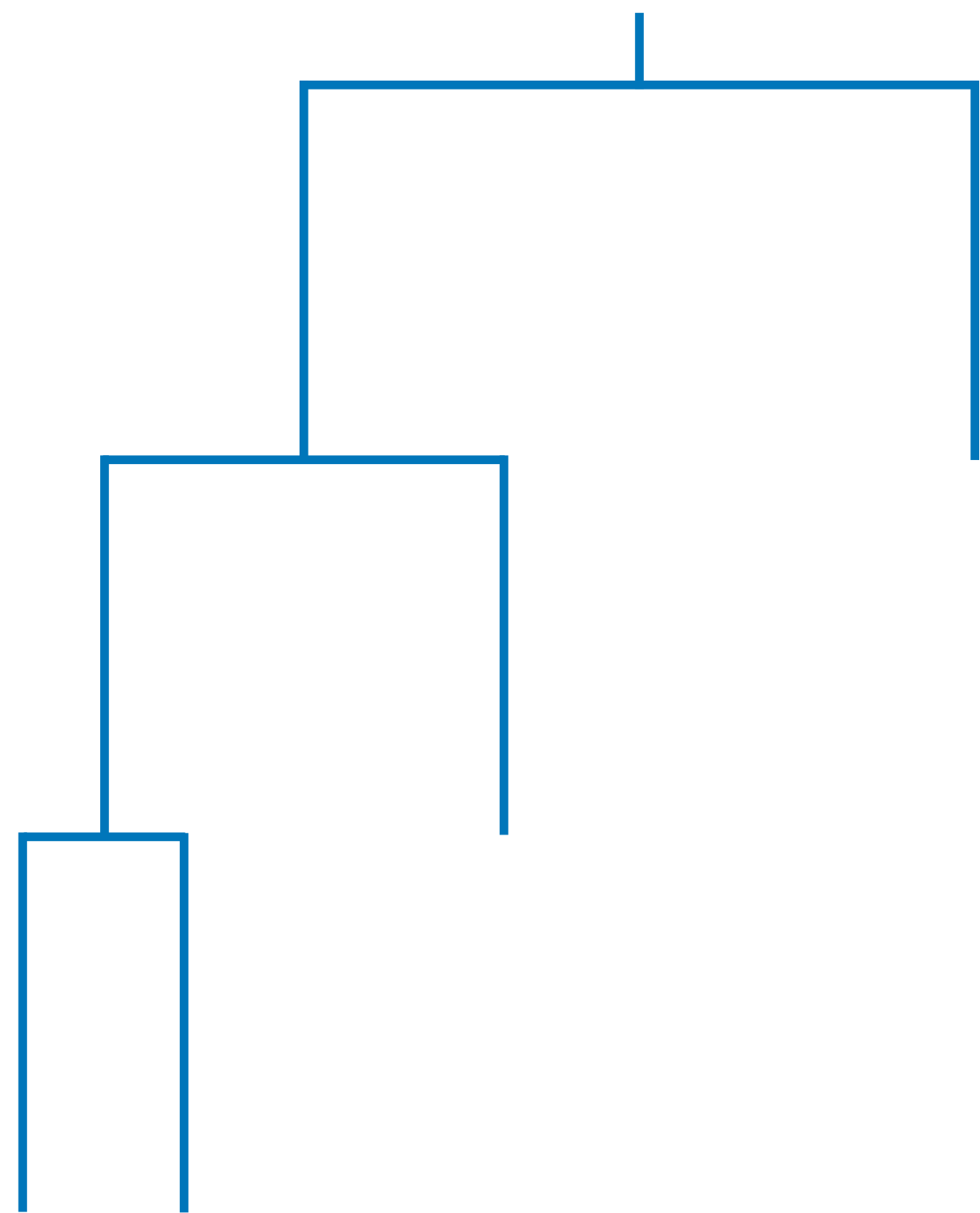
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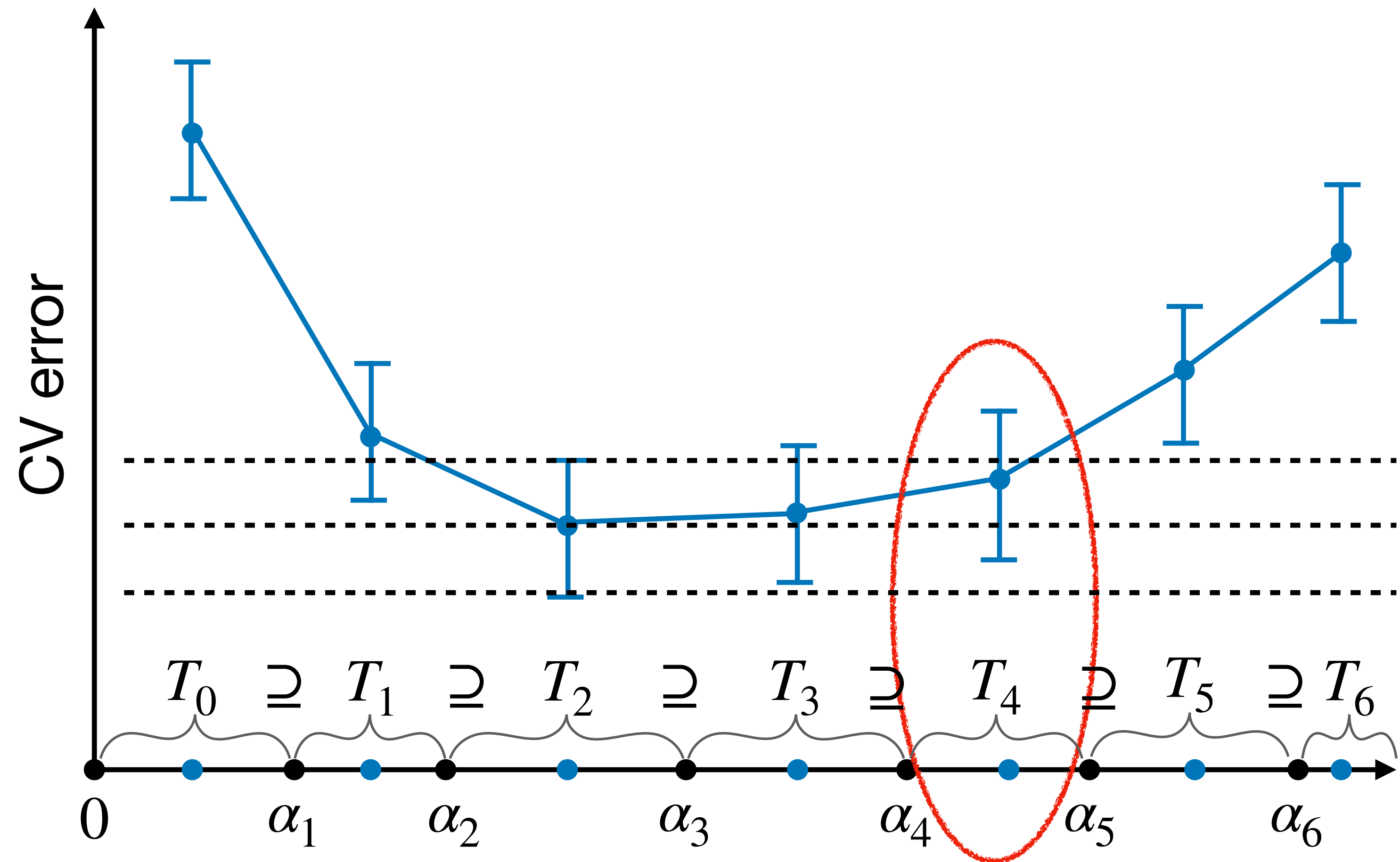
$$T_\alpha = \arg \min_{T \subseteq T_0} \{ \text{RSS}(T) + \alpha |T| \}$$

Illustration: Tree growing and pruning

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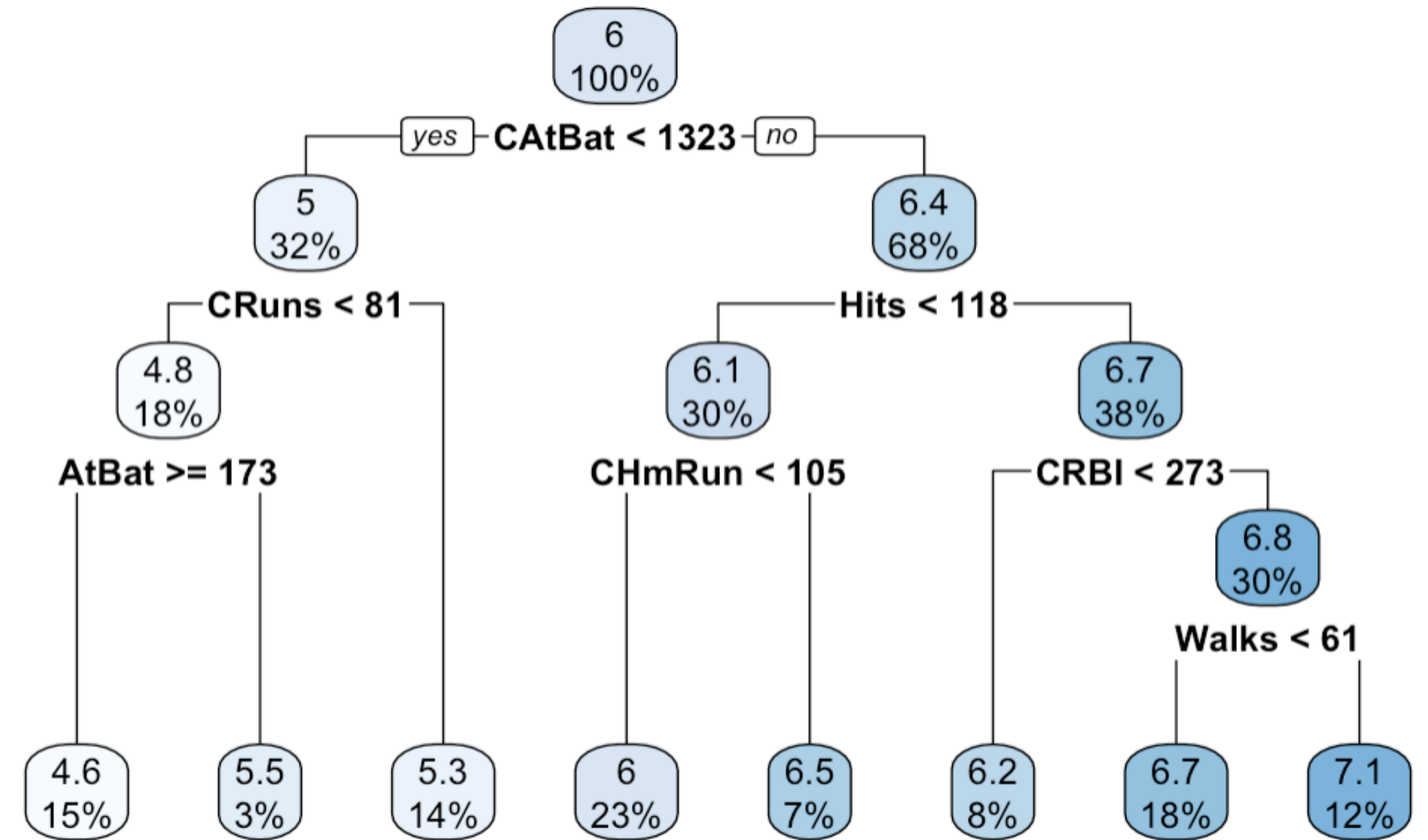
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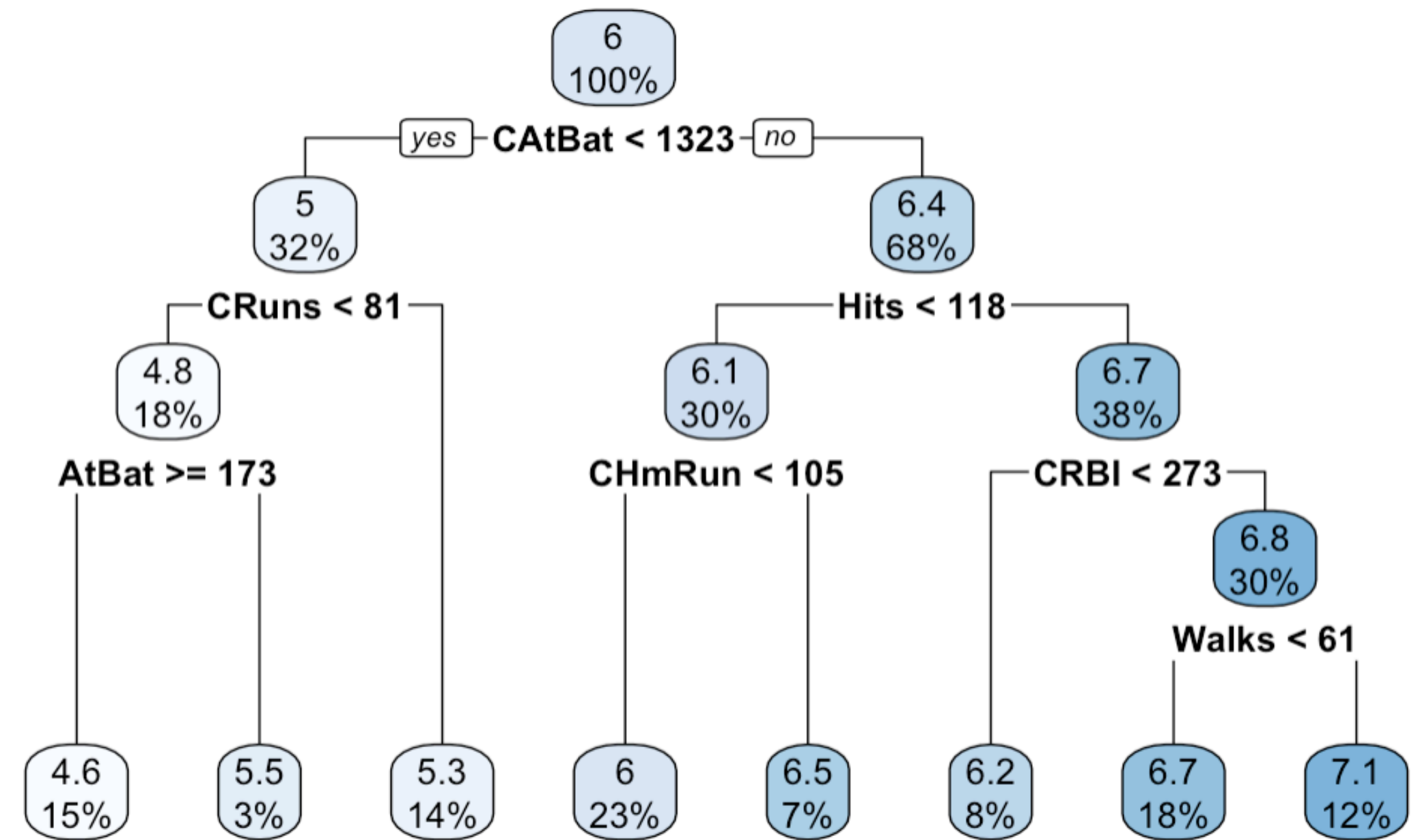
Growing and pruning both define a sequence of trees, but it may not be the same sequence. The sequence of trees for growing not used except to get the big tree T_0 ; the sequence of trees for pruning is the one used for cross-validation.

Summary: Decision Trees



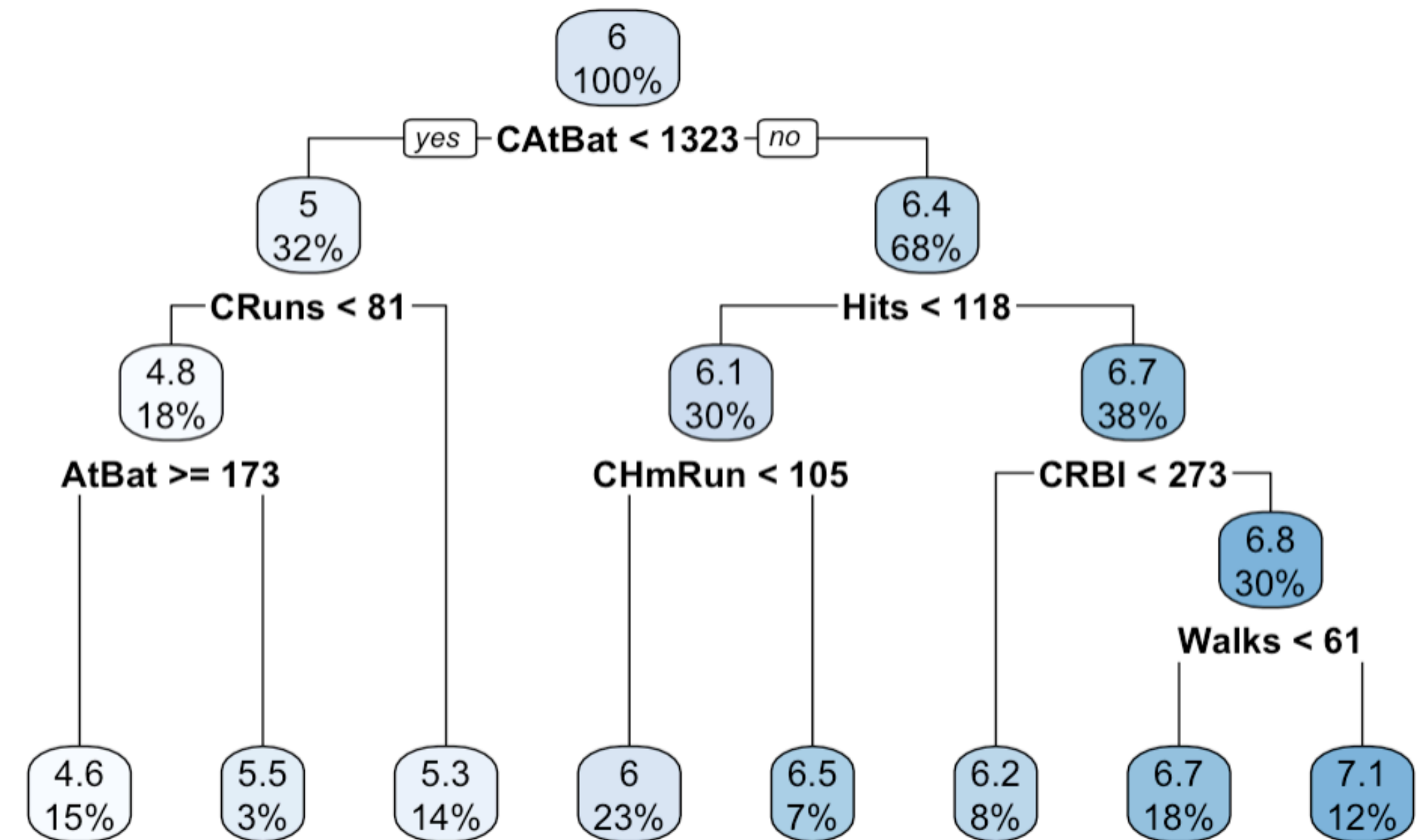
Summary: Decision Trees

- Nonlinear method for regression or classification based on recursive partitioning of feature space



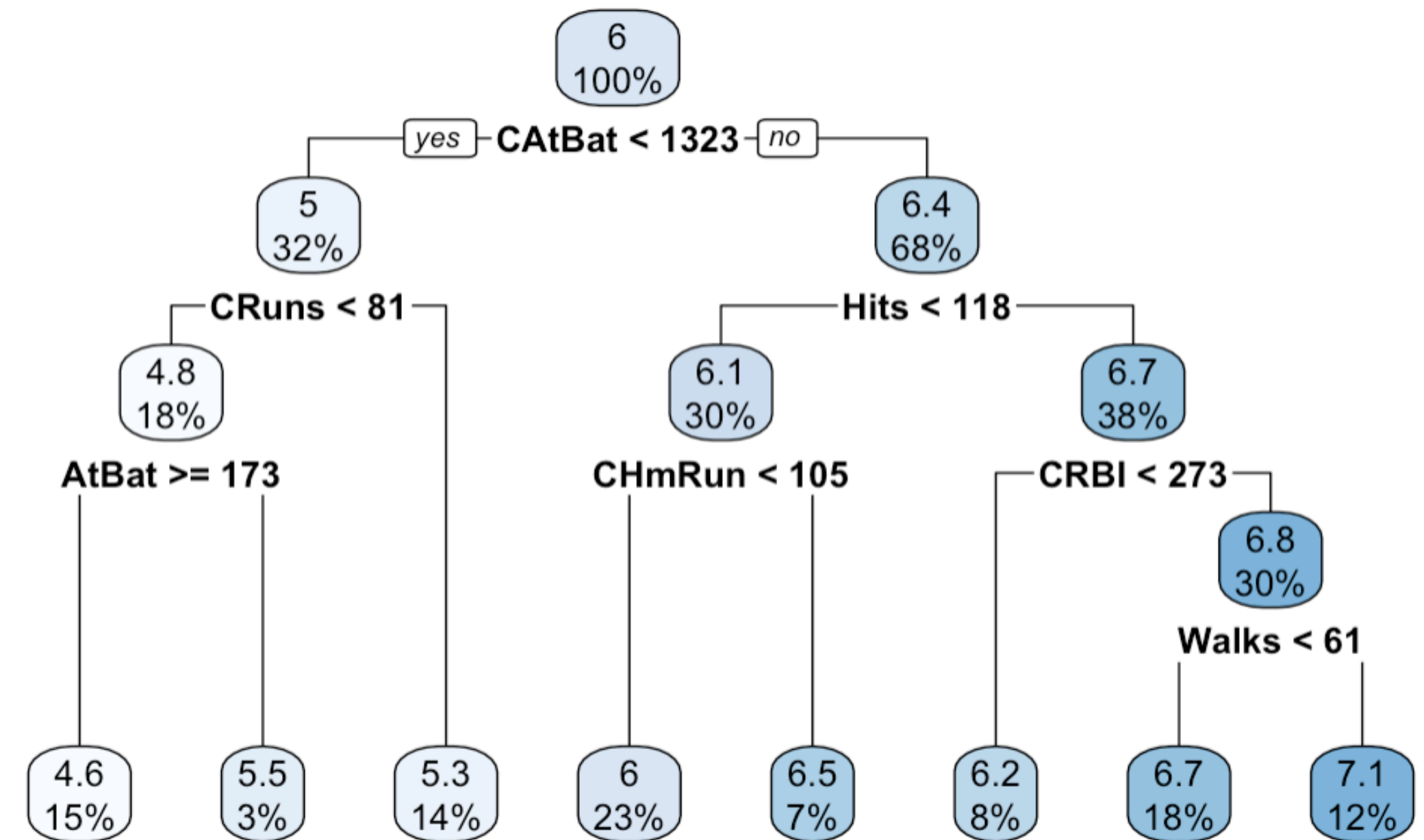
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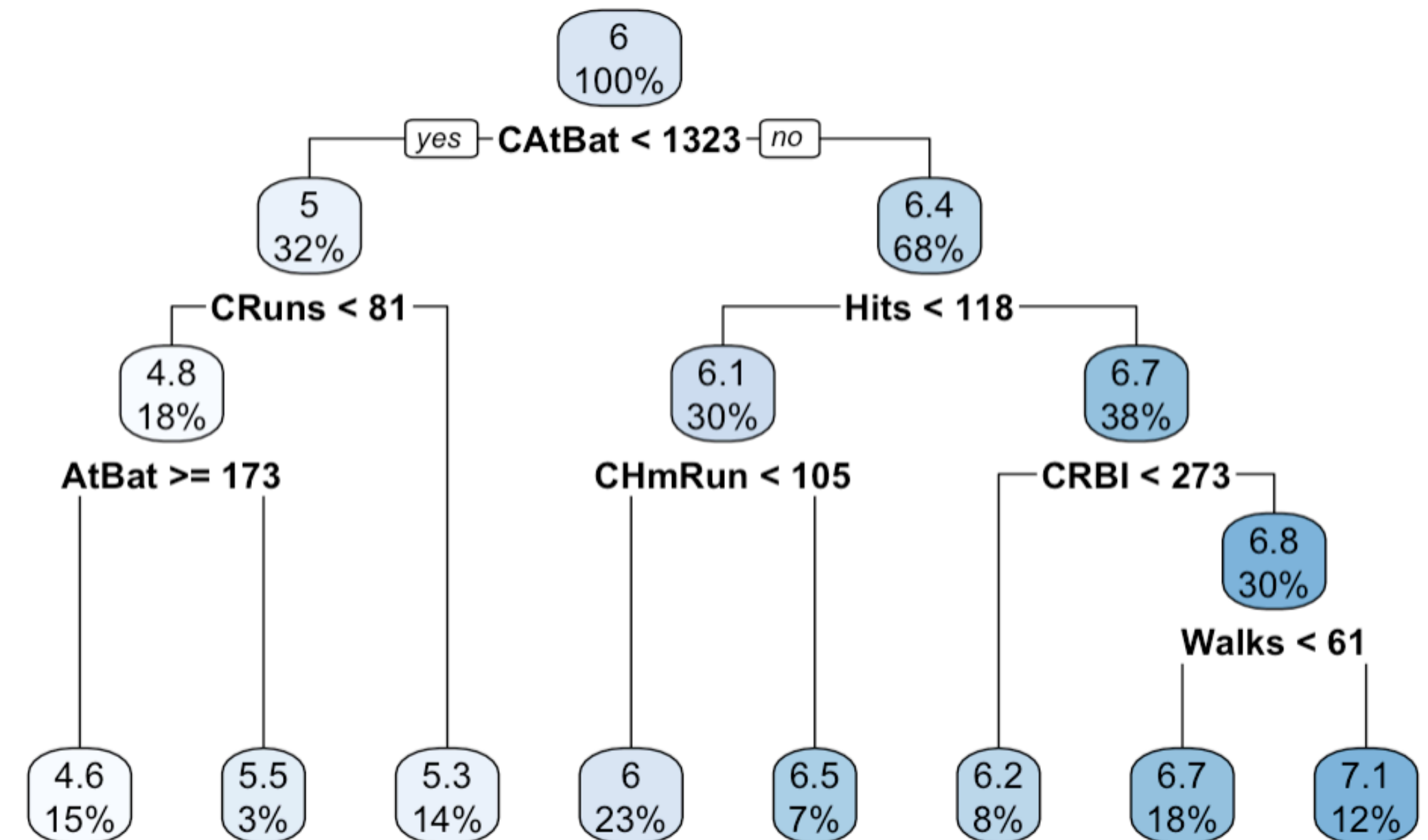
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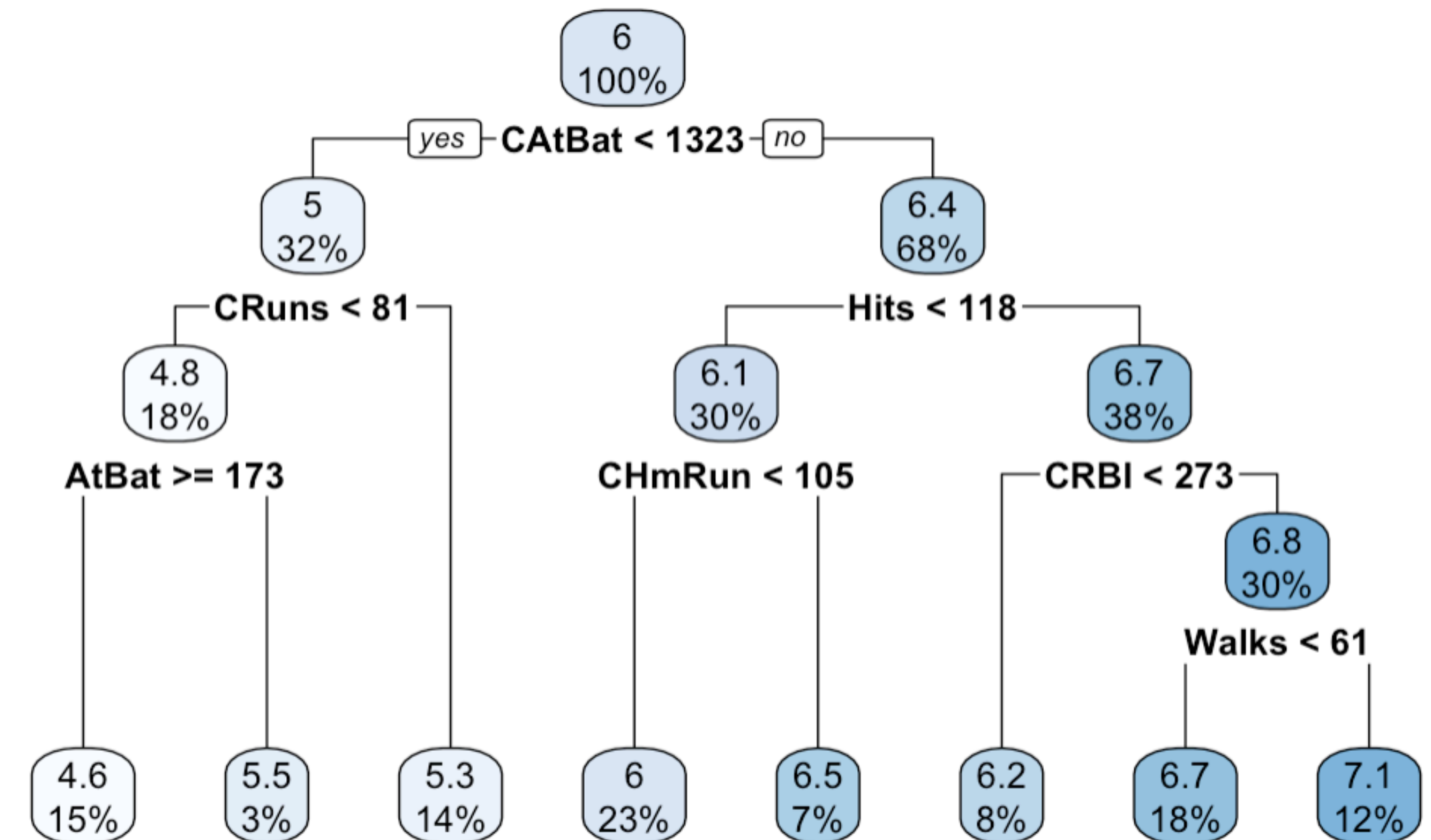
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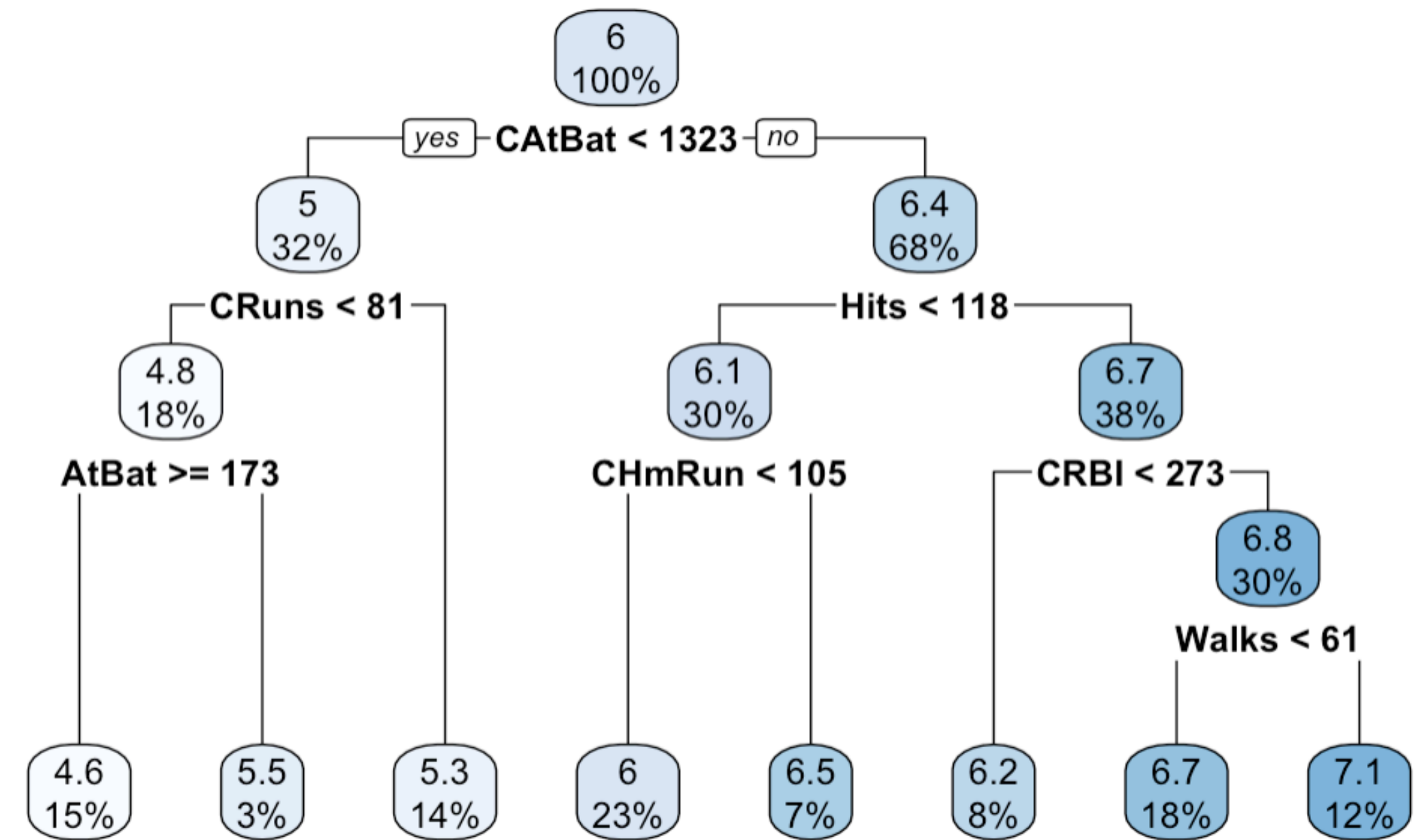
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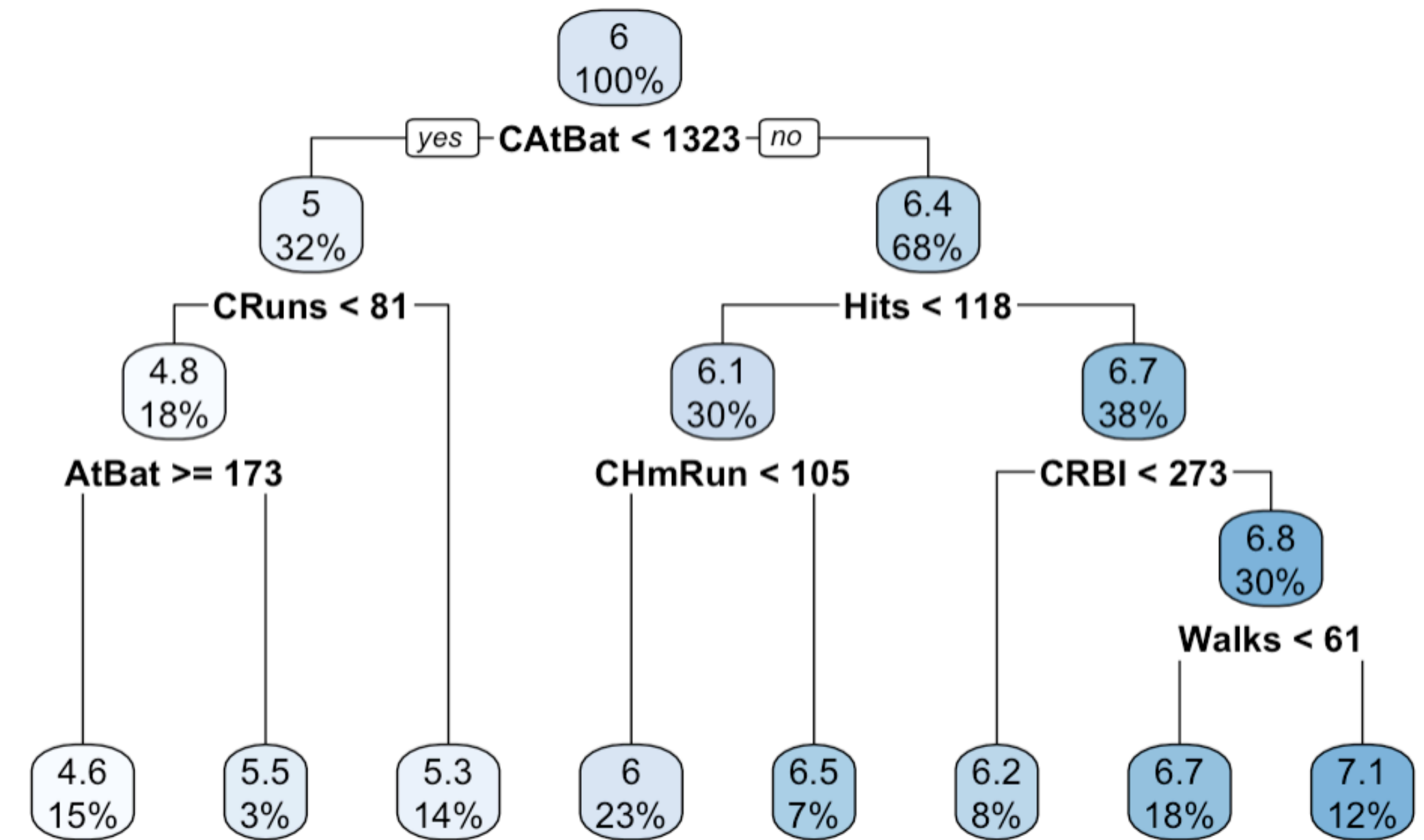
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Pros
Easily interpretable
Captures non-linear relationships

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Pros	Cons
Easily interpretable	Tree structure very sensitive to training data
Captures non-linear relationships	High variance predictions; suboptimal predictive performance

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Intuition: By averaging a bunch of trees, we are reducing the variance while keeping the bias about the same. This should yield better predictive performance!

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A **bootstrap sample** is a new data set with the same number of observations, generating by sampling observations from the original data **with replacement**.

The idea is that your bootstrap samples are slightly different versions of your training data, allowing you to fit different trees to these different training sets.

The bootstrap: An example

Original training data

Observation ID	X	Y
1	X_1	Y_1
2	X_2	Y_2
3	X_3	Y_3
4	X_4	Y_4
5	X_5	Y_5

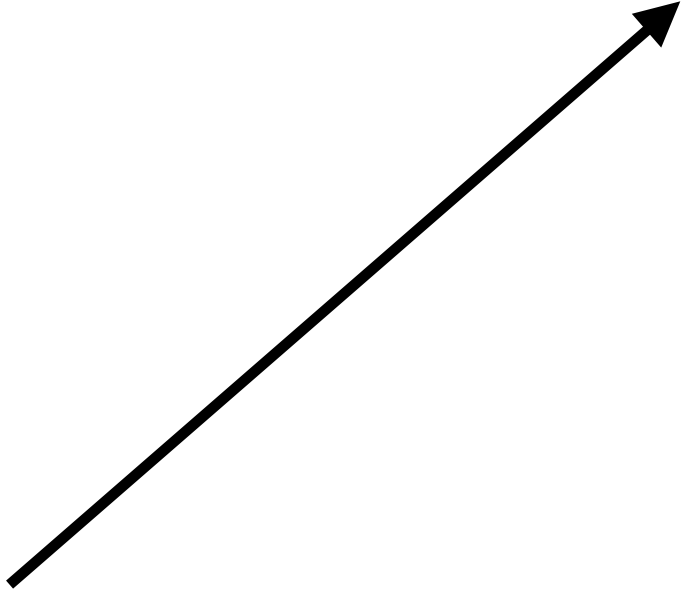
The bootstrap: An example

Bootstrap sample 1

Observation ID	X	Y
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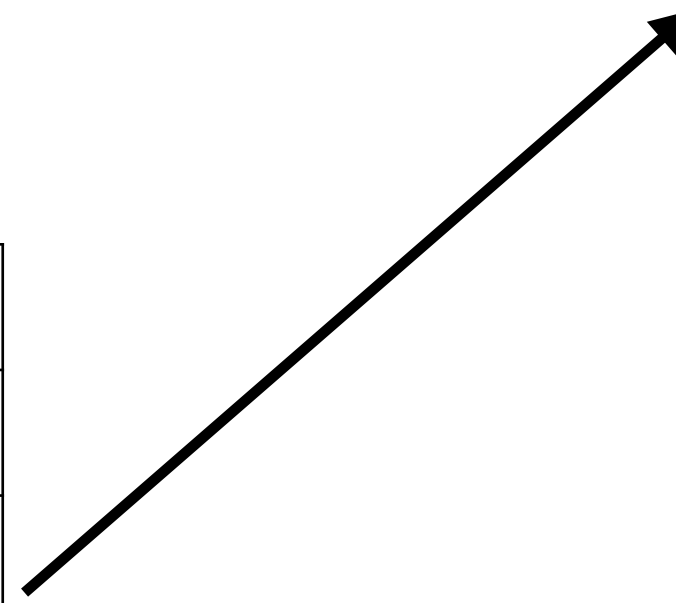
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Observation ID	X	Y
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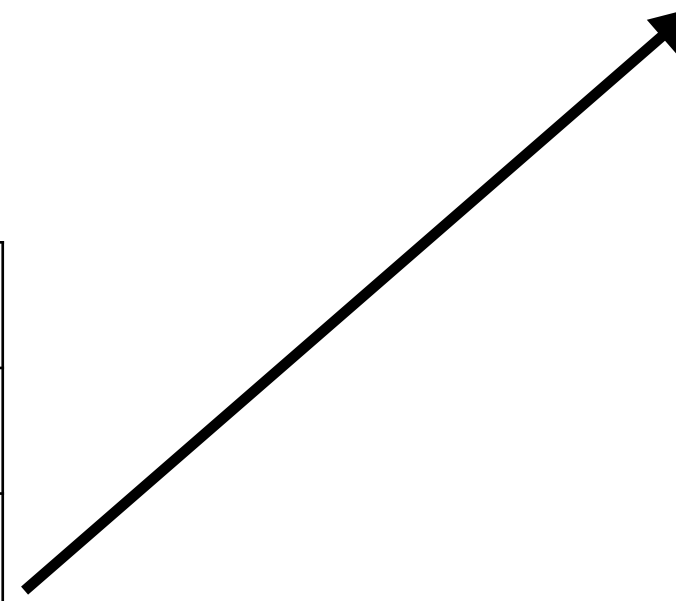
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Bootstrap sample 1

Observation ID	X	Y
5	X_5	Y_5
3	X_3	Y_3

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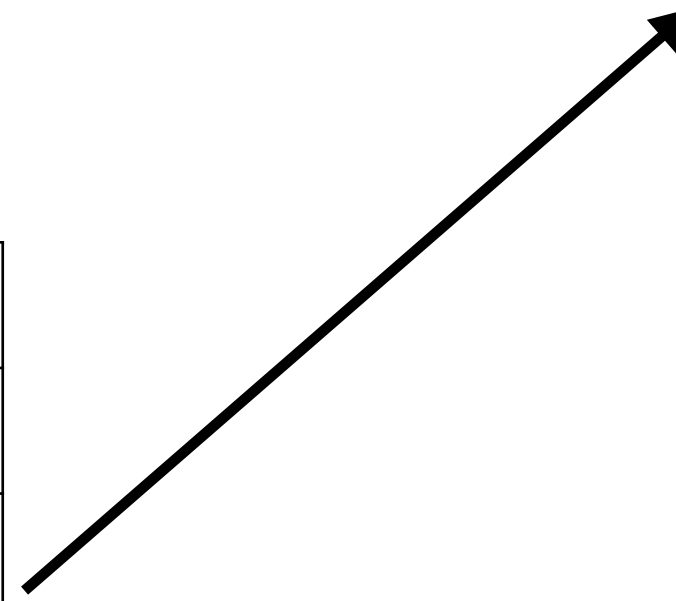
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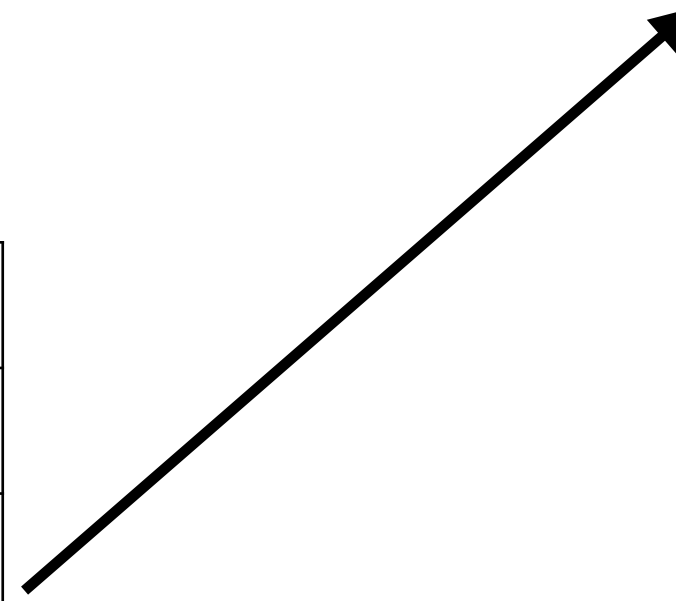
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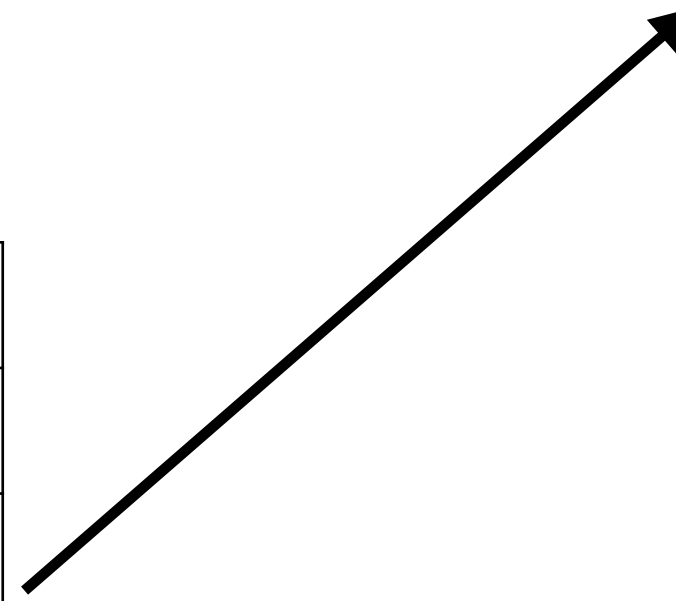
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5	X_5	Y_5
3	X_3	Y_3
2	X_2	Y_2
3	X_3	Y_3
1	X_1	Y_1

⋮

⋮

Bootstrap sample B

Observation ID	X	Y
4	X_4	Y_4
1	X_1	Y_1
1	X_1	Y_1
5	X_5	Y_5
4	X_4	Y_4

Bagging

Original training data

Obs ID	X	Y
1	X_1	Y_1
2	X_2	Y_2
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Bootstrap sample 1

Obs ID	X	Y
5	X_5	Y_5
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⋮

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→ T^{*1}

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→ T^{*1}

⋮

→ T^{*b}

⋮

⋮

Bootstrap sample B

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Obs ID	X	Y
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→ T^{*B}

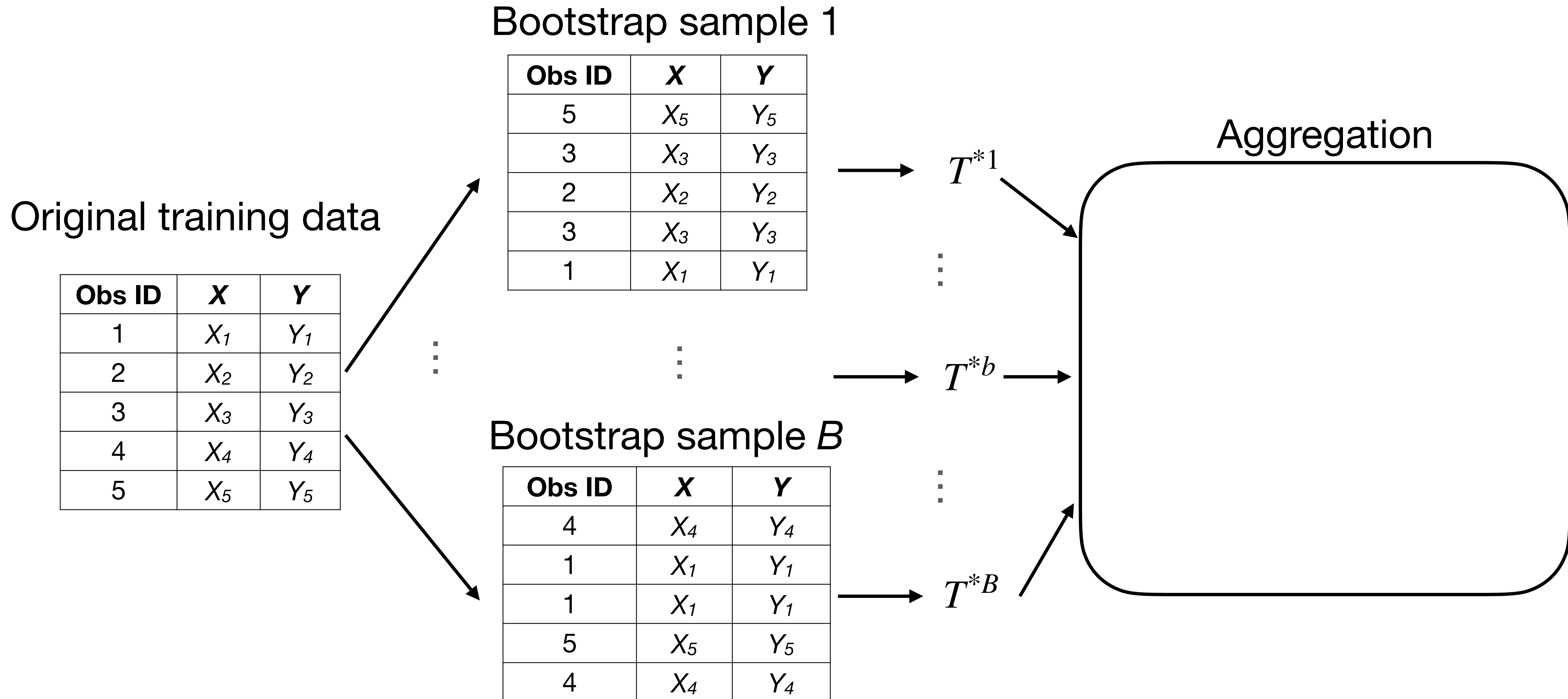
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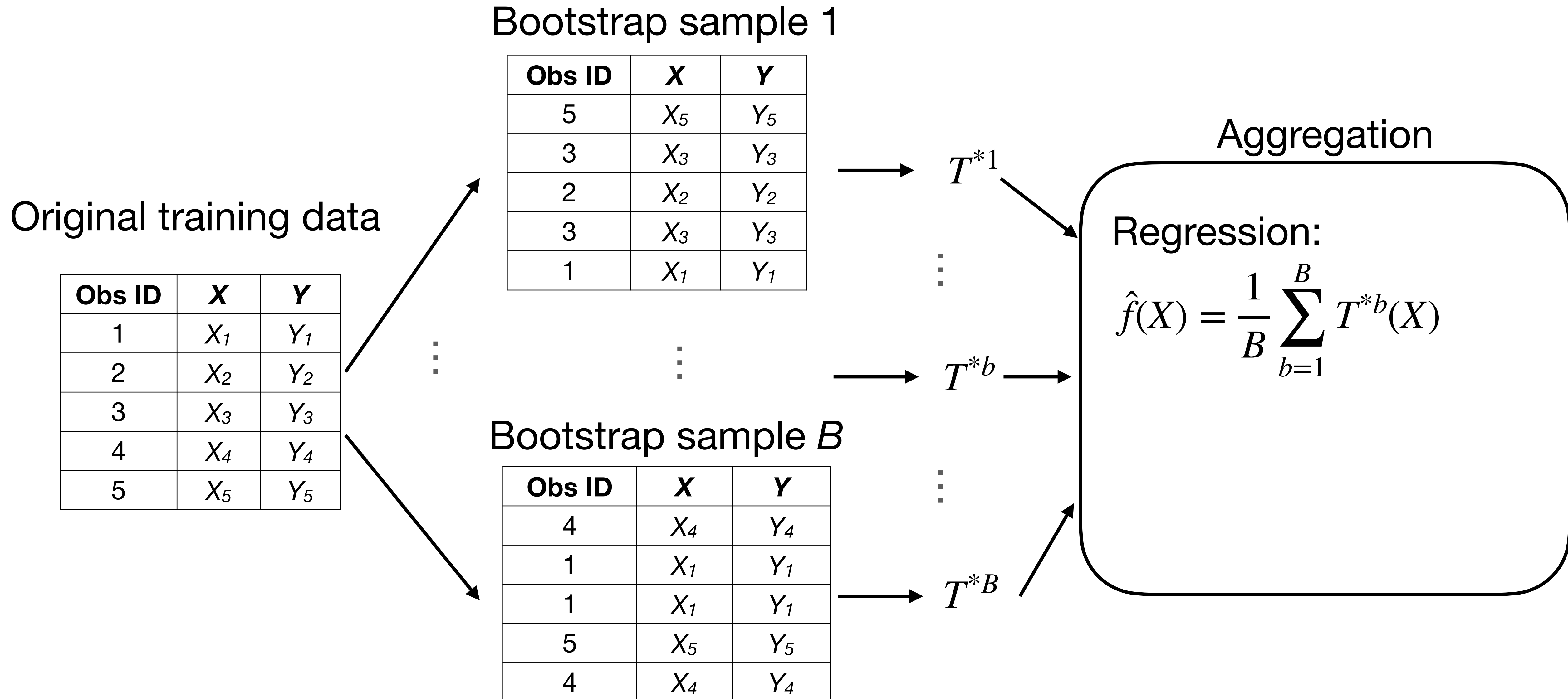
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