

On Computing Optimal Tree Ensembles

Christian Komusiewicz¹, Pascal Kunz^{2,3}, Frank Sommer¹, and Manuel Sorge⁴

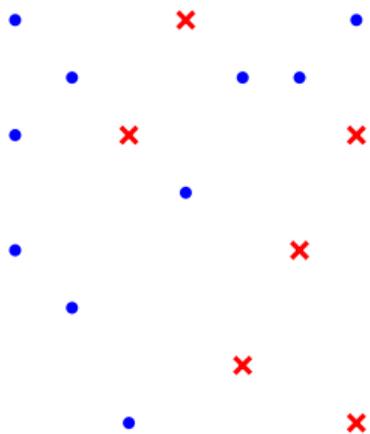
¹Friedrich-Schiller-Universität Jena, Germany

²TU Berlin, Germany

³HU Berlin, Germany

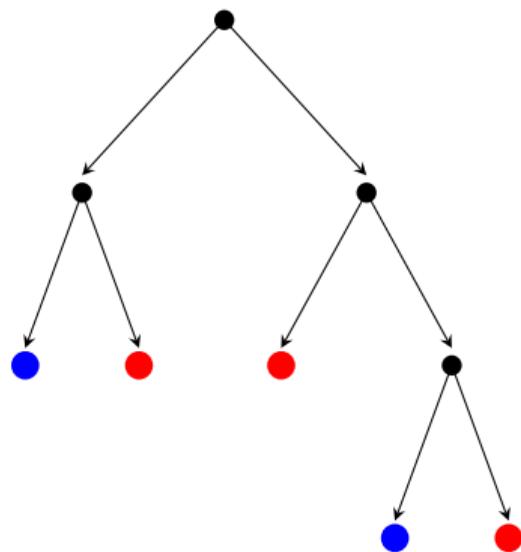
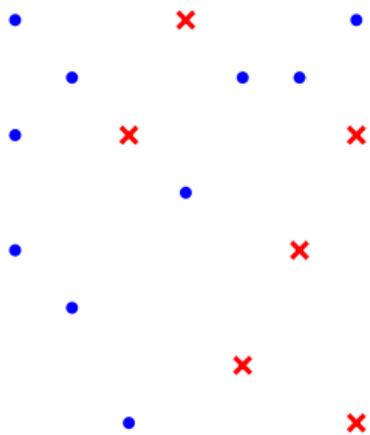
⁴TU Wien, Austria

ICML 2023



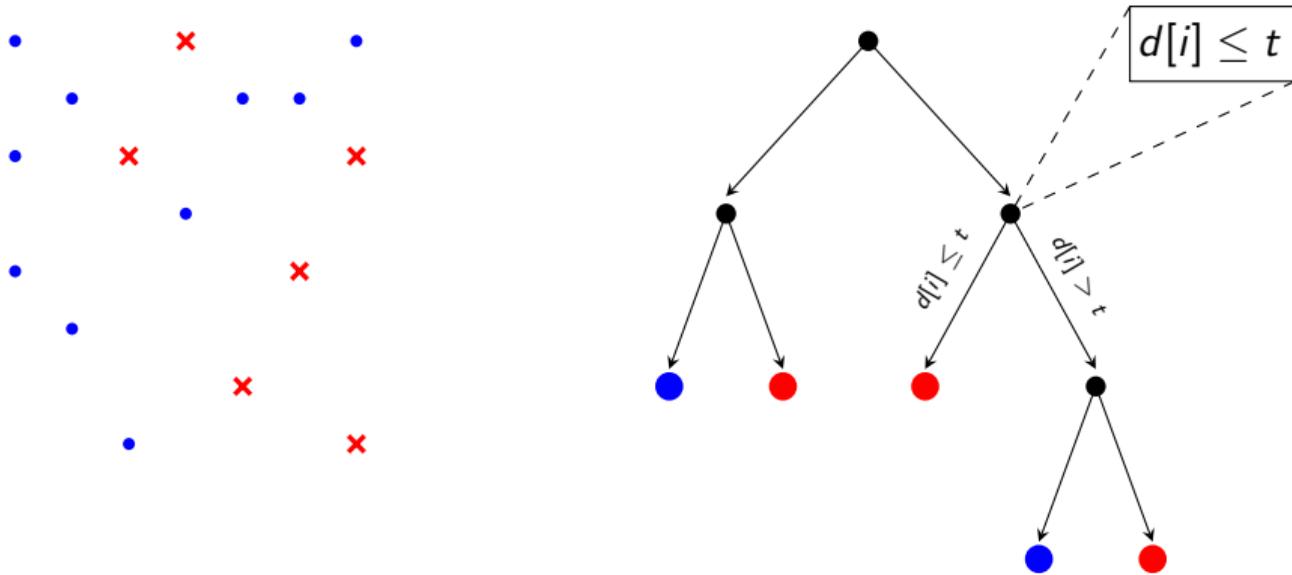
Input: Training data set of n points in d dimensions and two classes **red** and **blue**.

Task: Compute a decision tree of minimal size that classifies each example correctly.
(no misclassifications allowed)



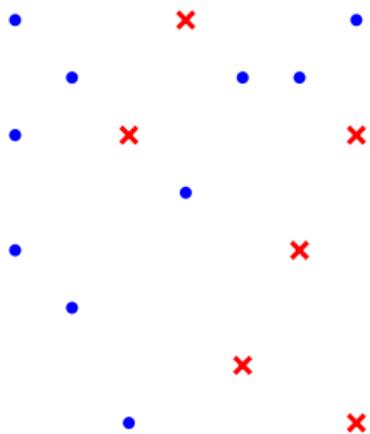
Input: Training data set of n points in d dimensions and two classes **red** and **blue**.

Task: Compute a decision tree of minimal size that classifies each example correctly.
(no misclassifications allowed)



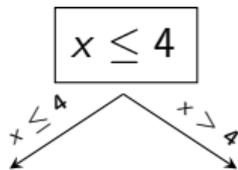
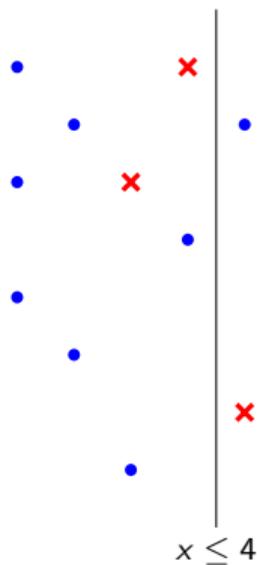
Input: Training data set of n points in d dimensions and two classes red and blue.

Task: Compute a decision tree of minimal size that classifies each example correctly.
(no misclassifications allowed)



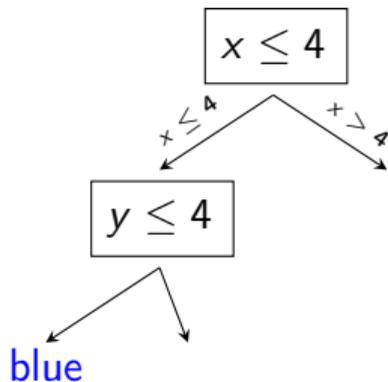
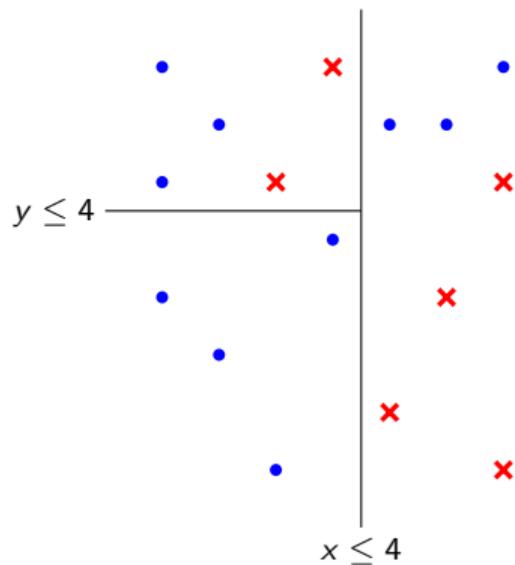
Input: Training data set of n points in d dimensions and two classes **red** and **blue**.

Task: Compute a decision tree of minimal size that classifies each example correctly.
(no misclassifications allowed)



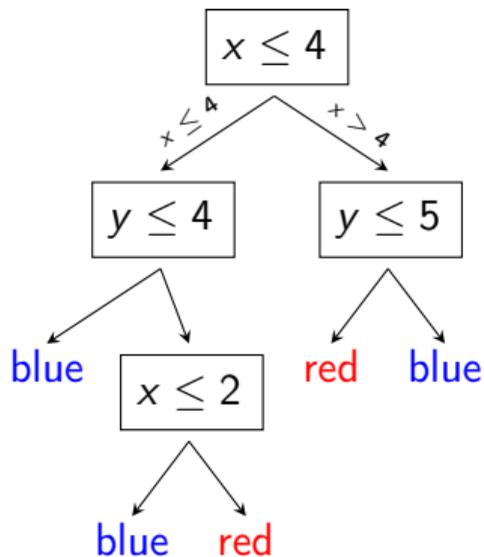
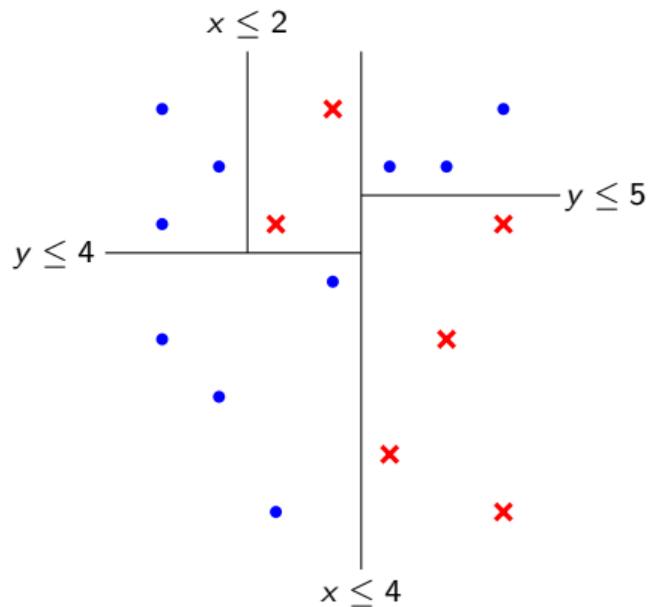
Input: Training data set of n points in d dimensions and two classes red and blue.

Task: Compute a decision tree of minimal size that classifies each example correctly.
(no misclassifications allowed)



Input: Training data set of n points in d dimensions and two classes **red** and **blue**.

Task: Compute a decision tree of minimal size that classifies each example correctly.
(no misclassifications allowed)



Input: Training data set of n points in d dimensions and two classes red and blue.

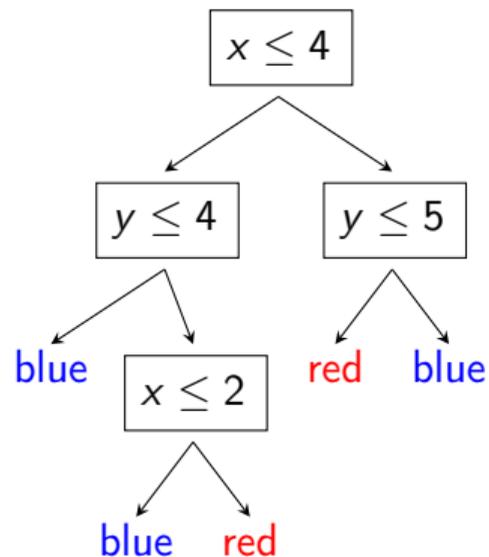
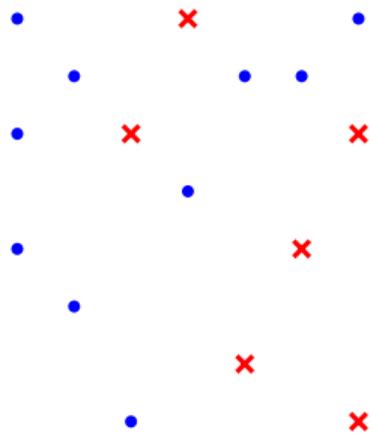
Task: Compute a decision tree of minimal size that classifies each example correctly.
(no misclassifications allowed)

Theorem (Hyafil and Rivest, *Inf. Process. Lett.* 1976)

Computing an optimal decision tree is NP-hard.

Theorem (Hyafil and Rivest, *Inf. Process. Lett.* 1976)

Computing an optimal decision tree is NP-hard.



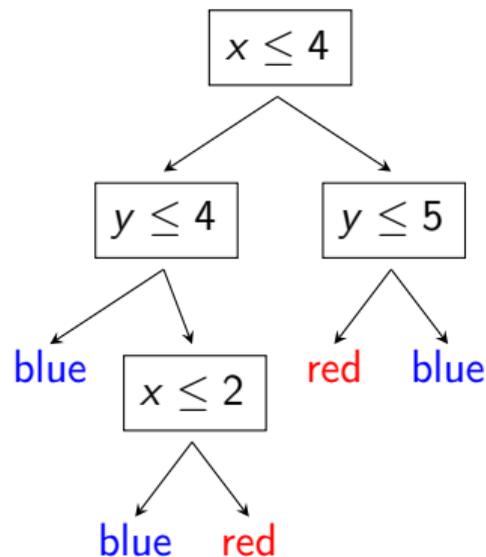
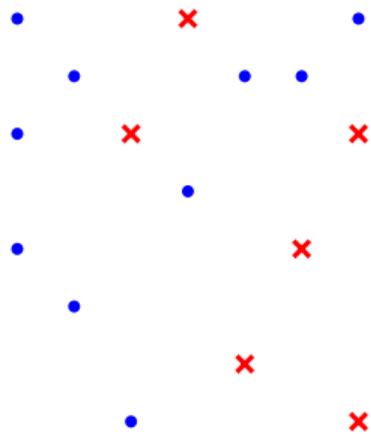
Parameters

s: Size of decision tree (# inner nodes)

4

Theorem (Hyafil and Rivest, *Inf. Process. Lett.* 1976)

Computing an optimal decision tree is NP-hard.



Parameters

s: Size of decision tree (# inner nodes)

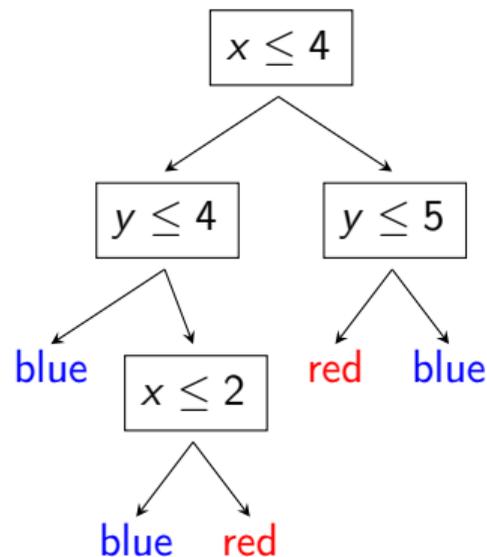
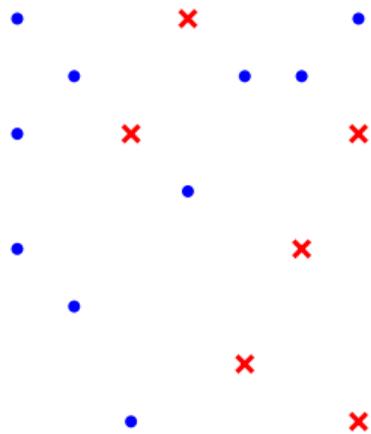
4

D: Maximal domain size (maximal # different values in one dimension)

8

Theorem (Hyafil and Rivest, *Inf. Process. Lett.* 1976)

Computing an optimal decision tree is NP-hard.



Parameters

s: Size of decision tree (# inner nodes)

4

D: Maximal domain size (maximal # different values in one dimension)

8

δ: Maximal # of dimensions in which a red and a blue example differ

2

Computing Optimal Decision Trees

Parameters

s: Size of decision tree (# inner nodes)

D: Maximal domain size (maximal # different values in one dimension)

δ : Maximal # of dimensions in which a red and a blue example differ

Computing Optimal Decision Trees

Parameters

s: Size of decision tree (# inner nodes)

D: Maximal domain size (maximal # different values in one dimension)

δ : Maximal # of dimensions in which a red and a blue example differ

Theorem (*Ordyniak and Szeider, AAAI 2021*)

An optimal decision tree can be computed in $\Omega(\delta^s \cdot (D^s 2\delta)^s \cdot 2^{s^2})$ time.

Computing Optimal Decision Trees

Parameters

s : Size of decision tree (# inner nodes)

D : Maximal domain size (maximal # different values in one dimension)

δ : Maximal # of dimensions in which a red and a blue example differ

Theorem (Ordyniak and Szeider, AAI 2021)

An optimal decision tree can be computed in $\Omega(\delta^s \cdot (D^s 2\delta)^s \cdot 2^{s^2})$ time.

Theorem (Our Work)

An optimal decision tree can be computed in $\mathcal{O}((6 \cdot \delta Ds)^s sn)$ time.

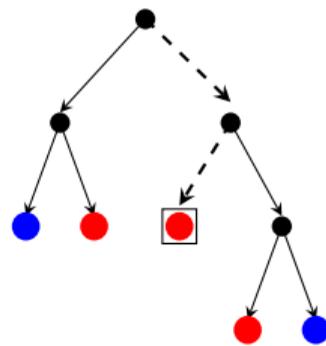
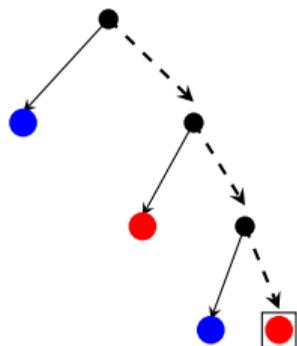
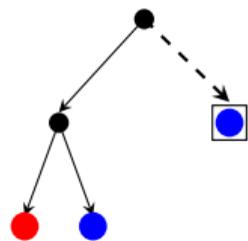
Outlook

Our algorithm with running time $\mathcal{O}((6 \cdot \delta Ds)^s sn)$ also works for Tree Ensembles!

Outlook

Our algorithm with running time $\mathcal{O}((6 \cdot \delta Ds)^5 sn)$ also works for Tree Ensembles!

Tree Ensembles: Majority vote of ℓ decision trees



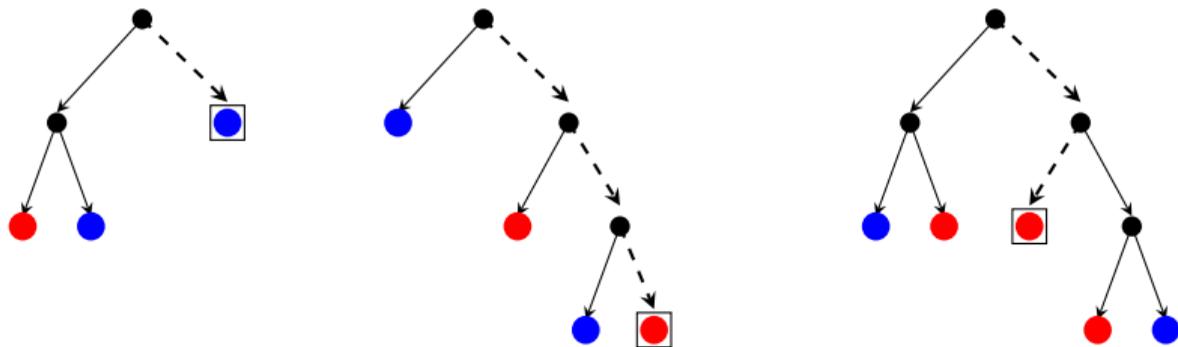
$$\ell = 3$$

example classified
as red

Outlook

Our algorithm with running time $\mathcal{O}((6 \cdot \delta Ds)^5 sn)$ also works for Tree Ensembles!

Tree Ensembles: Majority vote of ℓ decision trees



$\ell = 3$

example classified
as **red**

Future Work

- ▶ Algorithm engineering for our algorithm for decision trees
- ▶ Study variant which allows misclassifications