

LOGIC-BASED EXPLAINABLE ARTIFICIAL INTELLIGENCE

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ESSLLI, Bochum, Germany, July 2025

Brief bio sketch...

- Research:
 - Boolean satisfiability (SAT) – clause learning used in CDCL
 - Optimization & inconsistency
 - Quantification, model checking, uses of CEGAR
 - Logic encodings, description logics
 - Model-based diagnosis
 - ...
 - Rigorous explainability – new topic since 2019
- Career:
 - Research Professor – ICREA & Univ. Lleida, Catalunya, [Spain](#)
 - Directeur de Recherche – CNRS & IRIT, Toulouse, [France](#)
 - SFI Stokes Prof. of CS – Univ. College Dublin, [Ireland](#)
 - Full Professor of CS – Univ. Southampton, [United Kingdom](#)
 - Full Professor of CS – Univ. Lisbon – FCUL, [Portugal](#)
 - Full Professor of CS – Univ. Lisbon – IST, [Portugal](#)
 - ...
 - PhD at Univ. Michigan, Ann Arbor, MI, [USA](#) (1995)

Lecture 01

Remarkable ML successes – e.g. LLM ChatGPT for knowledge

Explain Sudoku puzzles. Give me an example.
Thanks!



What is Sudoku?

Sudoku is a logic-based number placement puzzle. It consists of a 9x9 grid divided into nine 3x3 subgrids, also called "regions." The goal is to fill the grid with numbers from 1 to 9 such that:

1. Each row contains the numbers 1 through 9, without repetition.
2. Each column contains the numbers 1 through 9, without repetition.
3. Each 3x3 subgrid contains the numbers 1 through 9, without repetition.

The puzzle starts with some numbers pre-filled, and your task is to fill in the blanks following the rules above. The difficulty of the puzzle depends on how many numbers are pre-filled and their arrangement.

Example Puzzle

Here's an example of a Sudoku puzzle:

5	3		7					
6			1	9	5			
	9	8				6		
8			6			3		
4			8	3		1		
7			2			6		
6			2	8				
			4	1	9	5		
			8			7	9	

Copy

How to Solve It

1. **Start with easy numbers:** Look for rows, columns, or subgrids where most numbers are already filled in. Use the process of elimination to determine the missing numbers.
2. **Use pencil marks:** If you're unsure, pencil in all possible candidates for a blank cell and narrow them down as you progress.
3. **Keep the rules in mind:** Continuously check the rows, columns, and subgrids to ensure you don't duplicate any numbers.
4. **Look for patterns:** Advanced strategies like "naked pairs" and "hidden singles" may help solve more challenging puzzles.

Would you like help solving this example or generating a new one?



Remarkable ML successes – e.g. LLM ChatGPT for programming

code for selecting columns of pandas
dataframe matching some value

To select columns in a pandas DataFrame that match a specific value, you can use a combination of boolean indexing and `.any()` or `.all()` methods. Here's a simple example:

Example Code

Let's assume you want to select all columns containing a specific value (say, 42).

```
python Copy  
  
import pandas as pd  
  
# Example DataFrame  
data = {  
    'A': [10, 42, 10],  
    'B': [5, 5, 42],  
    'C': [42, 1, 42],  
    'D': [2, 2, 2]  
}  
df = pd.DataFrame(data)  
  
# Specify the value to match  
value_to_match = 42  
  
# Selecting columns that contain the specified value  
matching_columns = df.columns[(df == value_to_match).  
  
# Filter the DataFrame to include only matching column  
df_matching = df[matching_columns]  
  
print(df_matching)
```

Explanation

1. `(df == value_to_match)` creates a DataFrame of booleans where `True` indicates cells that match the specified value.
2. `.any()` is used on columns (default `axis=0`) to determine if any cell in each column matches the value.
3. `df.columns[...]` is used to filter the columns to include only those with matching values.
4. `df[matching_columns]` creates a new DataFrame with only the matching columns.

Output

For the example given above, if `value_to_match` is 42, the output will be:

Copy

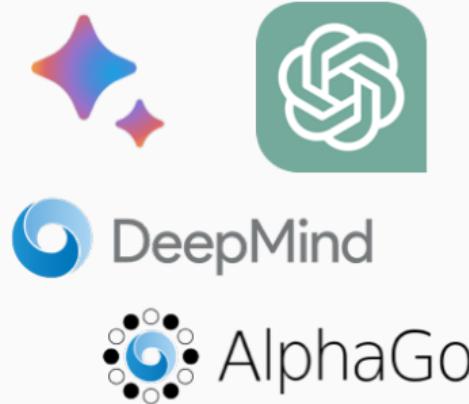
	A	B	C
0	10	5	42
1	42	5	1
2	10	42	42

Only columns A, B, and C are returned, as they contain the value 42.

Recent & ongoing ML successes

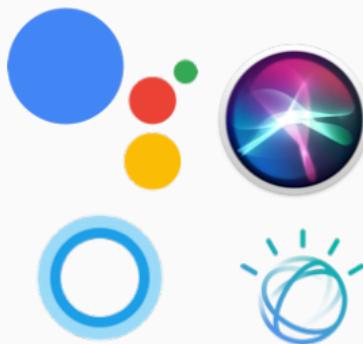
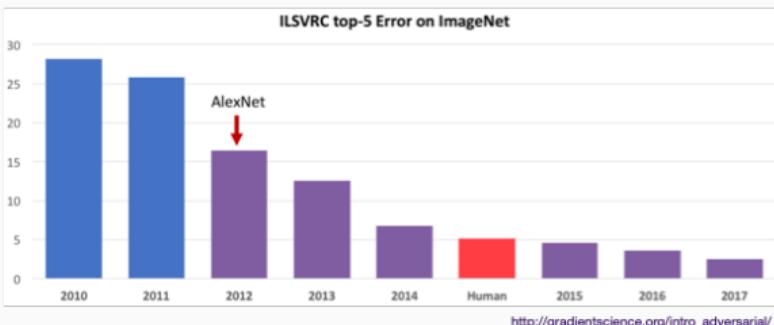


<https://en.wikipedia.org/wiki/Waymo>



AlphaGo Zero & Alpha Zero

Image & Speech Recognition



[https://fr.wikipedia.org/wiki/Pepper_\(robot\)](https://fr.wikipedia.org/wiki/Pepper_(robot))

Troubling ML issues – e.g. LLM ChatGPT for puzzles (Jan'25)

Count the number of occurrences of the letter 'L' in the word 'LOLLAPALOOZA'

To count the occurrences of the letter 'L' in the word **LOLLAPALOOZA**, we can visually inspect it:

The word is: **LOLLAPALOOZA**.

Now, let's count the 'L's:

- There are **3 L's** in the word.

Answer:

The number of occurrences of the letter 'L' is **3**.

<https://arxiv.org/html/2405.19616v2>

Troubling ML issues – e.g. LLM ChatGPT for puzzles (Jan'25)

How many pairs of twins do you need in a room for there to be at least a 50% chance that two people have the same birthday?

This question is a variation of the famous **Birthday Problem**, where the goal is to determine how many people are needed in a room for at least a 50% chance of two sharing the same birthday.

Here, you're dealing with **pairs of twins**. A pair of twins share the same birthday, so the effective number of unique birthdays to consider is reduced compared to regular individuals.

Step-by-Step Solution:

- 1. Revisiting the Regular Birthday Problem:** For a 50% chance of two people sharing a birthday in a room of unrelated individuals, you need about **23 people**. This assumes 365 equally likely days for a birthday.
- 2. Impact of Twins:**
 - Each pair of twins reduces the diversity of birthdays because both members of the pair share a single birthday.
 - Therefore, each pair of twins counts as **1 effective individual** in terms of the Birthday Problem.
- 3. Calculation for Pairs of Twins:**
 - For a 50% chance of a shared birthday, you need **23 effective individuals**.
 - Since each pair of twins is equivalent to **1 effective individual**, you need **23 pairs of twins** to achieve the same probability.

Final Answer:

You need **23 pairs of twins** in the room for at least a 50% chance that two people have the same birthday.

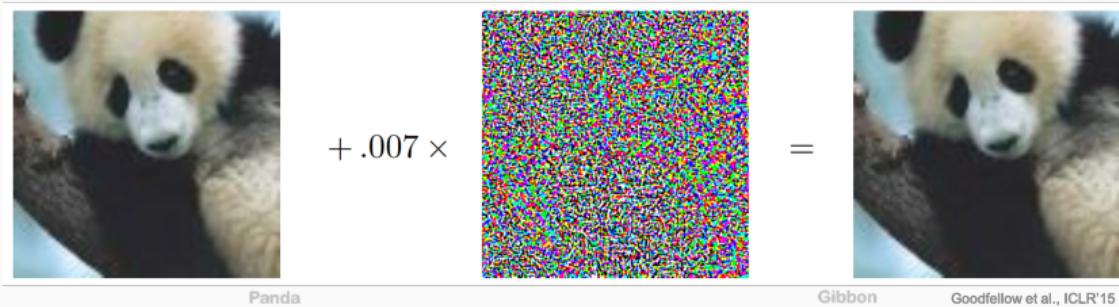
↓

<https://arxiv.org/html/2405.19616v2>

Can we trust ML models?

- Accuracy in training/test data
- Complex ML models are **brittle**
 - Extensive work on finding adversarial examples
 - Extensive work on learning robust ML models
- More recently, complex ML models **hallucinate**
 - LLMs also fail at basic reasoning tasks
- Need to validate operation of ML model, with rigor
 - Explanations; robustness; verification

ML models are brittle – adversarial examples



ML models are brittle – adversarial examples



ML models are brittle – adversarial examples



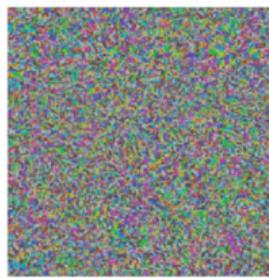
Adversarial examples can be very problematic

Original image



+ 0.04 ×

Adversarial noise



Adversarial example



Dermatoscopic image of a benign melanocytic nevus, along with the diagnostic probability computed by a deep neural network.



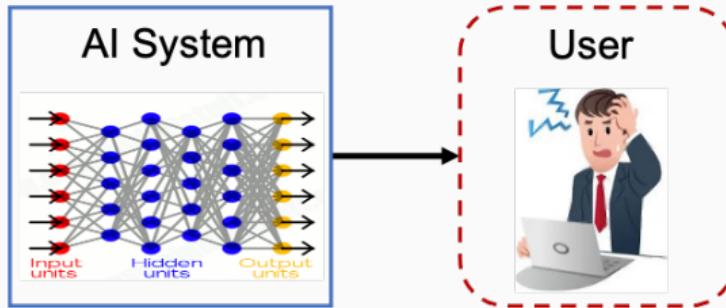
Perturbation computed by a common adversarial attack technique.

Combined image of nevus and attack perturbation and the diagnostic probabilities from the same deep neural network.



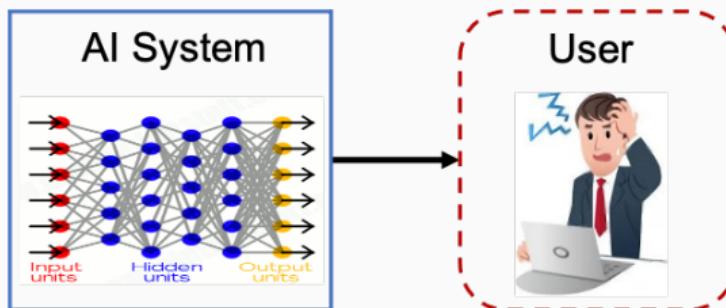
Finlayson et al., Nature 2019

The road to trust – eXplainable AI (XAI)



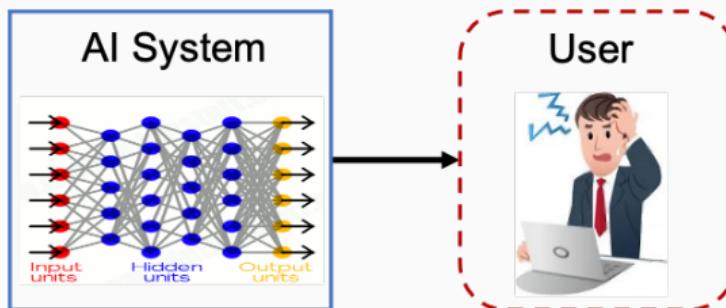
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- Goal of XAI: **to help humans understand ML models**

The road to trust – eXplainable AI (XAI)



- Complex ML models are **opaque**
- Goal of XAI: **to help humans understand ML models**
- How to XAI?
 - Answer to **Why (the prediction)?** questions
 - Answer to **Why Not (some other prediction)?** questions

The road to trust – eXplainable AI (XAI)



- Complex ML models are **opaque**
- Goal of XAI: **to help humans understand ML models**
- How to XAI?
 - Answer to **Why (the prediction)?** questions
 - Answer to **Why Not (some other prediction)?** questions
- What about **rigor**?
 - Sub-symbolic (i.e. non-symbolic) methods?
 - Symbolic (i.e. logic-based) methods?

Importance of XAI

REGULATION (EU) 2016/679 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL

of 27 April 2016

on the protection of natural persons with regard to the processing of personal data and on the free movement of such data, and repealing Directive 95/46/EC (General Data Protection Regulation)

(Text with EEA relevance)

European Union regulations on algorithmic decision-making
and a “right to explanation”

Bryce Goodman,^{1*} Seth Flaxman,²

We summarize the potential impact that the European Union's new General Data Protection Regulation will have on the routine use of machine-learning algorithms. Slated to take effect as law across the European Union in 2018, it will place restrictions on automated individual decision making (that is, algorithms that make decisions based on user-level predictors) that "significantly affect" users. When put into practice, the law may also effectively create a right to explanation, whereby a user can ask for an explanation of an algorithmic decision that significantly affects them. We argue that while this law may pose large challenges for industry, it highlights opportunities for computer scientists to take the lead in designing algorithms and evaluation frameworks that avoid discrimination and enable explanation.

Proposal for a

REGULATION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL

LAYING DOWN HARMONISED RULES ON ARTIFICIAL INTELLIGENCE
(ARTIFICIAL INTELLIGENCE ACT) AND AMENDING CERTAIN UNION
LEGISLATIVE ACTS

Explainable Artificial Intelligence (XAI)



David Gunning
DARPA/I2O
Program Update November 2017



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European Commission > Strategy > Digital Single Market > Reports and studies >

Digital Single Market

REPORT / STUDY | 8 April 2019

Ethics guidelines for trustworthy AI

Importance of XAI

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REGULATION (EU) 2016/679

In order to trust deployed AI systems, we must not only improve their robustness,⁵ but also develop ways to make their reasoning intelligible. Intelligibility will help us spot AI that makes mistakes due to distributional drift or incomplete representations of goals and features. Intelligibility will also facilitate control by humans in increasingly common collaborative human/AI teams. Furthermore, intelligibility will help humans learn from AI. Finally, there are legal reasons to want intelligible AI, including the European GDPR and a growing need to assign liability when AI errs.

Weld & Bansal, CACM, Jun'19
Due November 2017

THE COUNCIL

(Data and on the free movement of non-personal data and on the free movement of electronic communications (the "Data Protection Regulation))

Proposal for a

EAN PARLIAMENT AND OF THE COUNCIL

RULES ON ARTIFICIAL INTELLIGENCE (THE ACT) AND AMENDING CERTAIN UNION LEGISLATIVE ACTS

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REPORT / STUDY | 8 April 2019

Ethics guidelines for trustworthy AI



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Ethics guidelines for trustworthy AI

Following the publication of the draft ethics guidelines in December 2018 to which more than 500 comments were received, the independent expert group presents today their ethics guidelines for trustworthy artificial intelligence.

About Artificial intelligence

Blog posts

News

XAI & the principle of explicability



European Commission > Strategy > Digital Single Market > Reports and

Digital Single Market

REPORT / LIST

The principle of explicability

- **Explicability** is crucial for building and maintaining users' trust in AI systems. This means that processes need to be transparent, the capabilities and purpose of AI systems openly communicated, and decisions – to the extent possible – explainable to those directly and indirectly affected. Without such information, a decision cannot be duly contested. An explanation as to why a model has generated a particular output or decision (and what combination of input factors contributed to that) is not always possible. These cases are referred to as 'black box' algorithms and require special attention. In those circumstances, other explicability measures (e.g. traceability, auditability and transparent communication on system capabilities) may be required, provided that the system as a whole respects fundamental rights. The degree to which explicability is needed is highly dependent on the context and the severity of the consequences if that output is erroneous or otherwise inaccurate.³³

About Artificial
intelligence

Blog posts

News

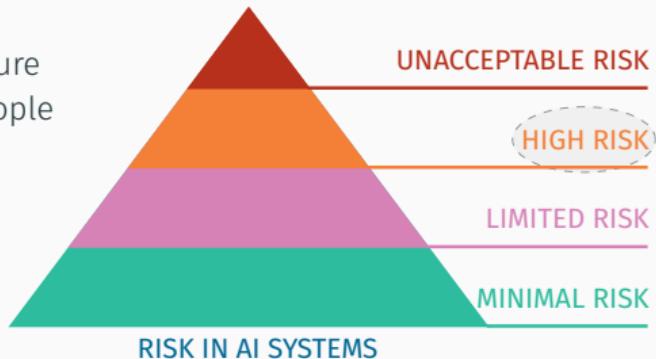
& thousands of recent papers!

XAI for high-risk & safety-critical applications

- **High-risk** (EU regulations):

- Law enforcement
- Management and operation of critical infrastructure
- Biometric identification and categorization of people
- ...

[EU21b, EU21a]



XAI for high-risk & safety-critical applications

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otherwise incorrect or unjust manner. Furthermore, the exercise of important procedural fundamental rights, such as the right to an effective remedy and to a fair trial as well as the right of defence and the presumption of innocence, could be hampered, in particular, where such AI systems are not sufficiently transparent, explainable and documented.

[21b, EU21a]

EU AI Act, 2021, page 27

HIGH RISK

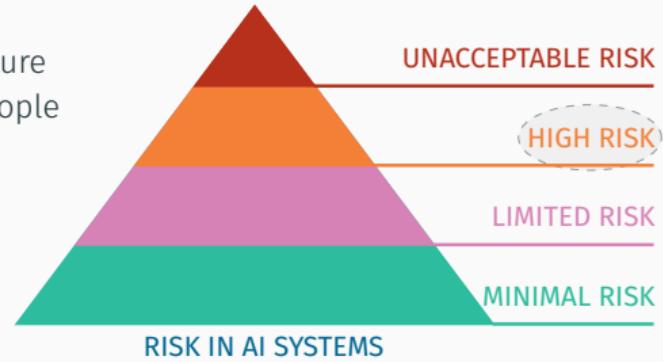


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[EU21b, EU21a]



- And **safety-critical**:

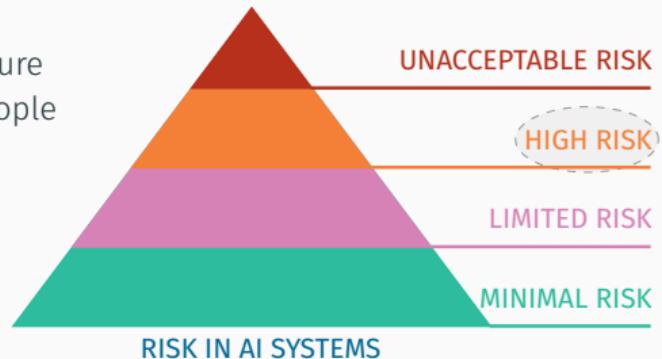
- Self-driving cars
- Autonomous vehicles
- Autonomous aerial devices
- ...

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Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead

Cynthia Rudin

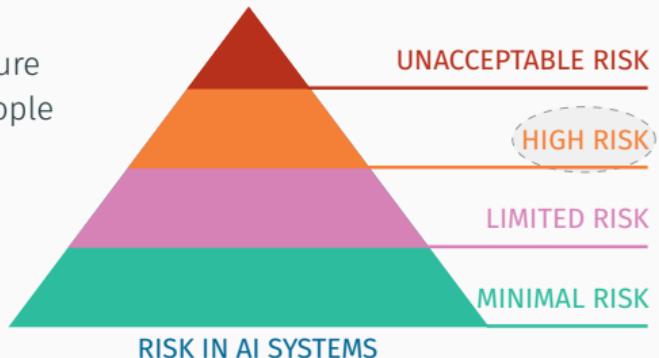
May 2019

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[EU21b, EU21a]



- And **safety-critical**:

- Self-driving cars
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- **Correctness of explanations is paramount!**

- To build trust
- To help debug AI systems
- To prevent (catastrophic) accidents
- ...

PERSPECTIVE

<https://doi.org/10.1038/s42256-019-0048-x>

nature
machine intelligence

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Cynthia Rudin

May 2019

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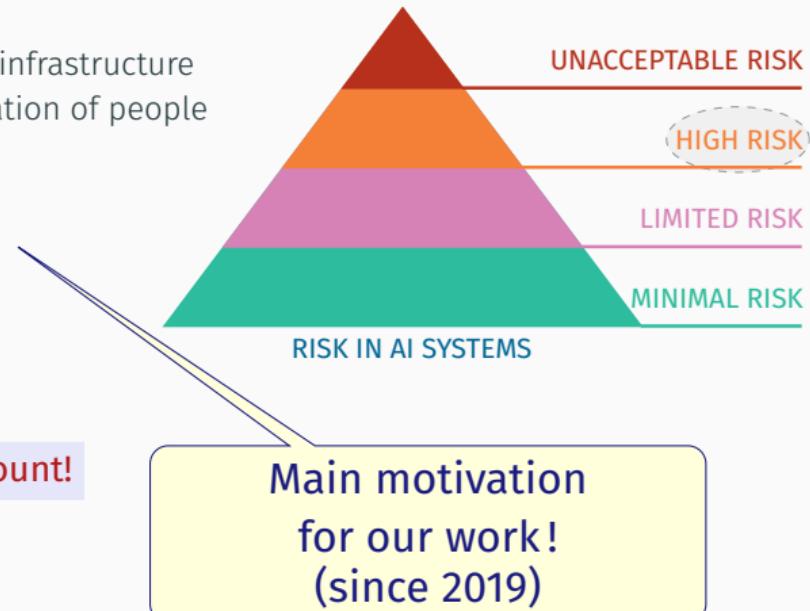
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Can we trust (non-symbolic) XAI? – some questions

- Many proposed **solutions** for XAI
 - Most, and the better-known, are heuristic
 - I.e. no guarantees of rigor
- Many proposed **uses** of XAI
- Regular complaints about issues with existing (heuristic) methods of XAI

Can we trust (non-symbolic) XAI? – some questions

- Many proposed **solutions** for XAI
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 - I.e. no guarantees of rigor
- Many proposed **uses** of XAI
- Regular complaints about issues with existing (heuristic) methods of XAI
- **Q:** Can heuristic XAI be trusted in high-risk and/or safety-critical domains?
- **Q:** Can we validate results of heuristic XAI?

What have we been up to? 1. Created the field of symbolic (formal) XAI – I

[MI22, Mar22, MS23, Mar24]

- Rigorous, logic-based, definitions of explanations
 - Relationship with abduction – abductive explanations (AXps)
 - Contrastive explanations (CXps) [Mil19]
- Duality between AXps & CXps
 - AXps are MHSes of CXps and vice-versa

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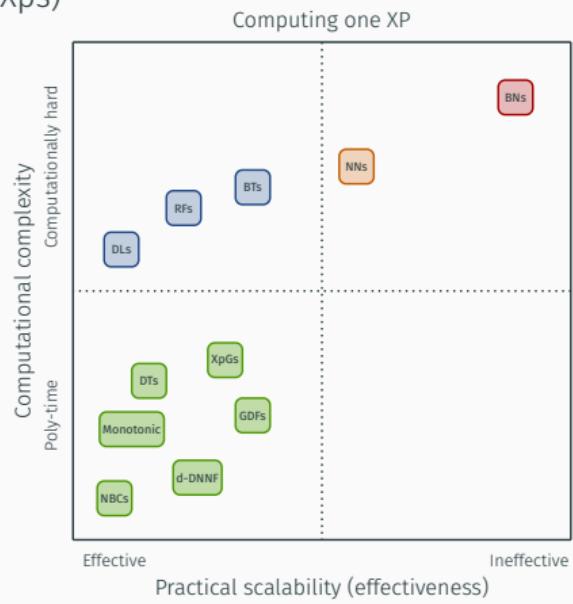
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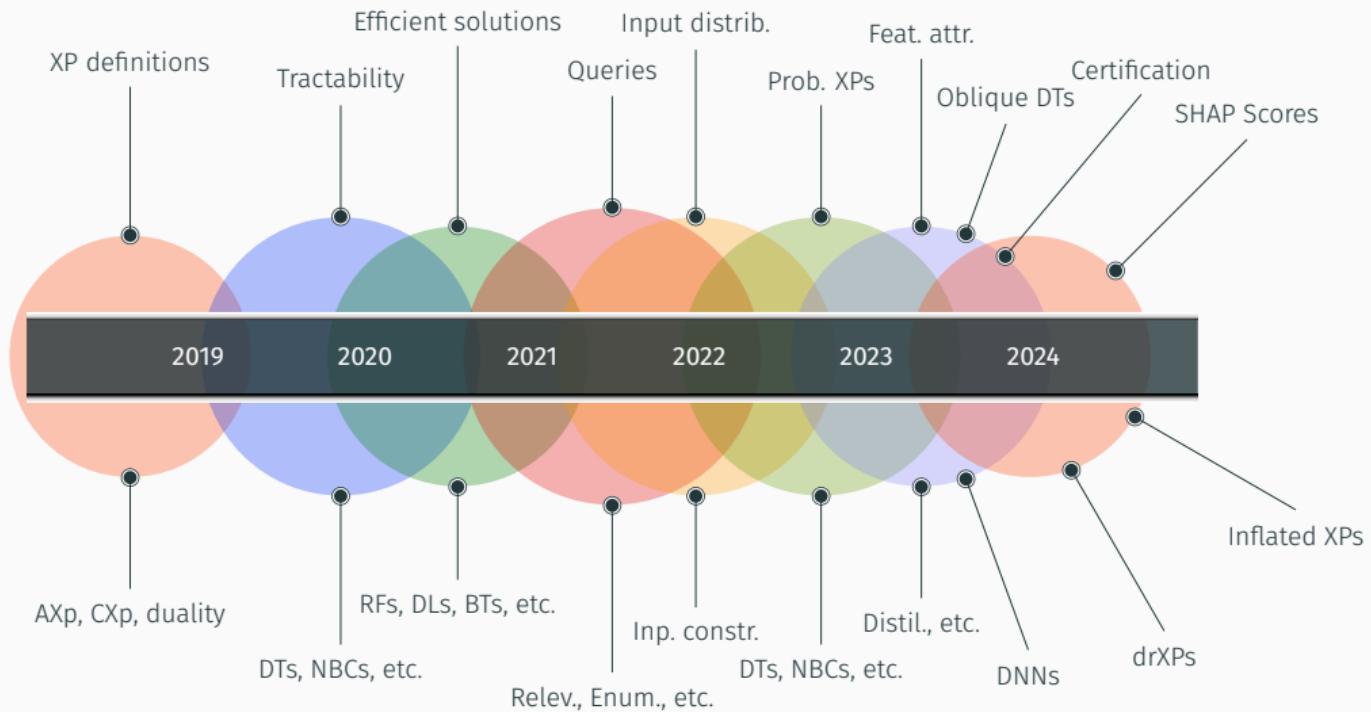
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What have we been up to? 1. Created the field of symbolic (formal) XAI – II

[MI22, Mar22, MS23, Mar24]



What have we been up to? 2. Uncovered key myths of non-symbolic XAI – I

[RSG16, LL17, RSG18, Rud19]

LIME “Why Should I Trust You?” Explaining the Predictions of Any Classifier

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PERSPECTIVE

<https://doi.org/10.1038/s42256-019-0048-x>

nature
machine intelligence

Stop explaining black box machine learning
models for high stakes decisions and use
interpretable models instead

Intrinsic Interpretability

Cynthia Rudin



A Unified Approach to Interpreting Model Predictions

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Anchors: High-Precision Model-Agnostic Explanations

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Anchor

[MSH24, HMS24, HM23c]

research and advances



DOI:10.1145/3635301

When the decisions of ML models impact people, one should expect explanations to offer the strongest guarantees of rigor. However, the most popular XAI approaches offer none.

BY JOAO MARQUES-SILVA AND XUANXIANG HUANG

Explainability Is Not a Game

» key insights

- Shapley values find extensive uses in explaining machine learning models and serve to assign importance to the features of the model.
- Shapley values for explainability also find ever-increasing uses in high-risk and safety-critical domains, for example, medical diagnosis.
- This article proves that the existing definition of Shapley values for explainability can produce misleading information regarding feature importance, and so can induce human decision makers in error.

Plan for this course

- Lecture 01 – unit(s):
 - #01: Foundations
- Lecture 02 – unit(s):
 - #02: Principles of symbolic XAI – **feature selection**
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 – unit(s):
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 – unit(s):
 - #06: Recent, emerging & advanced topics
- Lecture 05 – unit(s):
 - #07: Principles of symbolic XAI – **feature attribution** (& myth of Shapley values in XAI)
 - #08: Corrected feature attribution – nuSHAP
 - #09: Conclusions & research directions

Unit #01

Foundations

Classification problems

- Set of features $\mathcal{F} = \{1, 2, \dots, m\}$, each feature i taking values from domain D_i
 - Features can be categorical, discrete or real-valued
 - Feature space: $\mathbb{F} = \Pi_{i=1}^m D_i$
- Set of classes $\mathcal{K} = \{c_1, \dots, c_K\}$

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 - \mathcal{M}_C is a tuple $(\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$

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 - \mathcal{M}_C is a tuple $(\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$
- Instance (\mathbf{v}, c) for point $\mathbf{v} = (v_1, \dots, v_m) \in \mathbb{F}$, with prediction $c = \kappa(\mathbf{v})$, $c \in \mathcal{K}$
 - Goal: to compute explanations for (\mathbf{v}, c)

Regression problems

- For regression problems:
 - Codomain: \mathbb{V}
 - Regression function: $\rho : \mathbb{F} \rightarrow \mathbb{V}$ (non-constant)
 - ML model: \mathcal{M}_R is a tuple $(\mathcal{F}, \mathbb{F}, \mathbb{V}, \rho)$

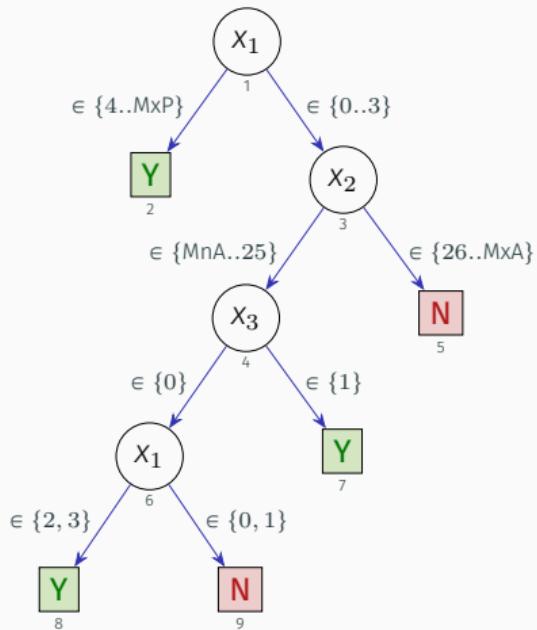
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 - Regression function: $\rho : \mathbb{F} \rightarrow \mathbb{V}$ (non-constant)
 - ML model: \mathcal{M}_R is a tuple $(\mathcal{F}, \mathbb{F}, \mathbb{V}, \rho)$
- General ML model:
 - \mathbb{T} : range of possible predictions
 - Non-constant function $\tau : \mathbb{F} \rightarrow \mathbb{T}$
 - ML model: \mathcal{M} is a tuple $(\mathcal{F}, \mathbb{F}, \mathbb{T}, \tau)$

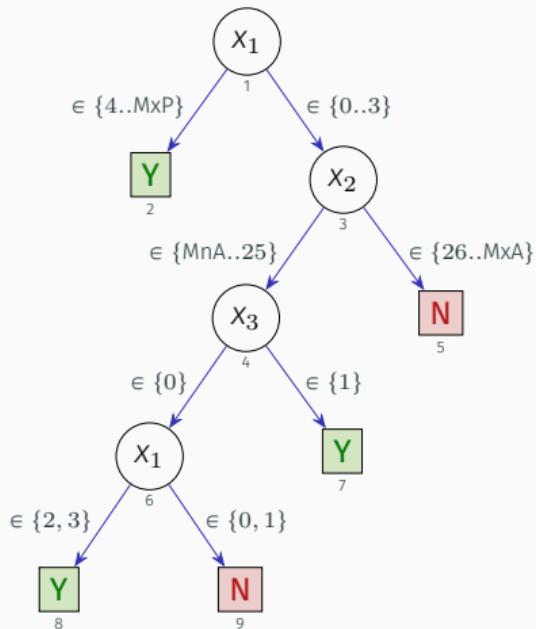
Regression problems

- For regression problems:
 - Codomain: \mathbb{V}
 - Regression function: $\rho : \mathbb{F} \rightarrow \mathbb{V}$ (non-constant)
 - ML model: \mathcal{M}_R is a tuple $(\mathcal{F}, \mathbb{F}, \mathbb{V}, \rho)$
- General ML model:
 - \mathbb{T} : range of possible predictions
 - Non-constant function $\tau : \mathbb{F} \rightarrow \mathbb{T}$
 - ML model: \mathcal{M} is a tuple $(\mathcal{F}, \mathbb{F}, \mathbb{T}, \tau)$
- Instance: $(\mathbf{v}, q), q \in \mathbb{T}$

Example ML models – classification – decision trees (DTs)

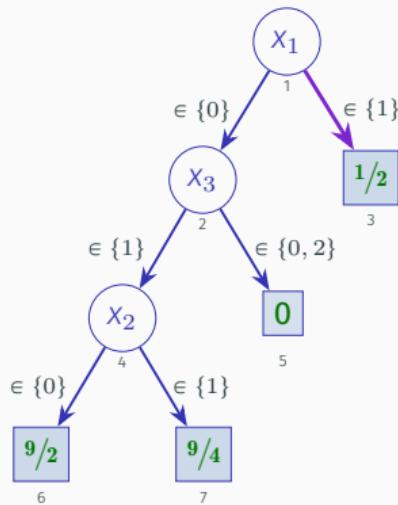


Example ML models – classification – decision trees (DTs)



- Literals in DTs can use $=$ or \in

Example ML models – regression – regression trees (RTs)



- Literals in RTs can use $=$ or \in

Example ML models – classification – rules

- Ordered rules – decision lists (DLs):

```
IF       $x_1 \wedge x_2$  THEN predict Y
ELSE IF  $\neg x_2 \vee x_3$  THEN predict N
ELSE          THEN predict Y
 $\mathcal{F} = \{1, 2, 3\}; \mathcal{D}_1 = \mathcal{D}_2 = \mathcal{D}_3 = \{0, 1\}; \mathcal{K} = \{Y, N\}$ 
```

Example ML models – classification – rules

- Ordered rules – decision lists (DLs):

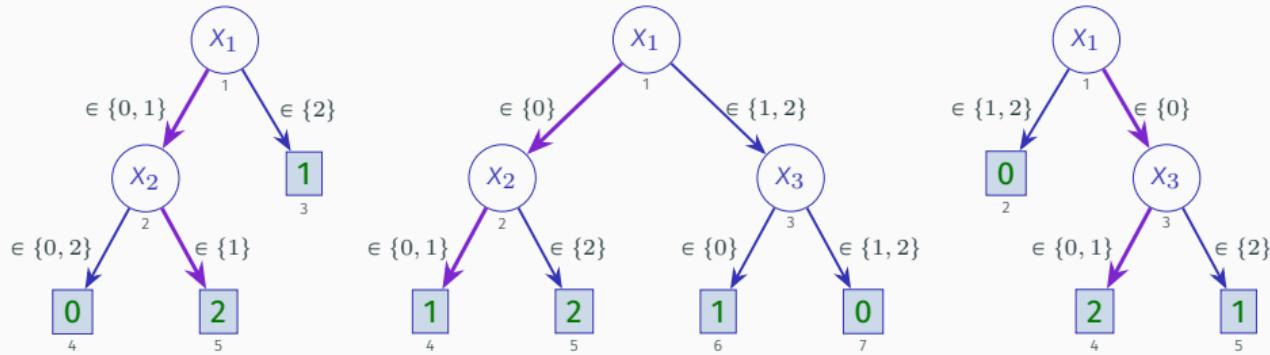
$$\begin{array}{lll} \text{IF } & x_1 \wedge x_2 & \text{THEN predict Y} \\ \text{ELSE IF } & \neg x_2 \vee x_3 & \text{THEN predict N} \\ \text{ELSE } & & \text{THEN predict Y} \\ \mathcal{F} = \{1, 2, 3\}; \mathcal{D}_1 = \mathcal{D}_2 = \mathcal{D}_3 = \{0, 1\}; \mathcal{K} = \{\text{Y}, \text{N}\} \end{array}$$

- Unordered rules – decision sets (DSs):

$$\begin{array}{lll} \text{IF } & x_1 + x_2 \geq 0 & \text{THEN predict } \blacksquare \\ \text{IF } & x_1 + x_2 < 0 & \text{THEN predict } \blacksquare \\ \mathcal{F} = \{1, 2\}; \mathcal{D}_1 = \mathcal{D}_2 = \mathbb{R}; \mathcal{K} = \{\blacksquare, \blacksquare\} \end{array}$$

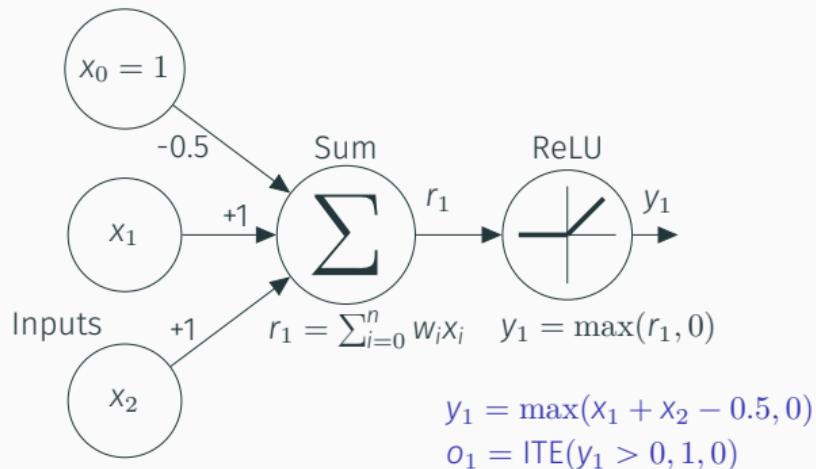
- Issues of DSs: overlap; incomplete coverage

Example ML models – classification – random forests (RFs)



- For each input, each DT picks a class
- Result uses majority or weighted voting of the DTs

Example ML models – classification – neural networks (NNs)



Outline – Unit #01

ML Models: Classification & Regression Problems

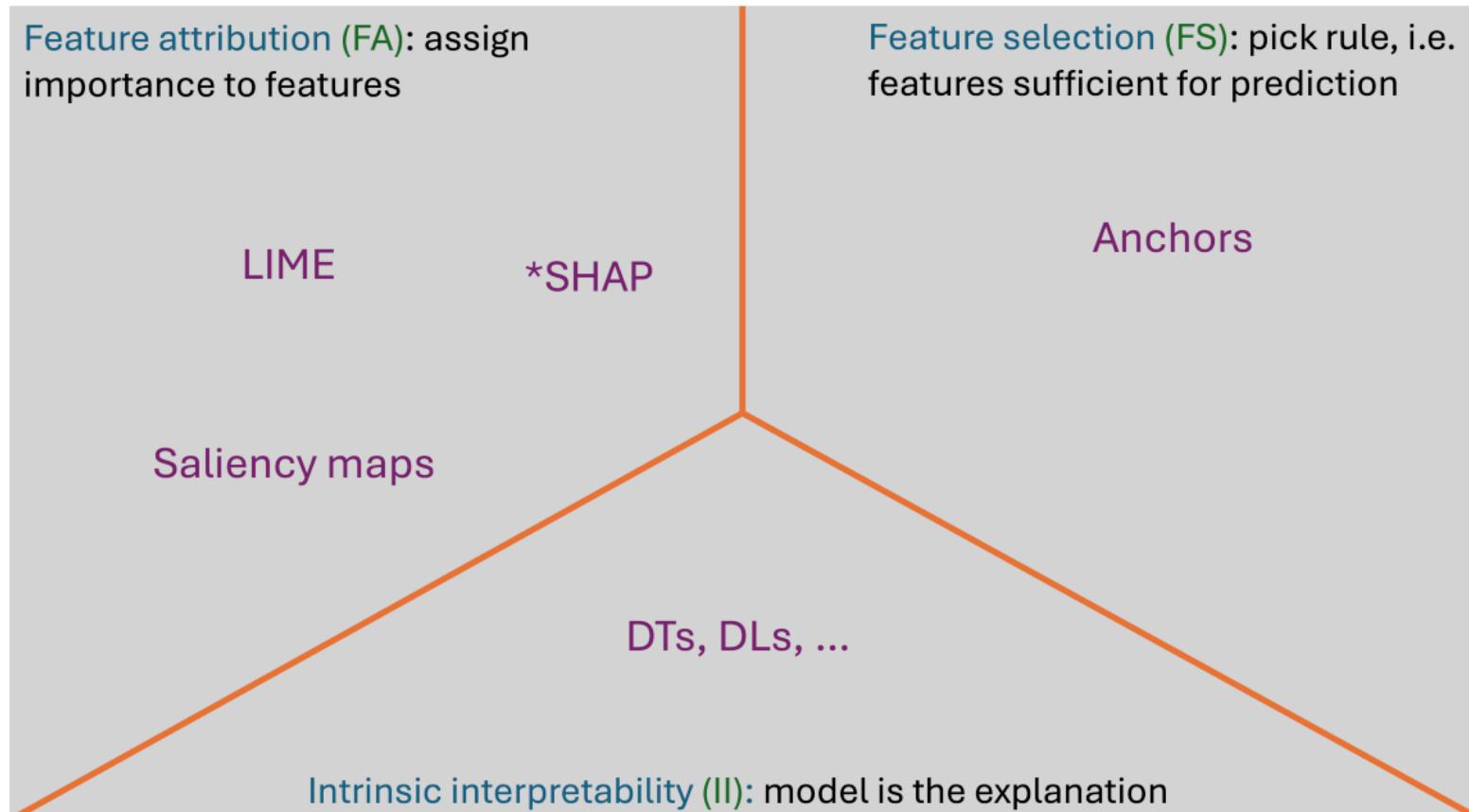
Basics of (non-symbolic) XAI

Motivation for Explanations

Brief Glimpse of Logic

Reasoning About ML Models

Understanding Intrinsic Interpretability

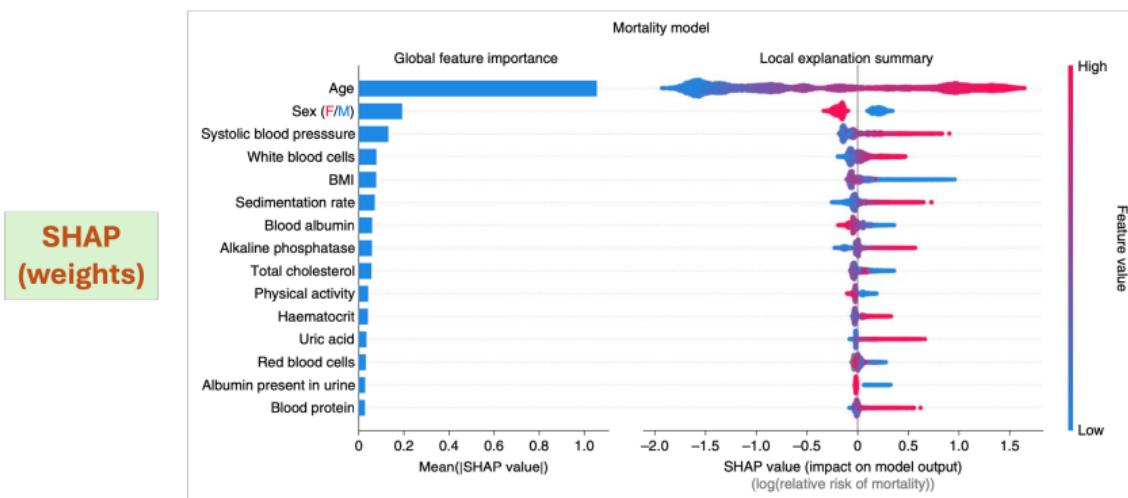


Some non-symbolic XAI methods

[LL17, RSG18]

**IF Country = United-States AND Capital Loss = Low
AND Race = White AND Relationship = Husband
AND Married AND $28 < \text{Age} \leq 37$
AND Sex = Male AND High School grad
AND Occupation = Blue-Collar
THEN PREDICT Salary > \$50K**

**Anchors
(rules)**



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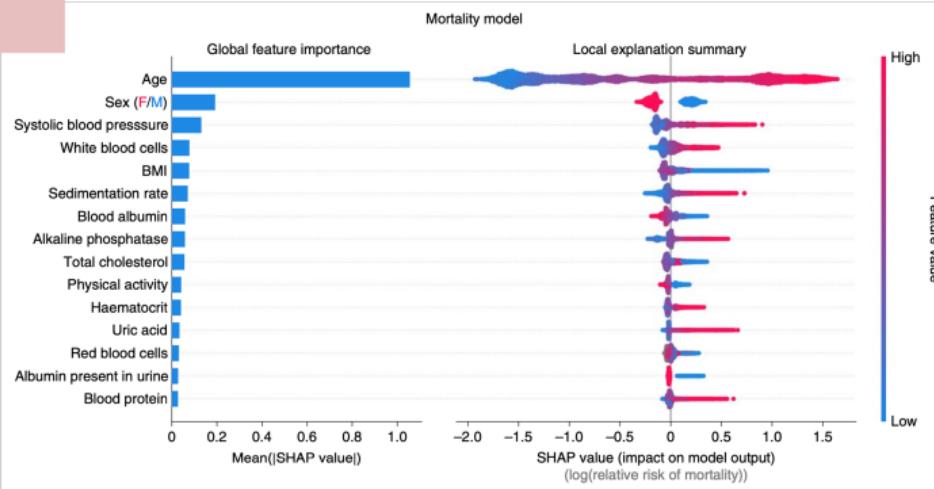
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**Anchors
(rules)**

model-agnostic, sample-based,
& no guarantees of rigor...

**SHAP
(weights)**



Outline – Unit #01

ML Models: Classification & Regression Problems

Basics of (non-symbolic) XAI

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What explanations do we seek? I.e. how to answer **Why?** questions?

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[RSG16]

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- We also seek the algorithms for the rigorous computation of such rules

[RSG16]

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A decision list example

```
IF       $\neg x_1 \wedge x_2$  THEN predict Y
ELSE IF  $\neg x_1 \wedge x_3$  THEN predict Y
ELSE IF  $x_4 \wedge x_5$  THEN predict N
ELSE                THEN predict Y
```

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- Explanation for why $\kappa(1, 1, 1, 1) = \text{N}$?

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 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$,
 - IF** $(x_1 = 1) \wedge (x_4 = 1) \wedge (x_5 = 1)$ **THEN** $\kappa(\mathbf{x}) = \text{N}$
 - I.e. $\{x_1 = 1, x_4 = 1, x_5 = 1\}$ suffice for DL to predict **N**

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IF       $\neg x_1 \wedge x_2$  THEN predict Y  
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A decision list example

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IF       $\neg x_1 \wedge x_2$  THEN predict Y  
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ELSE IF  $x_4 \wedge x_5$  THEN predict N  
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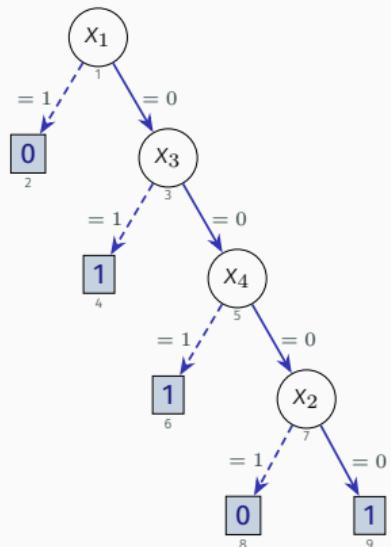
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- Explanation for **why** $\kappa(1, 0, 0, 0, 0) = \text{Y}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$,
IF $(x_4 = 0)$ **THEN** $\kappa(\mathbf{x}) = \text{Y}$
 - I.e. $\{x_4 = 0\}$ suffices for DL to predict **Y**

A decision list example

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IF       $\neg x_1 \wedge x_2$  THEN predict Y  
ELSE IF  $\neg x_1 \wedge x_3$  THEN predict Y  
ELSE IF  $x_4 \wedge x_5$  THEN predict N  
ELSE                THEN predict Y
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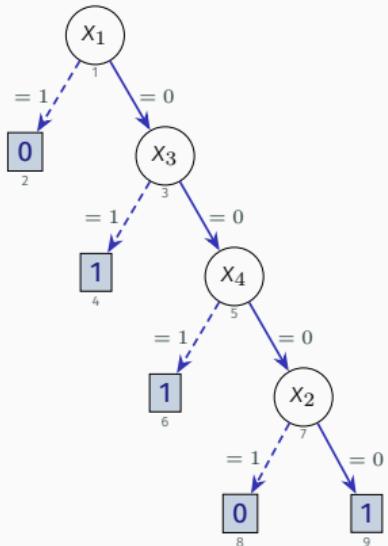
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 - I.e. $\{x_1 = 1, x_4 = 1, x_5 = 1\}$ suffice for DL to predict **N**
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IF $(x_4 = 0)$ **THEN** $\kappa(\mathbf{x}) = \text{Y}$
 - I.e. $\{x_4 = 0\}$ suffices for DL to predict **Y**
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$,
IF $(x_5 = 0)$ **THEN** $\kappa(\mathbf{x}) = \text{Y}$
 - I.e. $\{x_5 = 0\}$ also suffices for DL to predict **Y**

A decision tree example



x_1	x_2	x_3	x_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0

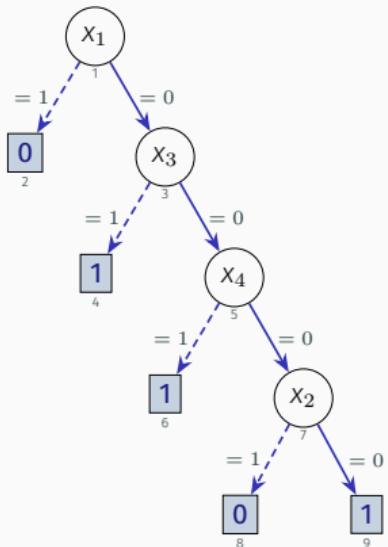
A decision tree example



- Explanation for **why** $\kappa(0, 0, 0, 0) = 1$?

x_1	x_2	x_3	x_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0

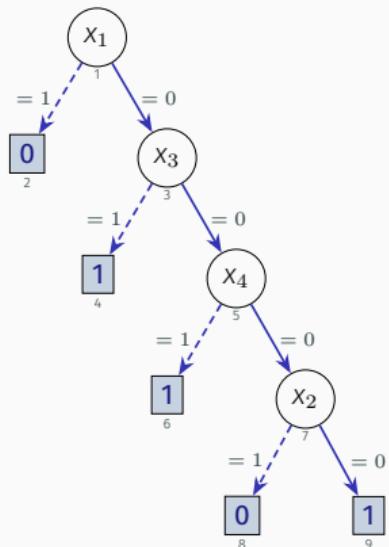
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- Explanation for **why** $\kappa(0, 0, 0, 0) = 1$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$,
 - IF** $(x_1 = 0) \wedge (x_2 = 0)$ **THEN** $\kappa(\mathbf{x}) = 1$
 - i.e. $\{x_1 = 0, x_2 = 0\}$ suffice for DT to predict 1

x_1	x_2	x_3	x_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0

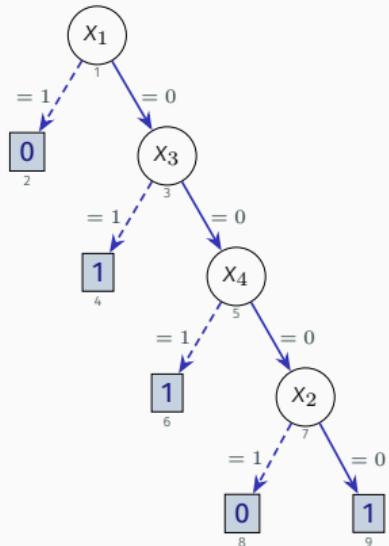
A decision tree example



- Explanation for why $\kappa(0, 0, 0, 0) = 1$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$,
 - IF $(x_1 = 0) \wedge (x_2 = 0)$ THEN $\kappa(\mathbf{x}) = 1$
 - i.e. $\{x_1 = 0, x_2 = 0\}$ suffice for DT to predict 1
- Explanation for why $\kappa(1, 1, 1, 1) = 0$?

x_1	x_2	x_3	x_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0

A decision tree example

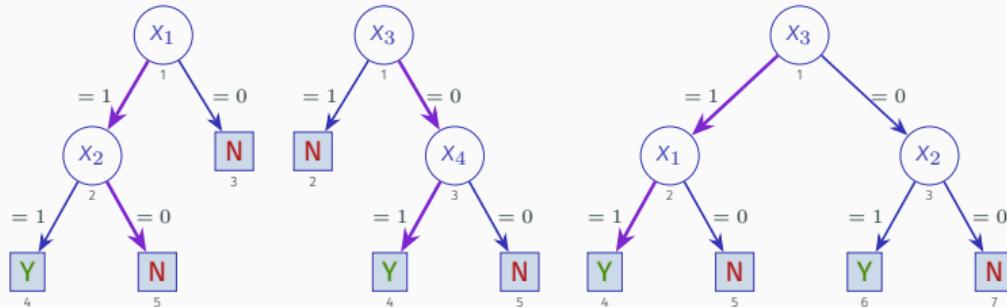


- Explanation for **why** $\kappa(0, 0, 0, 0) = 1$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$,
IF $(x_1 = 0) \wedge (x_2 = 0)$ **THEN** $\kappa(\mathbf{x}) = 1$
 - i.e. $\{x_1 = 0, x_2 = 0\}$ suffice for DT to predict **1**
- Explanation for **why** $\kappa(1, 1, 1, 1) = 0$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$,
IF $(x_1 = 1)$ **THEN** $\kappa(\mathbf{x}) = 0$
 - i.e. $\{x_1 = 1\}$ suffices for DT to predict **0**

x_1	x_2	x_3	x_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0

A random forest example

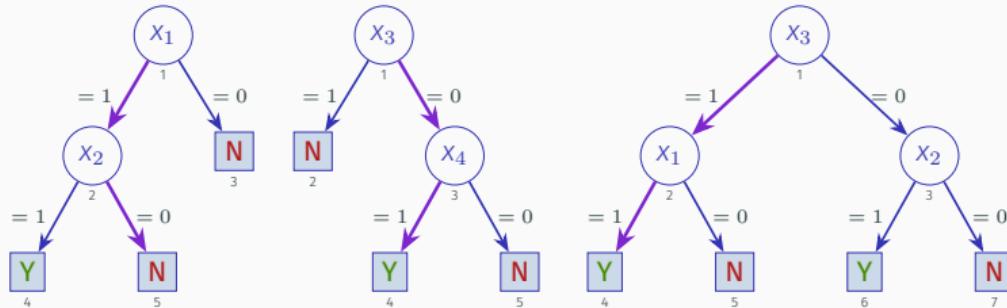
[IMS21]



X ₁	X ₂	X ₃	X ₄	T ₁	T ₂	T ₃	$\kappa(\mathbf{x})$
0	0	0	0	N	N	N	N
0	0	0	1	N	Y	N	N
0	0	1	0	N	N	N	N
0	0	1	1	N	N	N	N
0	1	0	0	N	N	Y	N
0	1	0	1	N	Y	Y	Y
0	1	1	0	N	N	N	N
0	1	1	1	N	N	N	N
1	0	0	0	N	N	N	N
1	0	0	1	N	Y	N	N
1	0	1	0	N	N	Y	N
1	0	1	1	N	N	Y	N
1	1	0	0	Y	N	Y	Y
1	1	0	1	Y	Y	Y	Y
1	1	1	0	Y	N	Y	Y
1	1	1	1	Y	N	Y	Y

A random forest example

[IMS21]

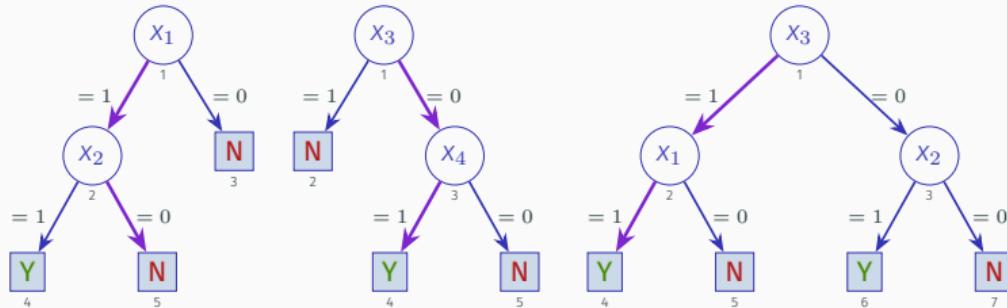


- Explanation for why $\kappa(1, 0, 0, 1) = \text{N}$?

X ₁	X ₂	X ₃	X ₄	T ₁	T ₂	T ₃	$\kappa(\mathbf{x})$
0	0	0	0	N	N	N	N
0	0	0	1	N	Y	N	N
0	0	1	0	N	N	N	N
0	0	1	1	N	N	N	N
0	1	0	0	N	N	Y	N
0	1	0	1	N	Y	Y	Y
0	1	1	0	N	N	N	N
0	1	1	1	N	N	N	N
1	0	0	0	N	N	N	N
1	0	0	1	N	Y	N	N
1	0	1	0	N	N	Y	N
1	0	1	1	N	N	Y	N
1	1	0	0	Y	N	Y	Y
1	1	0	1	Y	Y	Y	Y
1	1	1	0	Y	N	Y	Y
1	1	1	1	Y	N	Y	Y

A random forest example

[IMS21]

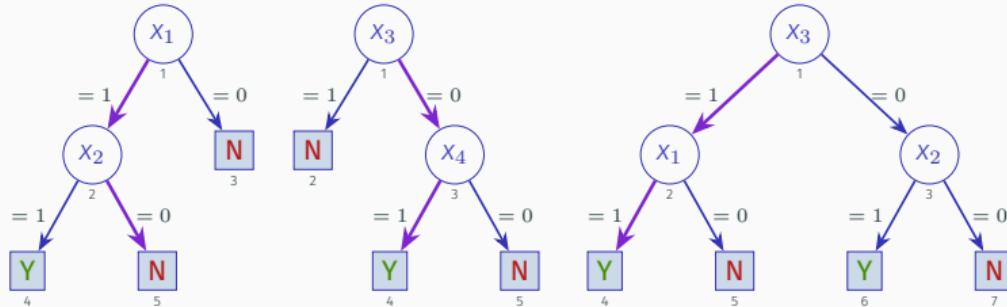


- Explanation for why $\kappa(1, 0, 0, 1) = \mathbf{N}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, IF ($x_2 = 0$) THEN $\kappa(\mathbf{x}) = \mathbf{N}$
 - i.e. $\{x_2 = 0\}$ suffices for RF to predict **N**

x_1	x_2	x_3	x_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	N	N	N	N
0	0	0	1	N	Y	N	N
0	0	1	0	N	N	N	N
0	0	1	1	N	N	N	N
0	1	0	0	N	N	Y	N
0	1	0	1	N	Y	Y	Y
0	1	1	0	N	N	N	N
0	1	1	1	N	N	N	N
1	0	0	0	N	N	N	N
1	0	0	1	N	Y	N	N
1	0	1	0	N	N	Y	N
1	0	1	1	N	N	Y	N
1	1	0	0	Y	N	Y	Y
1	1	0	1	Y	Y	Y	Y
1	1	1	0	Y	N	Y	Y
1	1	1	1	Y	N	Y	Y

A random forest example

[IMS21]

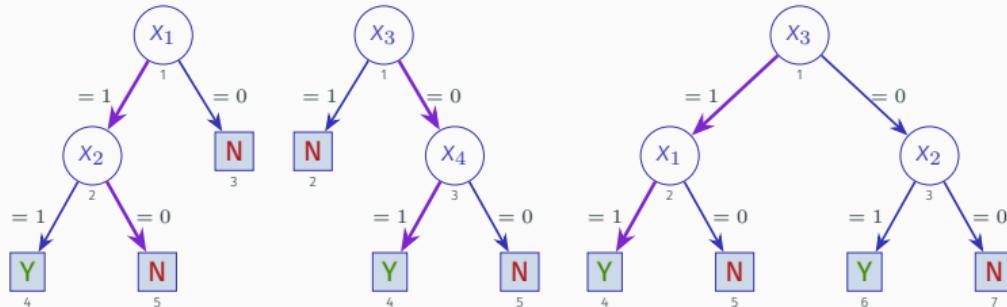


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- Explanation for why $\kappa(1, 1, 1, 1) = \text{Y}$?

x_1	x_2	x_3	x_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	N	N	N	N
0	0	0	1	N	Y	N	N
0	0	1	0	N	N	N	N
0	0	1	1	N	N	N	N
0	1	0	0	N	N	Y	N
0	1	0	1	N	Y	Y	Y
0	1	1	0	N	N	N	N
0	1	1	1	N	N	N	N
1	0	0	0	N	N	N	N
1	0	0	1	N	Y	N	N
1	0	1	0	N	N	Y	N
1	0	1	1	N	N	Y	N
1	1	0	0	Y	N	Y	Y
1	1	0	1	Y	Y	Y	Y
1	1	1	0	Y	N	Y	Y
1	1	1	1	Y	N	Y	Y

A random forest example

[IMS21]

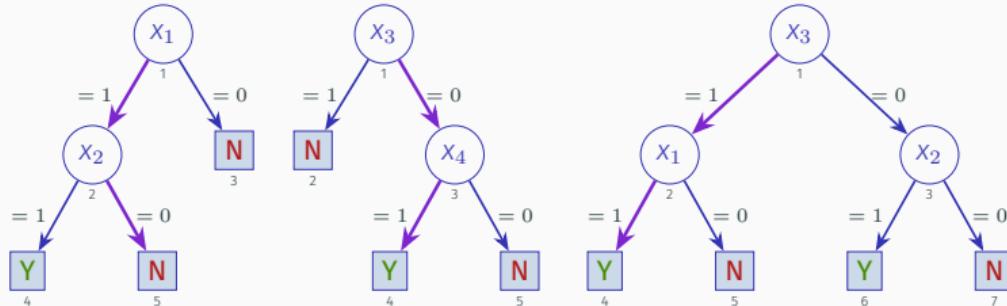


- Explanation for why $\kappa(1, 0, 0, 1) = \text{N}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, IF $(x_2 = 0)$ THEN $\kappa(\mathbf{x}) = \text{N}$
 - I.e. $\{x_2 = 0\}$ suffices for RF to predict **N**
- Explanation for why $\kappa(1, 1, 1, 1) = \text{Y}$?
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x_1	x_2	x_3	x_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	N	N	N	N
0	0	0	1	N	Y	N	N
0	0	1	0	N	N	N	N
0	0	1	1	N	N	N	N
0	1	0	0	N	N	Y	N
0	1	0	1	N	Y	Y	Y
0	1	1	0	N	N	N	N
0	1	1	1	N	N	N	N
1	0	0	0	N	N	N	N
1	0	0	1	N	Y	N	N
1	0	1	0	N	N	Y	N
1	0	1	1	N	N	Y	N
1	1	0	0	Y	N	Y	Y
1	1	0	1	Y	Y	Y	Y
1	1	1	0	Y	N	Y	Y
1	1	1	1	Y	N	Y	Y

A random forest example

[IMS21]

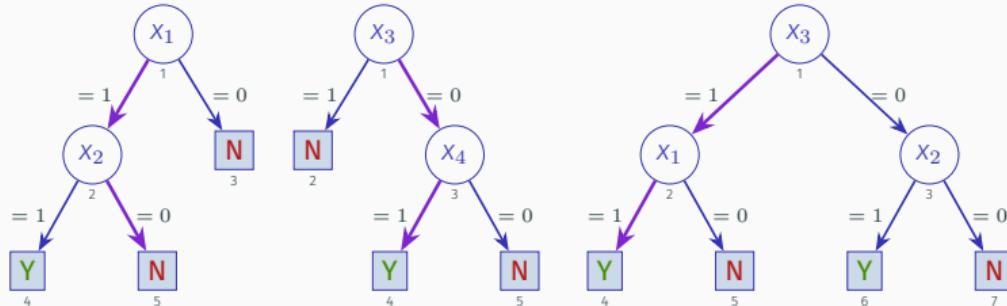


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0	1	0	0	N	N	Y	N
0	1	0	1	N	Y	Y	Y
0	1	1	0	N	N	N	N
0	1	1	1	N	N	N	N
1	0	0	0	N	N	N	N
1	0	0	1	N	Y	N	N
1	0	1	0	N	N	Y	N
1	0	1	1	N	N	Y	N
1	1	0	0	Y	N	Y	Y
1	1	0	1	Y	Y	Y	Y
1	1	1	0	Y	N	Y	Y
1	1	1	1	Y	N	Y	Y

A random forest example

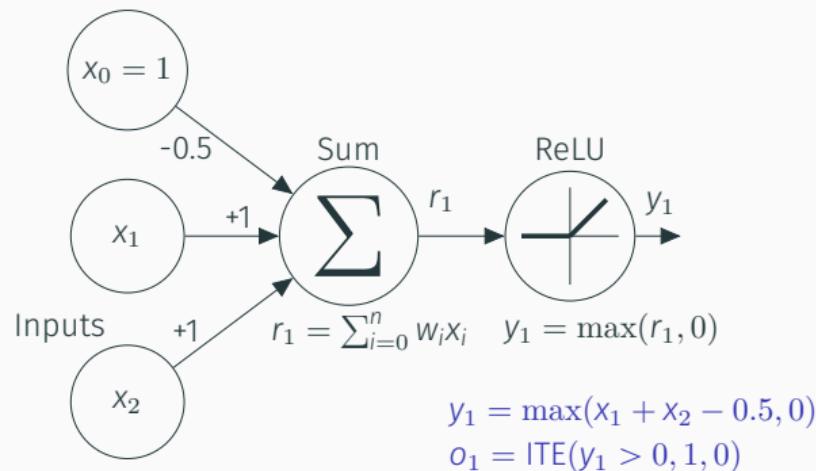
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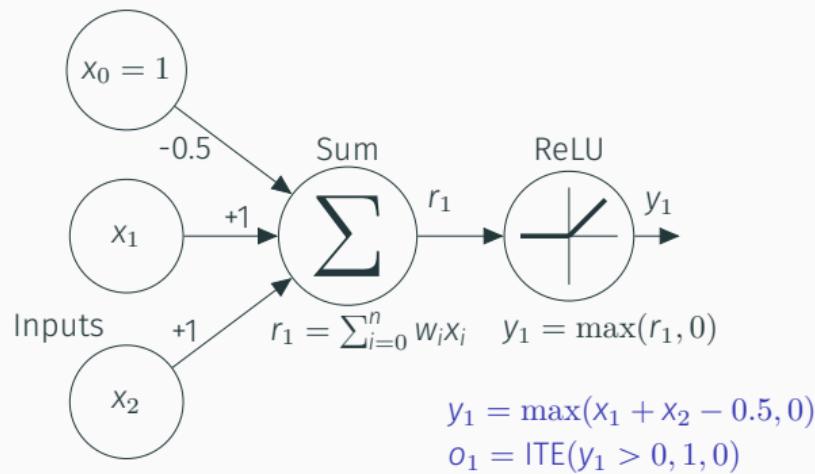
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1	0	1	0	N	N	Y	N
1	0	1	1	N	N	Y	N
1	1	0	0	Y	N	Y	Y
1	1	0	1	Y	Y	Y	Y
1	1	1	0	Y	N	Y	Y
1	1	1	1	Y	N	Y	Y

A neural network example



x_1	x_2	r_1	y_1	$\kappa(\mathbf{x})$
0	0	-0.5	0	0
0	1	0.5	0.5	1
1	0	0.5	0.5	1
1	1	1.5	1.5	1

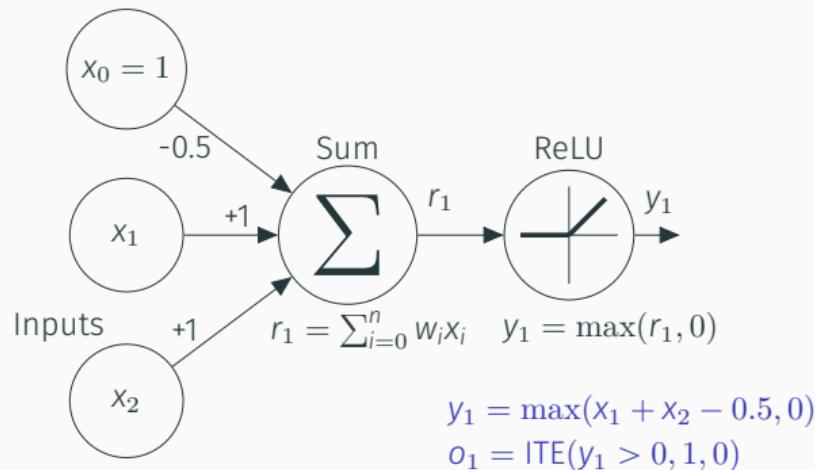
A neural network example



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0	0	-0.5	0	0
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- Explanation for why $\kappa(1, 1) = 1$?

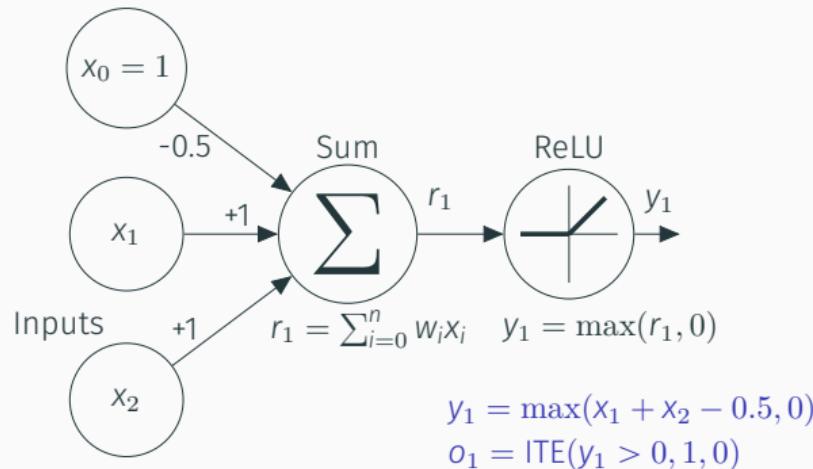
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An arbitrary classifier

- Classification function:

$$\kappa(x_1, x_2, x_3, x_4) = \neg x_1 \wedge \neg x_2 \vee x_1 \wedge x_2 \wedge x_4 \vee \neg x_1 \wedge x_2 \wedge \neg x_3 \vee \neg x_2 \wedge x_3 \wedge x_4$$

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0	0	1	0	1
0	0	1	1	1
0	1	0	0	1
0	1	0	1	1
0	1	1	0	0
0	1	1	1	0
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	1
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Outline – Unit #01

ML Models: Classification & Regression Problems

Basics of (non-symbolic) XAI

Motivation for Explanations

Brief Glimpse of Logic

Reasoning About ML Models

Understanding Intrinsic Interpretability

Standard tools of the trade

- **SAT**: decision problem for propositional logic
 - Formulas most often represented in CNF
 - There are optimization variants: MaxSAT, PBO, MinSAT, etc.
 - There are quantified variants: QBF, QMaxSAT, etc.
- **SMT**: decision problem for (decidable) fragments of first-order logic (**FOL**)
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- Background on SAT/SMT:
 - <https://alexeyignatiev.github.io/ssa-school-2019/>
 - <https://alexeyignatiev.github.io/ijcai19tut/>

Basic knowledge on
SAT & SMT assumed.
See links below.

[BHvMW09]

SAT/SMT/MILP/CP solvers used as oracles – more detail later

- Deciding satisfiability, entailment
- Computing prime implicants/implicates
- Computing MUSes, MCSes
 - Algorithms: Deletion, QuickXplain, Progression, Dichotomic, etc. [MM20]
- Enumeration of MUSes, MCSes
 - Algorithms: Marco, Camus, etc. [LS08, LPMM16]
- Solving MaxSAT, MaxSMT
 - Algorithms: Core-guided, Minimum hitting sets, branch&bound, etc. [MHL⁺13]
- Solving quantification problems, e.g. QBF
 - Algorithms: Abstraction refinement [JKMC16]

Basic definitions in propositional logic

- Atoms ($\{x, x_1, \dots\}$) & literals ($x_1, \neg x_1$)
- Well-formed formulas using $\neg, \wedge, \vee, \dots$
- Clause: disjunction of literals
- Term: conjunction of literals
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- Simple to generalize to more expressive domains

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- Conjunctive normal form (CNF): conjunction of clauses
- Disjunctive normal form (DNF): disjunction of terms
- Simple to generalize to more expressive domains
- $\text{CO}(\psi(\mathbf{x}))$ decides whether $\psi(\mathbf{x})$ is **satisfiable** (i.e. whether it is **consistent**), using an oracle for SAT/SMT/MILP/CP/etc.

Entailment

- Let φ represent some formula, defined on feature space \mathbb{F} , and representing a function $\varphi : \mathbb{F} \rightarrow \{0, 1\}$
- Let τ represent some other formula, also defined on \mathbb{F} , and with $\tau : \mathbb{F} \rightarrow \{0, 1\}$

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- An example:
 - $\mathbb{F} = \{0, 1\}^2$
 - $\varphi(x_1, x_2) = x_1 \vee \neg x_2$
 - Clearly, $x_1 \vDash \varphi$ and $\neg x_2 \vDash \varphi$
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- Another example:
 - $\mathbb{F} = \{0, 1\}^3$
 - $\varphi(x_1, x_2, x_3) = x_1 \wedge x_2 \vee x_1 \wedge x_3$
 - Clearly, $x_1 \wedge x_2 \vDash \varphi$ and $x_1 \wedge x_3 \vDash \varphi$
 - Also, $\text{CO}(x_1 \wedge x_2 \wedge ((\neg x_1 \vee \neg x_2) \wedge (\neg x_1 \vee \neg x_3)))$ does not hold

Entailment & explanations – how do we construct explanations?

- Classification function:

$$\kappa(x_1, x_2, x_3, x_4) = \neg x_1 \wedge \neg x_2 \vee x_1 \wedge x_2 \wedge x_4 \vee \neg x_1 \wedge x_2 \wedge \neg x_3 \vee \neg x_2 \wedge x_3 \wedge x_4$$

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1	0	0	1	0
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1	0	1	1	1
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Outline – Unit #01

ML Models: Classification & Regression Problems

Basics of (non-symbolic) XAI

Motivation for Explanations

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Reasoning About ML Models

Understanding Intrinsic Interpretability

Decision sets with boolean features

- Example ML model:

Features: $x_1, x_2, x_3, x_4 \in \{0, 1\}$ (boolean)

Rules:

IF	$x_1 \wedge \neg x_2 \wedge x_3$	THEN	predict \boxplus
IF	$x_1 \wedge \neg x_3 \wedge x_4$	THEN	predict \boxminus
IF	$x_3 \wedge x_4$	THEN	predict \boxminus

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IF	$x_1 \wedge \neg x_2 \wedge x_3$	THEN	predict \blacksquare
IF	$x_1 \wedge \neg x_3 \wedge x_4$	THEN	predict \square
IF	$x_3 \wedge x_4$	THEN	predict \square

- Q:** Can the model predict both \blacksquare and \square for some instance, i.e. is there overlap?

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- Yes, certainly: pick $(x_1, x_2, x_3, x_4) = (1, 0, 1, 1)$

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- Yes, certainly: pick $(x_1, x_2, x_3, x_4) = (1, 0, 1, 1)$
- A formalization:

$$\begin{aligned}y_{p,1} &\leftrightarrow (x_1 \wedge \neg x_2 \wedge x_3) \wedge \\y_{n,1} &\leftrightarrow (x_1 \wedge \neg x_3 \wedge x_4) \wedge \\y_{n,2} &\leftrightarrow (x_3 \wedge x_4) \wedge (y_p \leftrightarrow y_{p,1}) \wedge \\(y_n &\leftrightarrow (y_{n,1} \vee y_{n,2})) \wedge (y_p) \wedge (y_n)\end{aligned}$$

... and solve with SAT solver (after clausification)

Or use PySAT

[Tse68, PG86]

[IMM18]

\therefore There exists a model iff there exists a point in feature space yielding both predictions

Decision sets with ordinal features

- Example ML model:

Features: $x_1, x_2 \in \{0, 1, 2\}$ (integer)

Rules:

IF $2x_1 + x_2 > 0$ THEN predict 田

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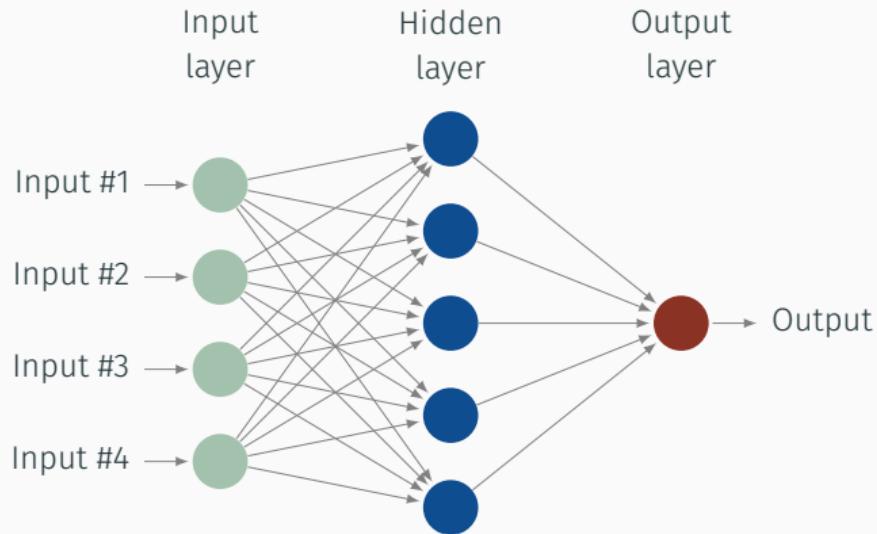
- Yes, of course: pick $x_1 = 0$ and $x_2 = 1$
- A formalization:

$$y_p \leftrightarrow (2x_1 + x_2 > 0) \wedge y_n \leftrightarrow (2x_1 - x_2 \leq 0) \wedge (y_p) \wedge (y_n)$$

... and solve with SMT solver (many alternatives)

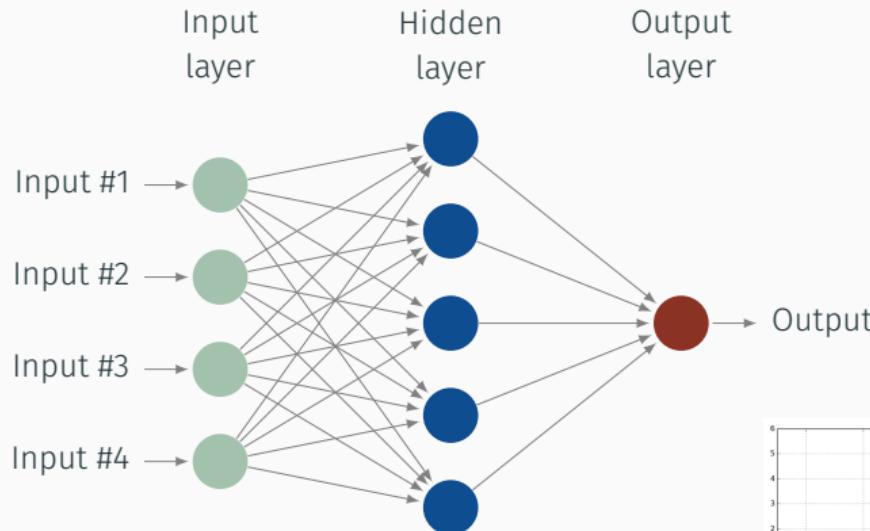
∴ There exists a model iff there exists a point in feature space yielding both predictions

Neural networks

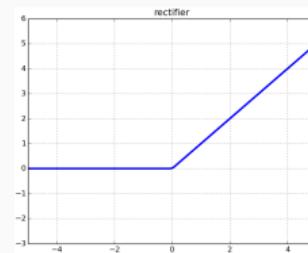


- Each layer (except first) viewed as a **block**, and
 - Compute \mathbf{x}' given input \mathbf{x} , weights matrix \mathbf{A} , and bias vector \mathbf{b}
 - Compute output \mathbf{y} given \mathbf{x}' and activation function

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 - Compute \mathbf{x}' given input \mathbf{x} , weights matrix \mathbf{A} , and bias vector \mathbf{b}
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- Each unit uses a **ReLU** activation function



[NH10]

Encoding NNs using MILP

Computation for a NN ReLU **block**, in two steps:

$$\mathbf{x}' = \mathbf{A} \cdot \mathbf{x} + \mathbf{b}$$

$$\mathbf{y} = \max(\mathbf{x}', \mathbf{0})$$

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Encoding each **block**:

[FJ18]

$$\sum_{j=1}^n a_{i,j}x_j + b_i = y_i - s_i$$

$$z_i = 1 \rightarrow y_i \leq 0$$

$$z_i = 0 \rightarrow s_i \leq 0$$

$$y_i \geq 0, s_i \geq 0, z_i \in \{0, 1\}$$

Simpler encodings exist, but **not** as effective

[KBD⁺17]

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Modeling ML models
with logic is not only
possible but also simple !

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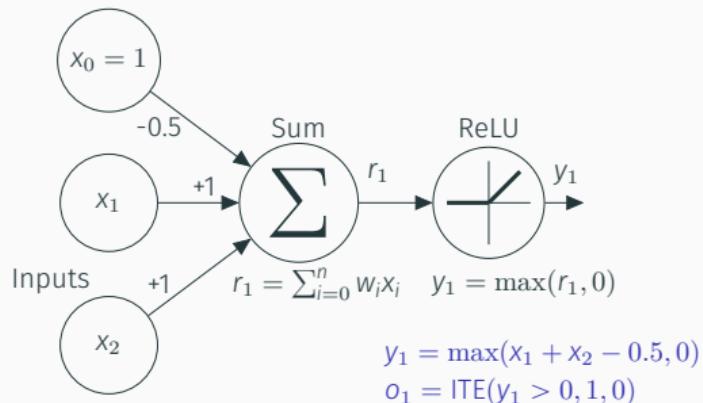
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Simpler encodings exist, but **not** as effective

[KBD⁺17]

Example – encoding a simple NN in MILP



x_1	x_2	r_1	y_1	o_1
0	0	-0.5	0	0
1	0	0.5	0.5	1
0	1	0.5	0.5	1
1	1	1.5	1.5	1

MILP encoding:

$$x_1 + x_2 - 0.5 = y_1 - s_1$$

$$z_1 = 1 \rightarrow y_1 \leq 0$$

$$z_1 = 0 \rightarrow s_1 \leq 0$$

$$o_1 = (y_1 > 0)$$

$$x_1, x_2, z_1, o_1 \in \{0, 1\}$$

$$y_1, s_1 \geq 0$$

Instance: $(\mathbf{x}, c) = ((1, 0), 1)$

$$1 + 0 - 0.5 = 0.5 - 0$$

$$1 \vee 0.5 \leq 0$$

$$0 \vee 0 \leq 0$$

$$1 = (0.5 > 0)$$

$$x_1 = 1, x_2 = 0, z_1 = 0, o_1 = 1$$

$$y_1 = 0.5, s_1 = 0$$

Checking: $\mathbf{x} = (0, 0)$

$$0 + 0 - 0.5 = 0 - 0.5$$

$$0 \vee 0 \leq 0$$

$$1 \vee 0.5 \leq 0$$

$$0 = (0 > 0)$$

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What is intrinsic interpretability?

- Goal is to deploy *interpretable* ML models
 - E.g. Decision trees, decision lists, decision sets, etc.
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[Rud19, Mol20, RCC⁺22, Rud22]

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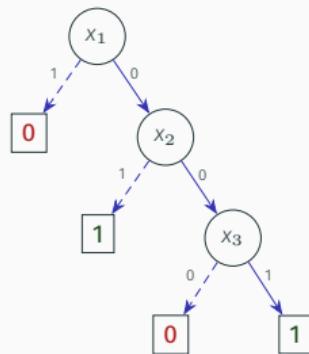
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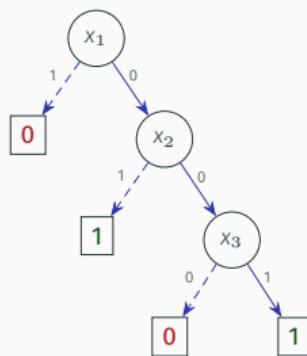
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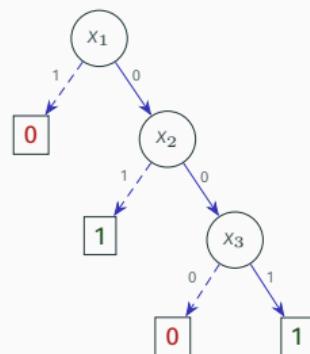


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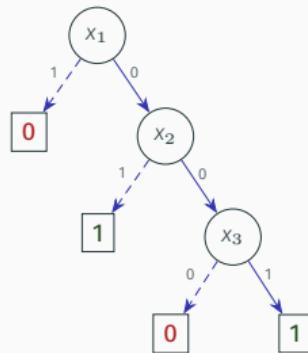
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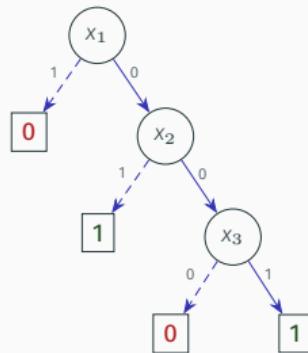
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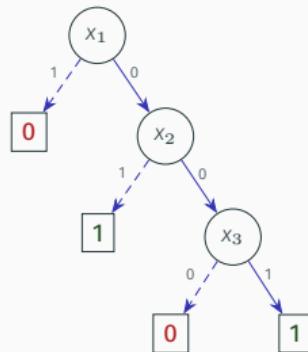
Really?

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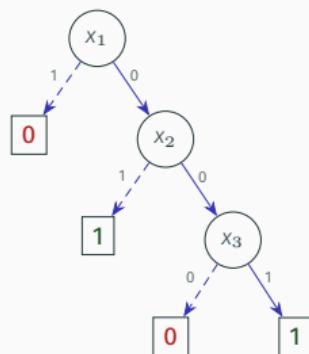
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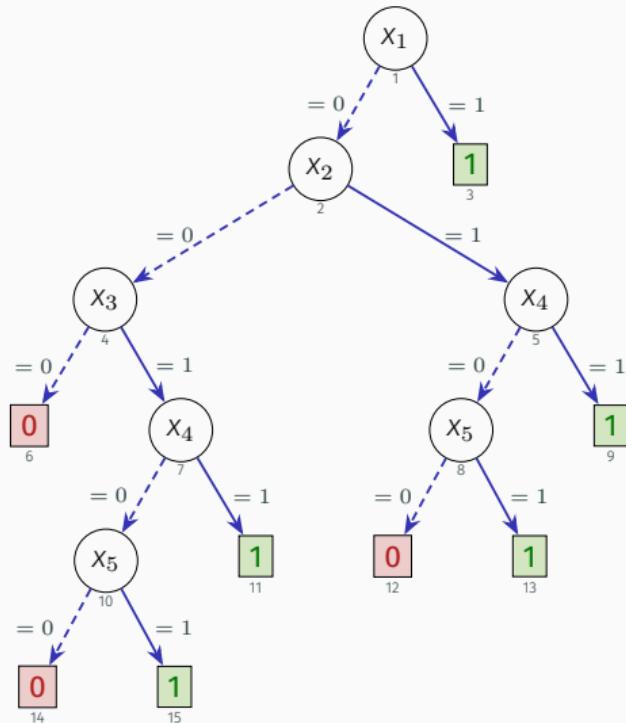
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- It is the case that: IF $\neg x_1 \wedge x_3$ THEN $\kappa(\mathbf{x}) = 1$
 - $\{1, 3\}$ is also *sufficient* for the prediction!
 - $\{1, 3\}$ is easier to grasp; also, it is *irreducible*

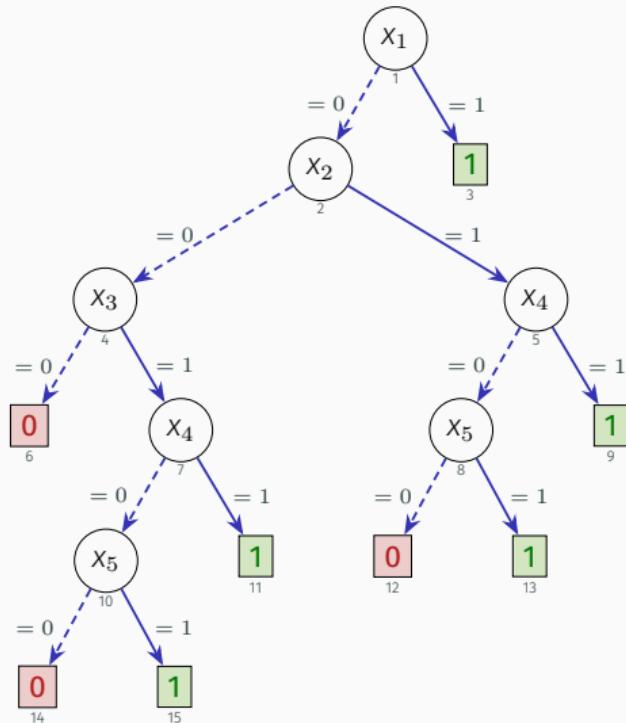
Are *interpretable* models really interpretable? – DTs



- Case of **optimal** decision tree (DT)
- Explanation for $(0, 0, 1, 0, 1)$, with prediction 1?

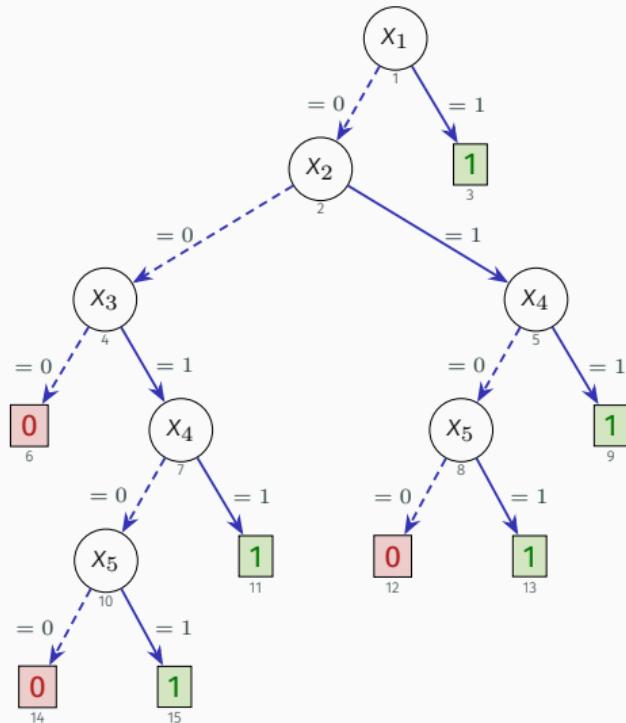
[HRS19]

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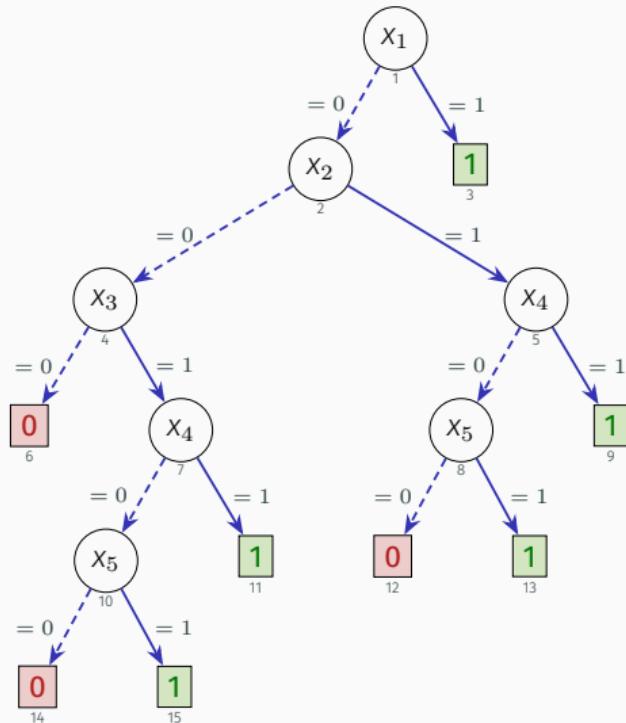
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 - But, x_1, x_2, x_4 are **irrelevant** for the prediction:

x_3	x_5	x_1	x_2	x_4	$\kappa(\mathbf{x})$
1	1	0	0	0	1
1	1	0	0	1	1
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1	1	1	1	1	1

\therefore fixing $\{3, 5\}$ suffices for the prediction
Compare with $\{1, 2, 3, 4, 5\}...$

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_2 :$	ELSE IF	$(x_2 \wedge x_4 \wedge x_6)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_3 :$	ELSE IF	$(\neg x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
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 - Would he/she be able to compute the set $\{3, 4, 6\}$, by manual inspection?

Questions?

Lecture 02

Recapitulate first lecture

- ML models: classification & regression

Recapitulate first lecture

- ML models: classification & regression
- Glimpse of heuristic XAI

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- Answers to **Why?** questions as logic rules

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- ML models: classification & regression
- Glimpse of heuristic XAI
- Answers to **Why?** questions as logic rules
- Logic-based reasoning of ML models
- Apparent difficulties with explaining interpretable models

Plan for this course

- Lecture 01 – unit(s):
 - #01: Foundations
- Lecture 02 – unit(s):
 - #02: Principles of symbolic XAI – **feature selection**
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 – unit(s):
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 – unit(s):
 - #06: Recent, emerging & advanced topics
- Lecture 05 – unit(s):
 - #07: Principles of symbolic XAI – **feature attribution** (& myth of Shapley values in XAI)
 - #08: Corrected feature attribution – nuSHAP
 - #09: Conclusions & research directions

Unit #02

Principles of Symbolic XAI – Feature Selection

Outline – Unit #02

Definitions of Explanations

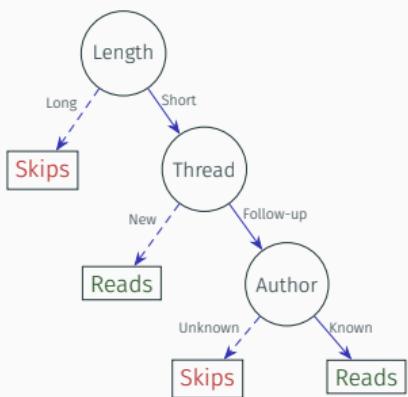
Duality Properties

Computational Problems

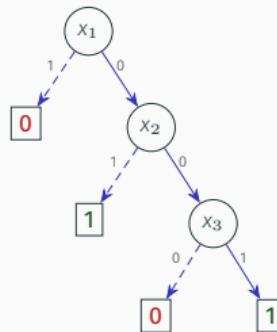
What is an explanation?

- Notation:

Original DT [PM17]



Rewritten DT



Mapping

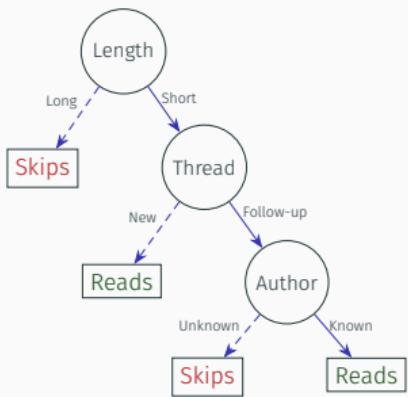
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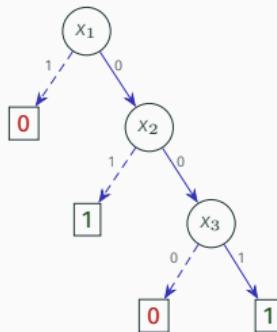
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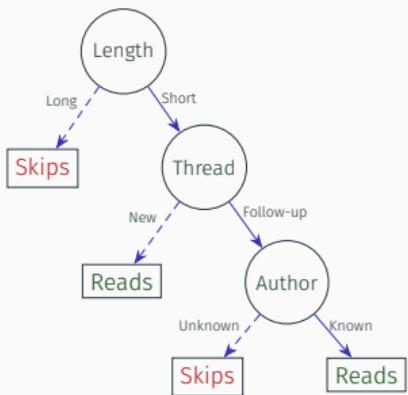
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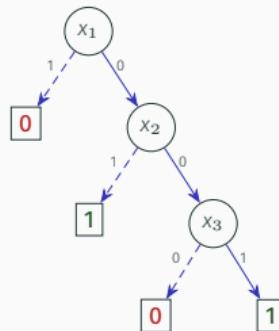
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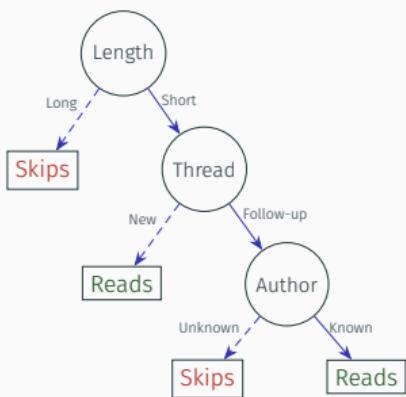
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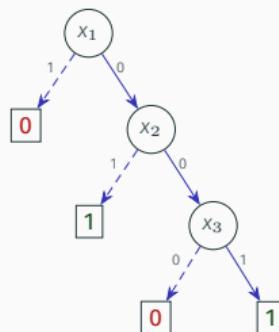
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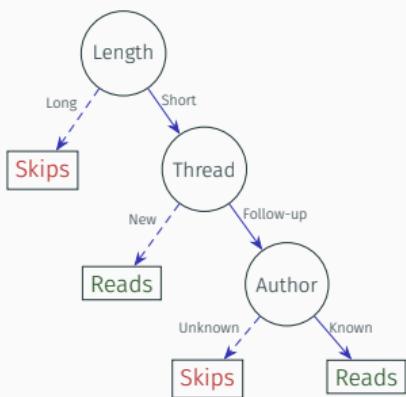
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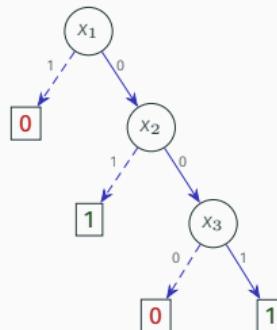
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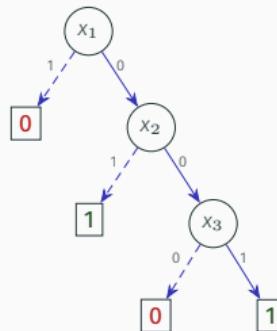
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- E.g.: explanation for $\mathbf{v} = (\neg x_1, \neg x_2, x_3)$?
 - It is the case that, **IF** $\neg x_1 \wedge \neg x_2 \wedge x_3$ **THEN** $\kappa(\mathbf{x}) = 1$
 - One possible explanation is $\{\neg x_1, \neg x_2, x_3\}$ or simply $\{1, 2, 3\}$

The similarity predicate

[Mar24]

- Recall ML models for classification & regression:

- Classification: $\mathcal{M}_C = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$
- Regression: $\mathcal{M}_R = (\mathcal{F}, \mathbb{F}, \mathbb{V}, \rho)$
- General: $\mathcal{M} = (\mathcal{F}, \mathbb{F}, \mathbb{T}, \tau)$

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- **Similarity predicate:** $\sigma : \mathbb{F} \rightarrow \{\top, \perp\}$
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- Bottom line:
Reason about symbolic explainability by abstracting away type of ML model

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[SCD18, INM19a]

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- Finding one AXp (example algorithm; many more exist):

[MM20]

- Let $\mathcal{X} = \mathcal{F}$, i.e. fix all features
- Invariant: $\text{WAXp}(\mathcal{X})$ must hold. Why?
- Analyze features in any order, one feature i at a time
 - If $\text{WAXp}(\mathcal{X} \setminus \{i\})$ holds, then remove i from \mathcal{X} , i.e. i becomes free

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- In general, **validity/consistency checked with SAT/SMT/MILP/CP reasoners**

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- Can feature 1 be removed, i.e. $\forall (\mathbf{x} \in \{0, 1\}^4). \neg x_2 \wedge \neg x_3 \wedge x_4 \rightarrow \kappa(x_1, x_2, x_3, x_4)$? **Yes**
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- Can feature 4 be removed, i.e. $\forall (\mathbf{x} \in \{0, 1\}^4). \top \rightarrow \kappa(x_1, x_2, x_3, x_4)$? **No**
- AXp $\mathcal{X} = \{4\}$
- In general, **validity/consistency checked with SAT/SMT/MILP/CP reasoners**
 - **Obs:** for some classes of classifiers, poly-time algorithms exist

Recap weak AXp: $\forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (x_j = v_j) \rightarrow (\sigma(\mathbf{x}))$

More notation

- Notation $\mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}$:

$$[\mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}] \equiv \bigwedge_{i \in \mathcal{S}} (x_i = v_i)$$

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Other definitions of WAXps/AXps

- Using probabilities, non-real-valued features:

[WMHK21, IH⁺22, ABOS22, IH⁺23]

$$\text{WAXp}(\mathcal{S}) \quad := \quad \Pr(\sigma(\mathbf{x}) \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}) = 1$$

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 - This is true when comparing against 1

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[Mil19, INAM20]

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- Finding one CXp:

[MM20]

- Let $\mathcal{Y} = \mathcal{F}$, i.e. **free all features**
- Invariant: $\text{WCXp}(\mathcal{Y})$ must hold. **Why?**
- Analyze features in any order, one feature i at a time
 - If $\text{WCXp}(\mathcal{Y} \setminus \{i\})$ holds, then remove i from \mathcal{Y} , i.e. i becomes **fixed**

A simple example – CXp's

- Classifier:

$$\kappa(x_1, x_2, x_3, x_4) = \bigvee_{i=1}^4 x_i$$

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- CXp $\mathcal{Y} = \{4\}$
- **Obs:** AXp is MHS of CXp and vice-versa...

Recap weak CXp: $\exists(\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (x_j = v_j) \wedge (\neg \sigma(\mathbf{x}))$

Other definitions of WCXps/CXps

- Using probabilities, non-real-valued features:

$$\text{WCXp}(\mathcal{S}) := \Pr(\sigma(\mathbf{x}) \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}) < 1$$

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- Definition of CXp remains unchanged

Detour: global explanations

[INM19b]

- AXps and CXps are defined locally (because of \mathbf{v}) but hold globally
 - Localized explanations
 - Can be viewed as attempt at formalizing local explanations
- One can define explanations without picking a given point in feature space
 - Let $q \in \mathbb{T}$, and refine the similarity predicate:
 - Classification: $\sigma(\mathbf{x}) = [\kappa(\mathbf{x}) = q]$
 - Regression: $\sigma(\mathbf{x}) = [|\kappa(\mathbf{x}) - q| \leq \delta]$, δ is user-specified
 - Let $\mathbb{L} = \{(x_i = v_i) \mid i \in \mathcal{F} \wedge v_i \in \mathbb{V}\}$
 - Let $\mathcal{S} \subsetneq \mathbb{L}$ be a subset of literals that does not repeat features, i.e. \mathcal{S} is not inconsistent
 - Then, \mathcal{S} is a global AXp if,

$$\forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{(x_i = v_i) \in \mathcal{S}} (x_i = v_i) \rightarrow (\sigma(\mathbf{x}))$$

- Counterexamples are minimal hitting sets of global AXps and vice-versa

[INM19b]

Outline – Unit #02

Definitions of Explanations

Duality Properties

Computational Problems

Duality in explainability – basic results

[INAM20, Mar22]

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$\mathcal{S} \subseteq \mathcal{F}$ is an AXp iff it is a minimal hitting set
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Duality in explainability – basic results

[INAM20, Mar22]

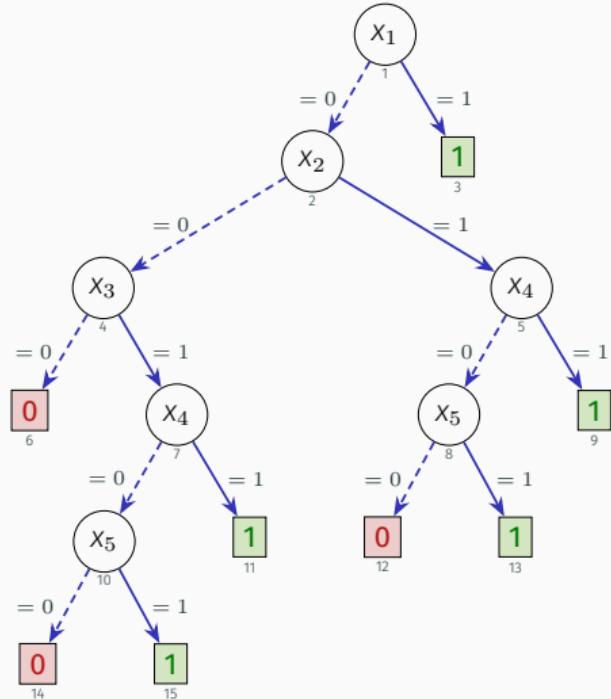
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[INAM20, Mar22]

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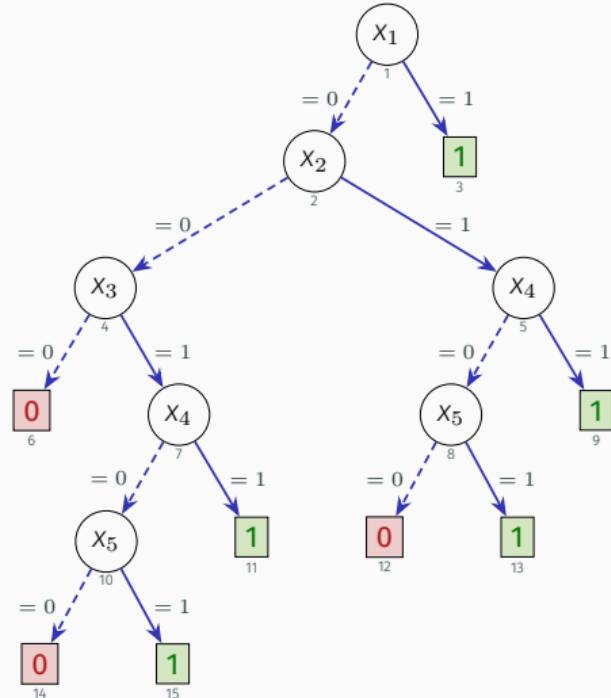
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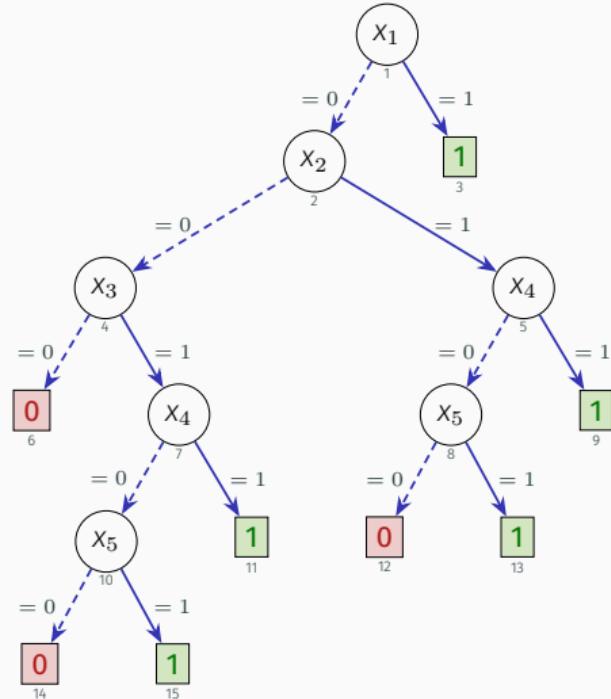
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[INAM20, Mar22]

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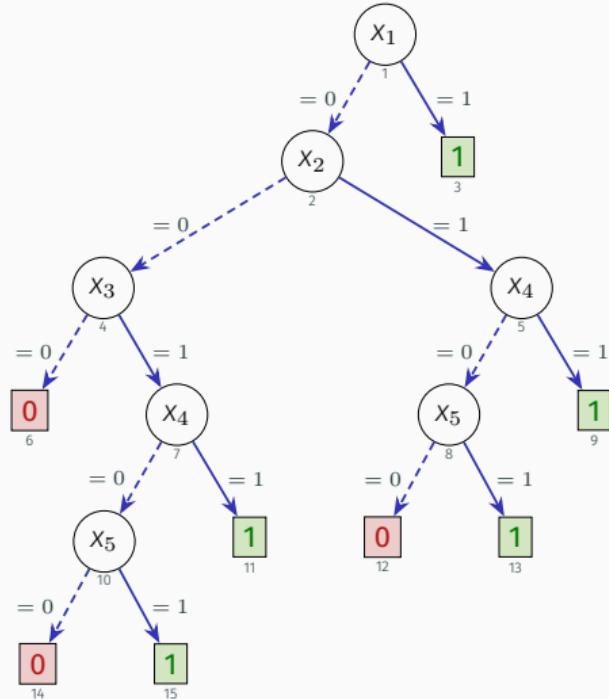
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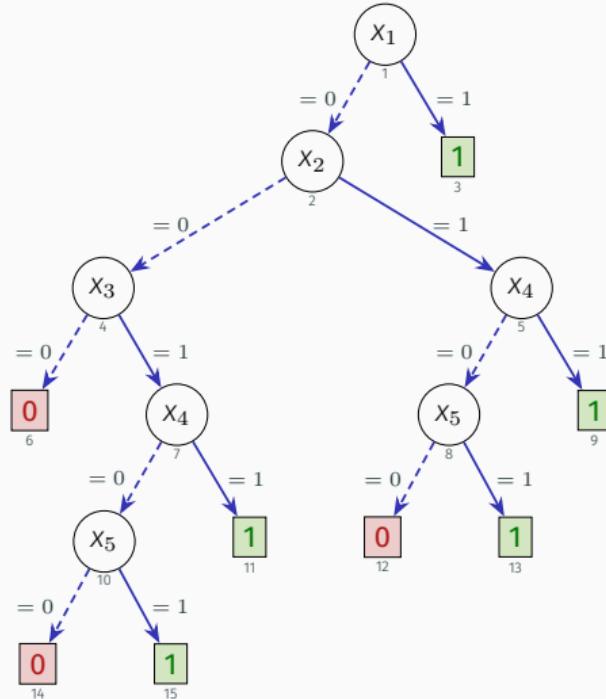
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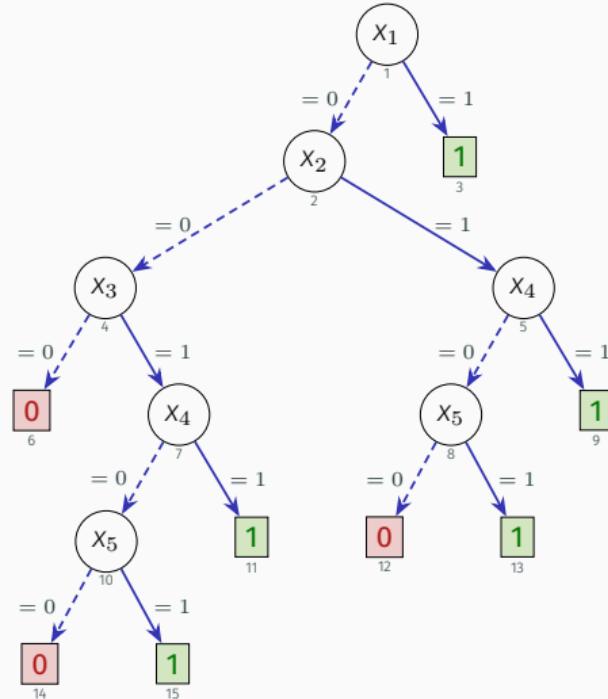
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- Each AXp is an MHS of the set of CXps
- Each CXp is an MHS of the set of AXps



Duality in explainability – basic results

[INAM20, Mar22]

- **Claim:**

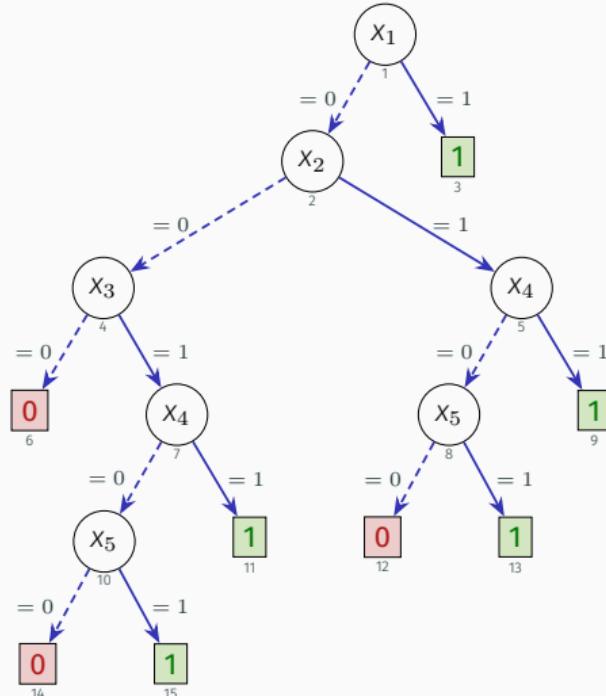
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 - $\{2, 5\}$ is **not** a CXp
 - $\{1, 2, 3, 4, 5\}, \{1, 2, 3, 5\}$ and $\{1, 3, 5\}$ are **not** AXps



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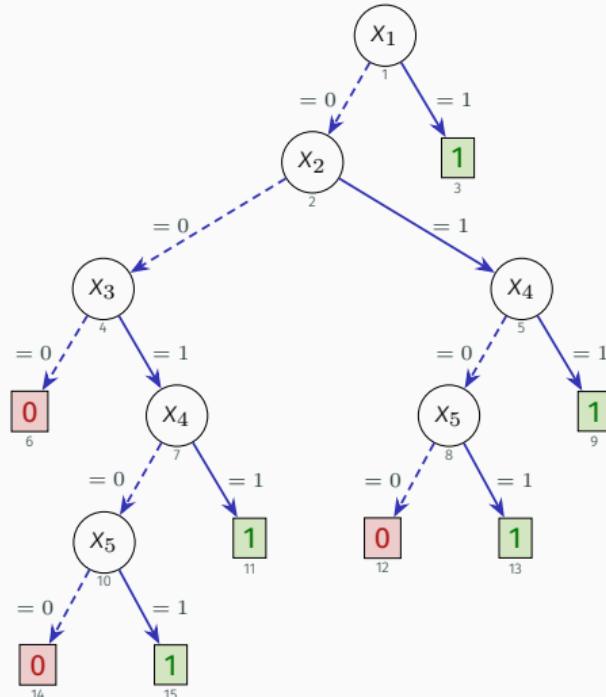
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 - **Why?**



Outline – Unit #02

Definitions of Explanations

Duality Properties

Computational Problems

Computational problems in (formal) explainability

- Compute one abductive/contrastive explanation

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- Compute **one** abductive/contrastive explanation
- Enumerate **all** abductive/contrastive explanations

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- Decide whether feature included in **some** abductive/contrastive explanation

Computing one AXp/CXp

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- **Monotone** predicates for WAXp & WCXp:

$$\mathbb{P}_{\text{axp}}(\mathcal{S}) \triangleq \neg \text{CO} (\llbracket (\bigwedge_{i \in \mathcal{S}} (x_i = v_i)) \wedge (\neg \sigma(\mathbf{x})) \rrbracket) \quad \mathbb{P}_{\text{cxp}}(\mathcal{S}) \triangleq \text{CO} \left(\llbracket \left(\bigwedge_{i \in \mathcal{F} \setminus \mathcal{S}} (x_i = v_i) \right) \wedge (\neg \sigma(\mathbf{x})) \rrbracket \right)$$

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Input: Predicate \mathbb{P} , parameterized by \mathcal{T}, \mathcal{M}

Output: One XP \mathcal{S}

```
1: procedure oneXP( $\mathbb{P}$ )
2:    $\mathcal{S} \leftarrow \mathcal{F}$                                  $\triangleright$  Initialization:  $\mathbb{P}(\mathcal{S})$  holds
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5:        $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$ 
6:   return  $\mathcal{S}$                                  $\triangleright$  Update  $\mathcal{S}$  only if  $\mathbb{P}(\mathcal{S} \setminus \{i\})$  holds
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Exploiting MSMP, i.e.
basic algorithm used
for different problems.

- ▷ Initialization: $\mathbb{P}(\mathcal{S})$ holds
- ▷ Loop invariant: $\mathbb{P}(\mathcal{S})$ holds
- ▷ Update \mathcal{S} only if $\mathbb{P}(\mathcal{S} \setminus \{i\})$ holds
- ▷ Returned set \mathcal{S} : $\mathbb{P}(\mathcal{S})$ holds

Detour: More Connections with Automated Reasoning

Prime implicants & implicants

- A conjunction of literals π (which will be viewed as a set of literals where convenient) is a **prime implicant** of some function φ if,
 1. $\pi \vDash \varphi$
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- Example:
 - $\mathbb{F} = \{0, 1\}^3$
 - $\varphi(x_1, x_2, x_3) = x_1 \wedge x_2 \vee x_1 \wedge x_3$
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- A disjunction of literals η (also viewed as a set of literals where convenient) is a prime implicate of some function φ if
 1. $\varphi \vDash \eta$
 2. For any $\eta' \subsetneq \eta$, $\varphi \not\vDash \eta'$

- Formula $\mathcal{T} = \mathcal{B} \cup \mathcal{S}$, with
 - \mathcal{B} : background knowledge (base), i.e. hard constraints
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 - And, $\mathcal{T} \vDash \perp$
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[Rei87]

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- Variants:
 - Smallest(-cost) MCS, i.e. complement of maximum(-cost) satisfiability (MaxSAT)
 - Smallest(-cost) MUS

[Rei87]

Computing AXps (resp. CXps) as MUSes (resp. MCSes)

- Recap:

$$\text{WAXp}(\mathcal{X}) \quad := \quad \forall(\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (x_j = v_j) \rightarrow (\sigma(\mathbf{x}))$$

$$\text{WCXp}(\mathcal{Y}) \quad := \quad \exists(\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (x_j = v_j) \wedge (\neg\sigma(\mathbf{x}))$$

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- **Claim:** Each MUS of $(\mathcal{B}, \mathcal{S})$ is an AXp & each MCS of $(\mathcal{B}, \mathcal{S})$ is a CXp
 - Can use MUS/MCS algorithms for finding AXps/CXps

Unit #03

Tractability in Symbolic XAI

Outline – Unit #03

Explanations for Decision Trees

XAI Queries for DTs

Myth #01: Intrinsic Interpretability

Detour: From Decision Trees to Explained Decision Sets

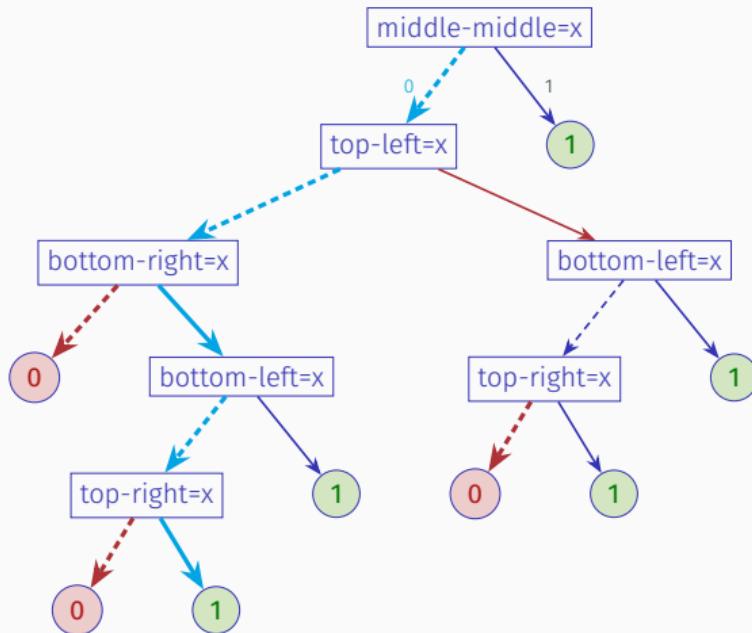
Explanations for Decision Graphs

Explanations for Monotonic Classifiers

Review examples

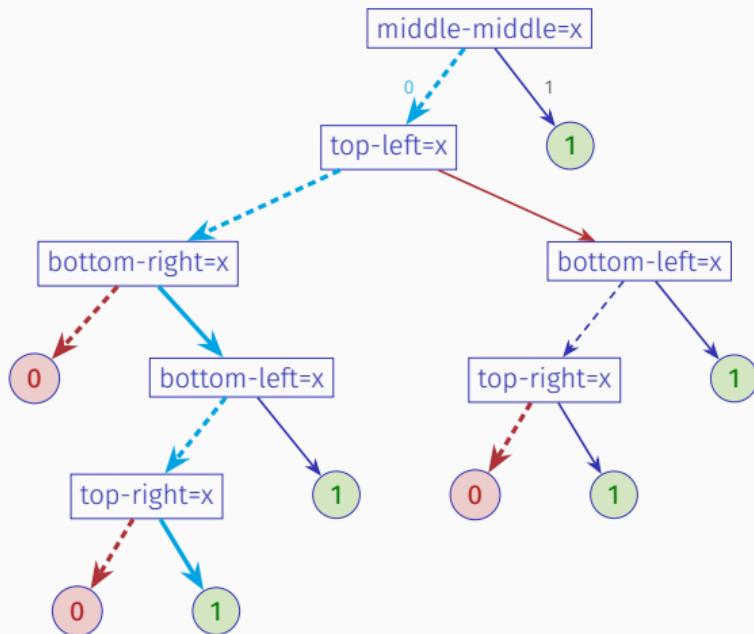
DT explanations

[IIM20]



DT explanations

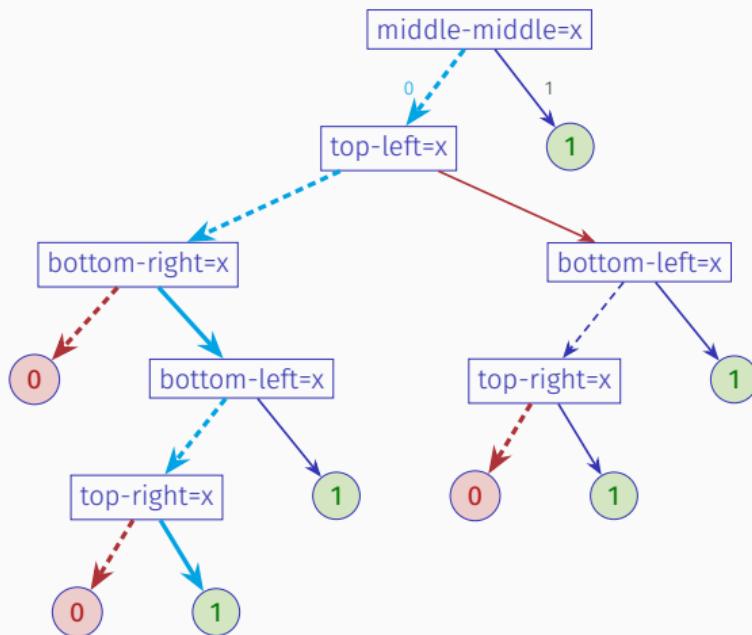
[IIM20]



- Run PI-explanation algorithm based on NP-oracles
 - Worst-case exponential time

DT explanations

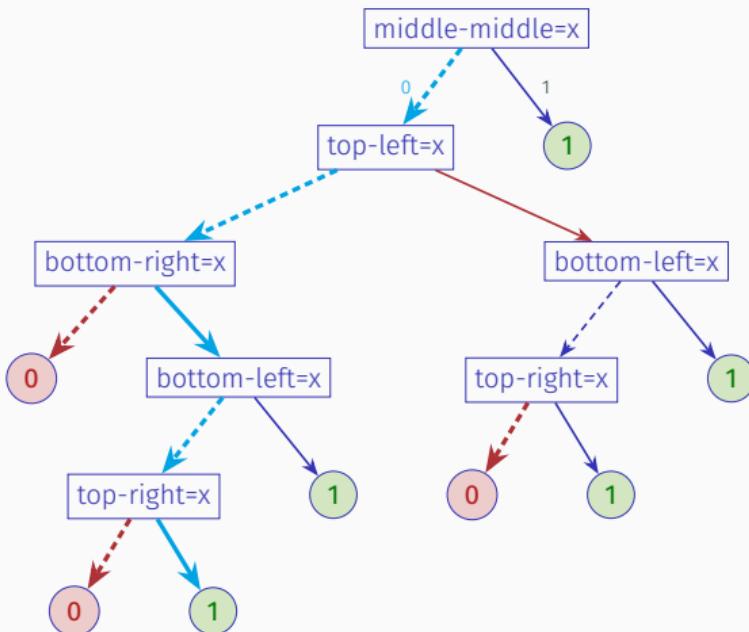
[IIM20]



- Run PI-explanation algorithm based on NP-oracles
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- For prediction **1**, it suffices to ensure **all** paths with prediction **0** remain inconsistent

DT explanations in polynomial time

[IIM20]



- Run PI-explanation algorithm based on NP-oracles
 - Worst-case exponential time
- For prediction **1**, it suffices to ensure **all** paths with prediction **0** remain inconsistent
 - I.e. find a **subset-minimal hitting set** of **all 0** paths; **these are the features to keep**
 - E.g. BR and TR suffice for prediction
 - Well-known to be solvable in **polynomial time**

[EG95]

Outline – Unit #03

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Answering queries in DTs

- Finding one AXp in polynomial-time – covered

Answering queries in DTs

- Finding one AXp in polynomial-time – covered
- Finding one CXp in polynomial-time

Answering queries in DTs

- Finding one AXp in polynomial-time – covered
- Finding one CXp in polynomial-time
- Finding all CXps in polynomial-time

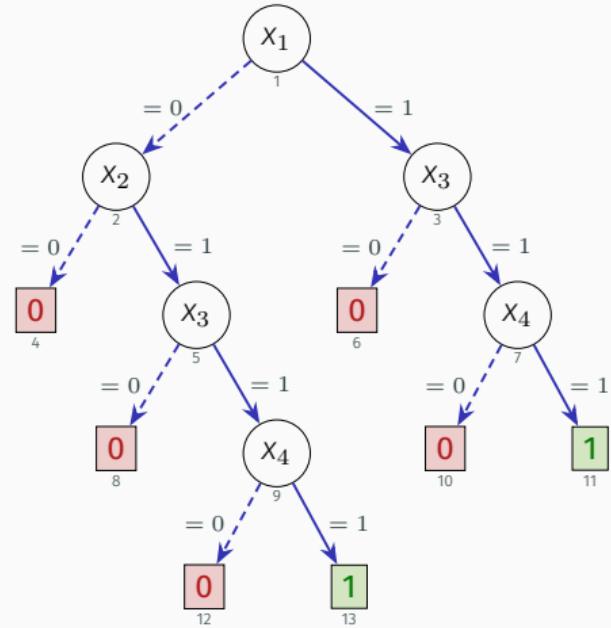
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- Finding one AXp in polynomial-time – covered
- Finding one CXp in polynomial-time
- Finding all CXps in polynomial-time; hence, finding one CXp also in polynomial-time
- Practically efficient enumeration of AXps – later

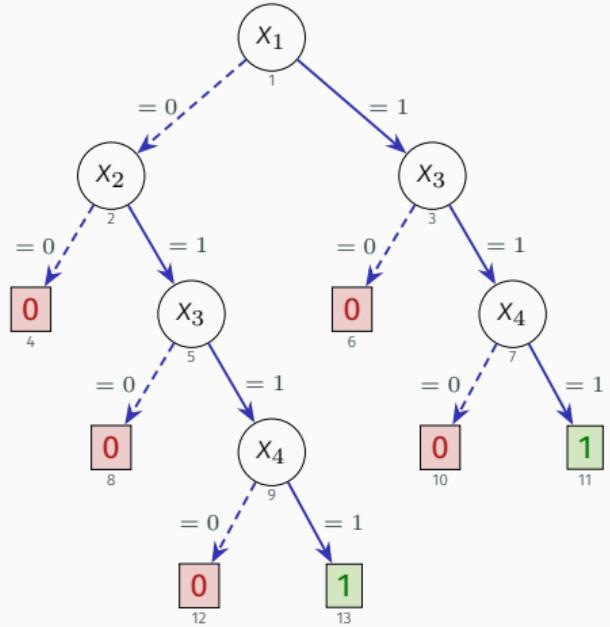
Finding all CXps in polynomial-time

- Basic algorithm:
 - $\mathcal{L} = \emptyset$



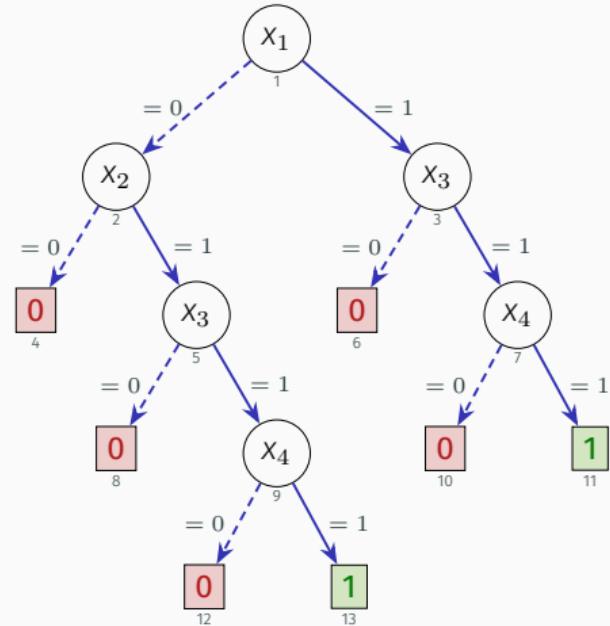
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 - For each leaf node not predicting q :



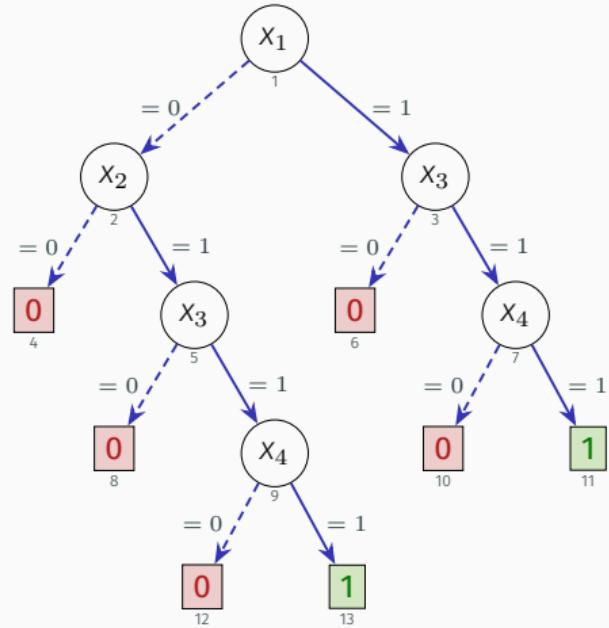
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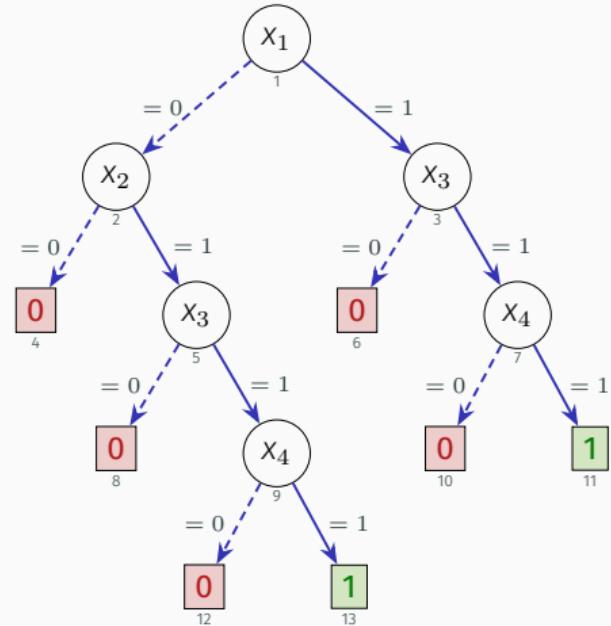
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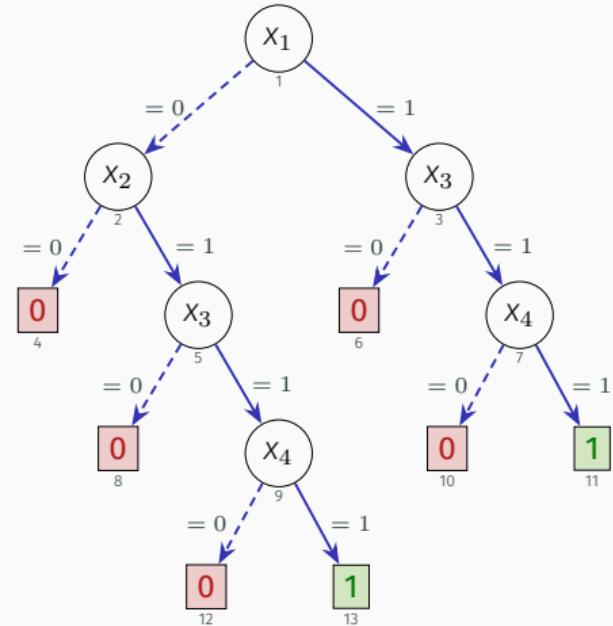
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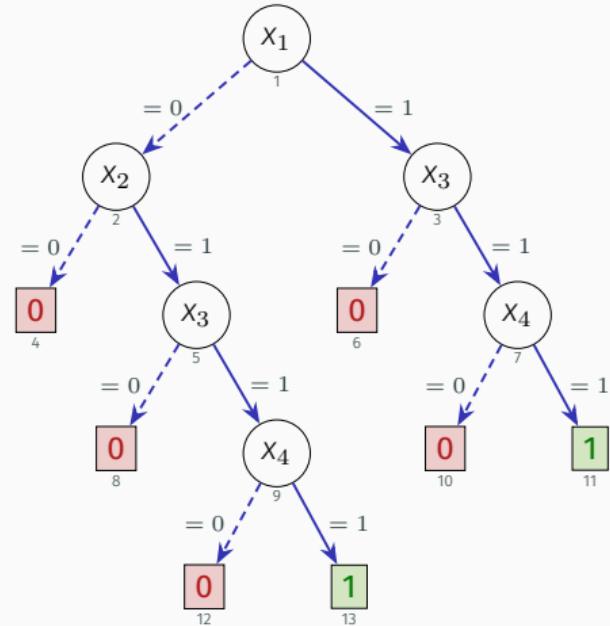
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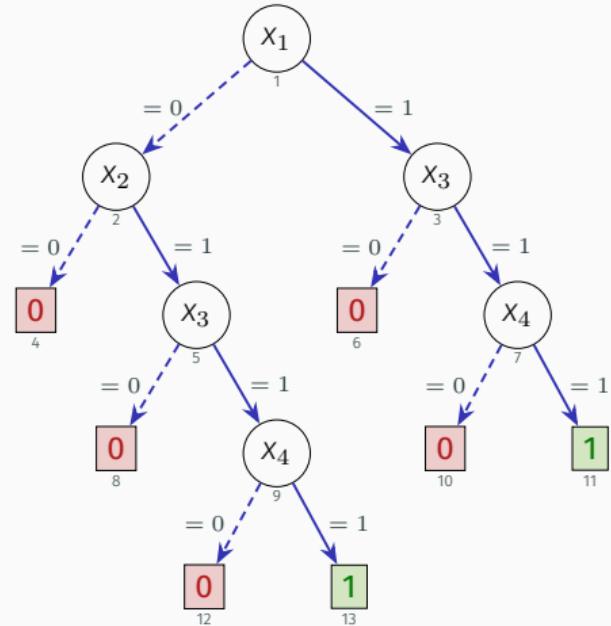
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- Example: instance is $((1, 1, 1, 1), 1)$



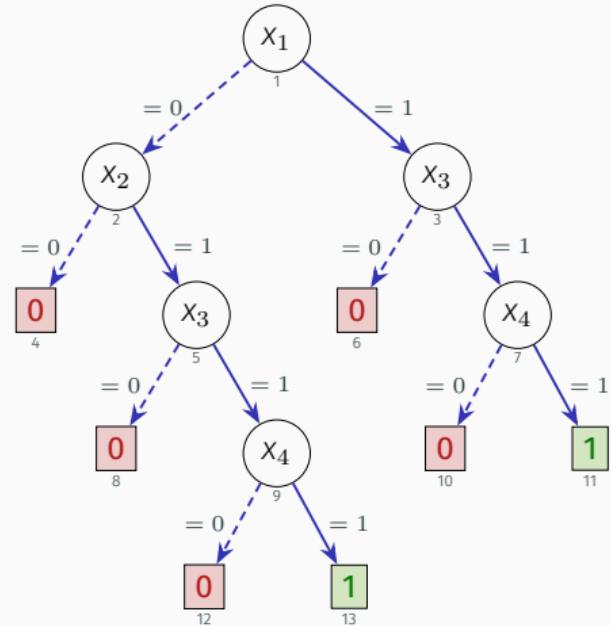
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 - Add \mathcal{I} to \mathcal{L}
 - Remove from \mathcal{L} non-minimal sets
 - \mathcal{L} contains all the CXps of the DT
- Example: instance is $((1, 1, 1, 1), 1)$
 - Add $\{1, 2\}$ to \mathcal{L}



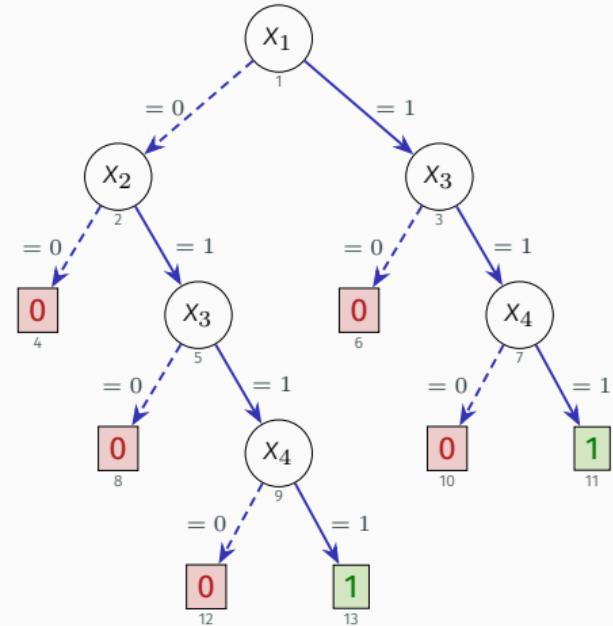
Finding all CXps in polynomial-time

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- Example: instance is $((1, 1, 1, 1), 1)$
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 - Add $\{1, 3\}$ to \mathcal{L}



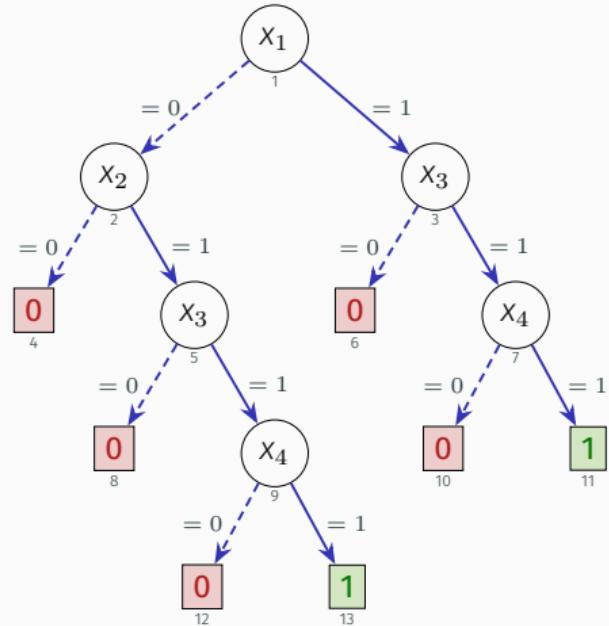
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 - Add $\{1, 3\}$ to \mathcal{L}
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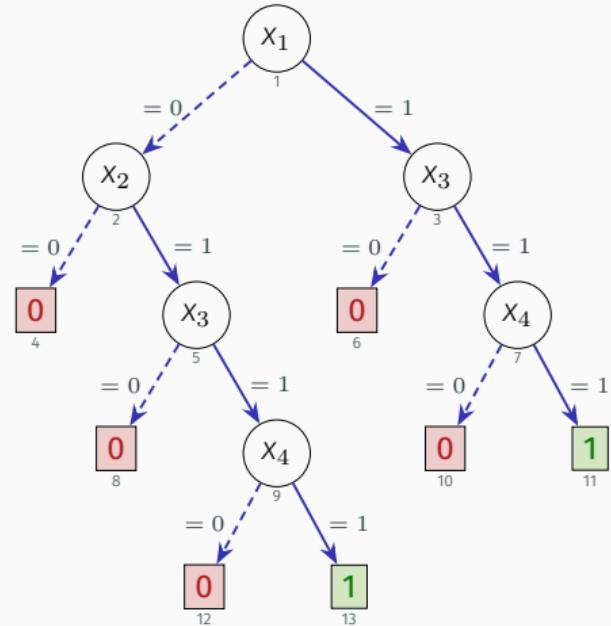
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- Example: instance is $((1, 1, 1, 1), 1)$
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 - Add $\{1, 3\}$ to \mathcal{L}
 - Add $\{1, 4\}$ to \mathcal{L}
 - Add $\{3\}$ to \mathcal{L}



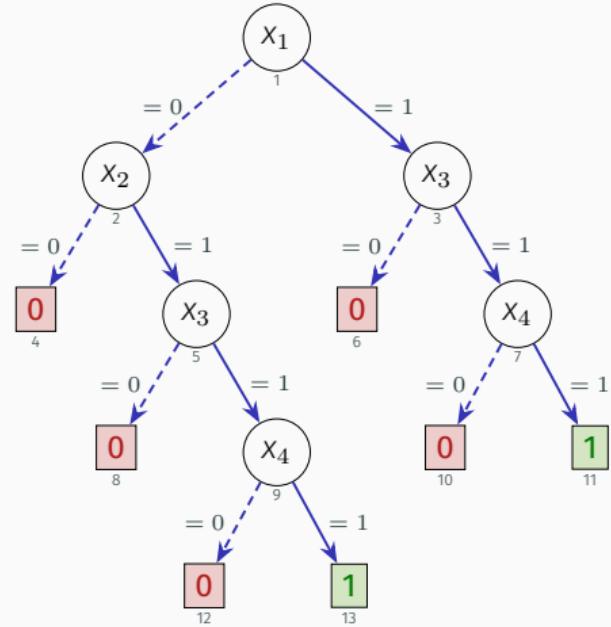
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 - Add $\{1, 4\}$ to \mathcal{L}
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 - Add $\{4\}$ to \mathcal{L}



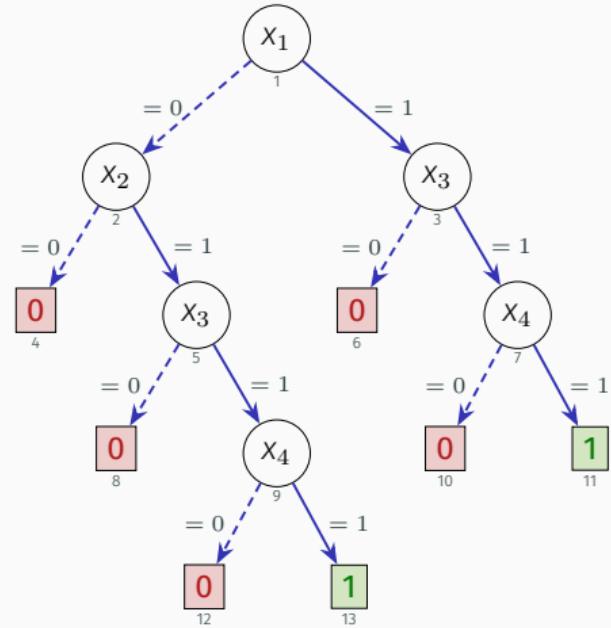
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 - Add $\{4\}$ to \mathcal{L}
 - Remove from \mathcal{L} : $\{1, 3\}$ and $\{1, 4\}$



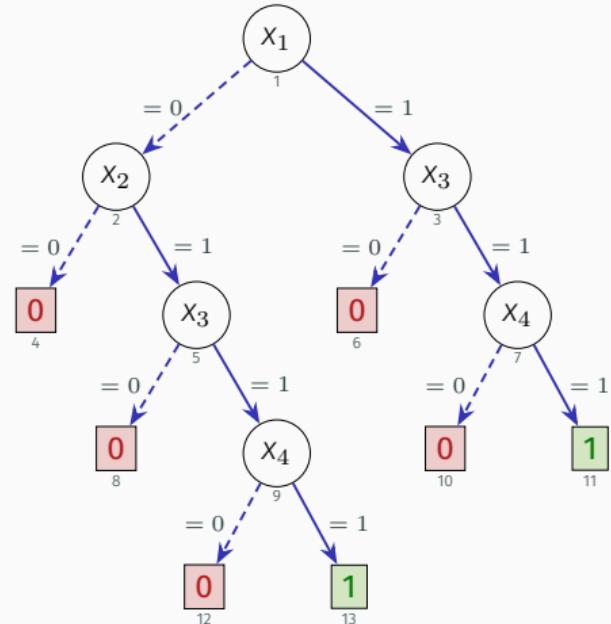
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Finding all CXps in polynomial-time

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 - Add $\{1, 4\}$ to \mathcal{L}
 - Add $\{3\}$ to \mathcal{L}
 - Add $\{4\}$ to \mathcal{L}
 - Remove from \mathcal{L} : $\{1, 3\}$ and $\{1, 4\}$
 - CXps: $\{\{1, 2\}, \{3\}, \{4\}\}$
 - AXps: $\{\{1, 3, 4\}, \{2, 3, 4\}\}$, by computing all MHSes



Outline – Unit #03

Explanations for Decision Trees

XAI Queries for DTs

Myth #01: Intrinsic Interpretability

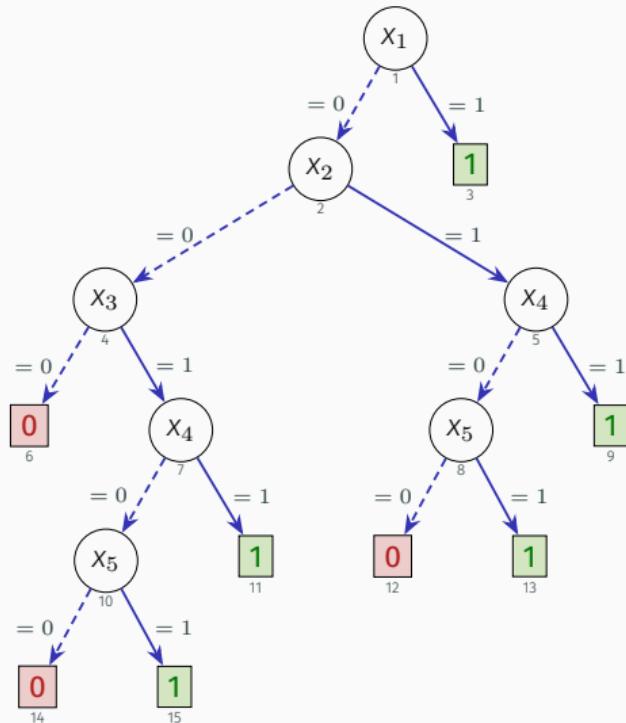
Detour: From Decision Trees to Explained Decision Sets

Explanations for Decision Graphs

Explanations for Monotonic Classifiers

Review examples

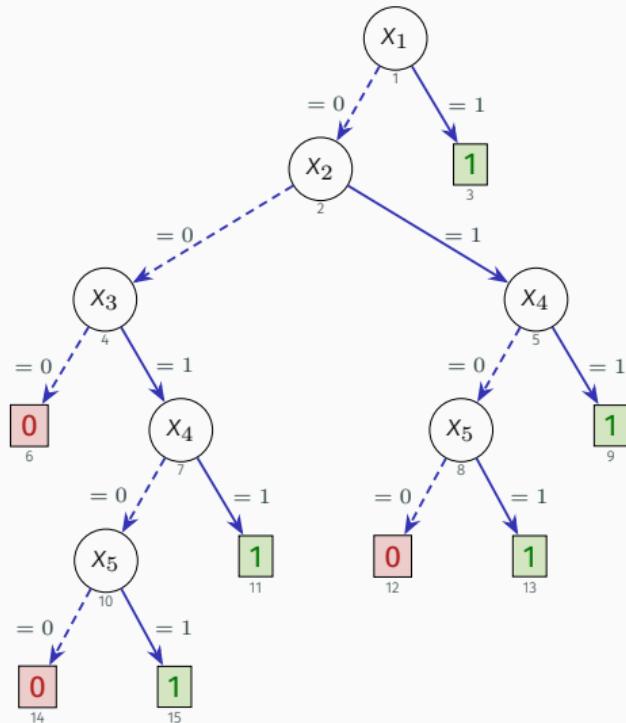
Are *interpretable* models really interpretable? – DTs



- Case of **optimal** decision tree (DT)
- Explanation for $(0, 0, 1, 0, 1)$, with prediction 1?

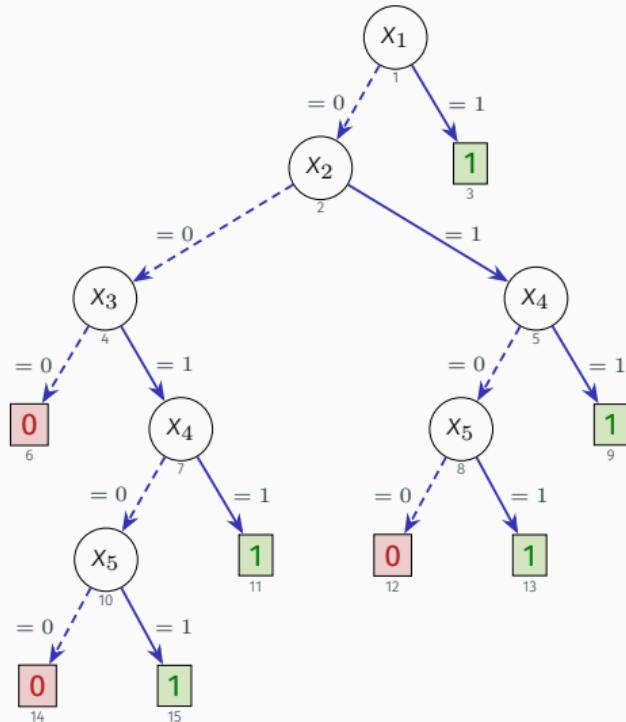
[HRS19]

Are *interpretable* models really interpretable? – DTs



- Case of **optimal** decision tree (DT) [HRS19]
- Explanation for $(0, 0, 1, 0, 1)$, with prediction 1?
 - Clearly, IF $\neg x_1 \wedge \neg x_2 \wedge x_3 \wedge \neg x_4 \wedge x_5$ THEN $\kappa(\mathbf{x}) = 1$

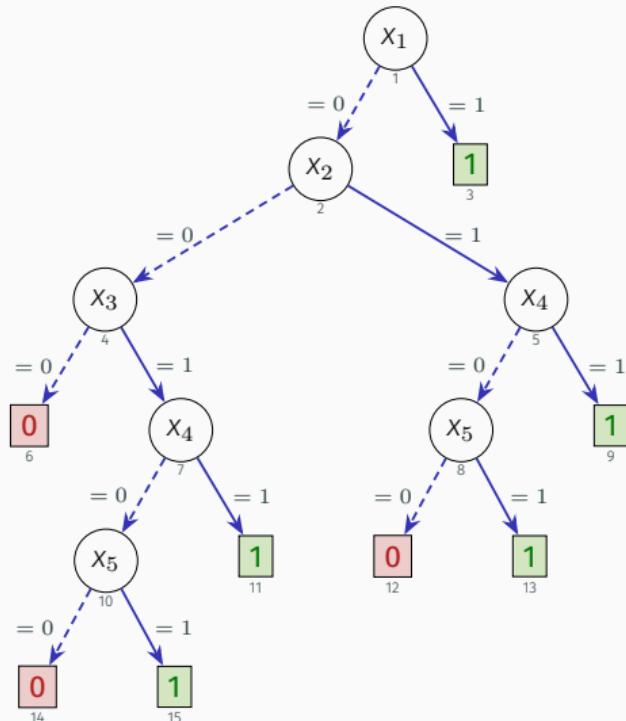
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- Explanation for $(0, 0, 1, 0, 1)$, with prediction 1?
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 - But, X_1, X_2, X_4 are **irrelevant** for the prediction:

x_3	x_5	x_1	x_2	x_4	$\kappa(\mathbf{x})$
1	1	0	0	0	1
1	1	0	0	1	1
1	1	0	1	0	1
1	1	0	1	1	1
1	1	1	0	0	1
1	1	1	0	1	1
1	1	1	1	0	1
1	1	1	1	1	1

Are *interpretable* models really interpretable? – DTs

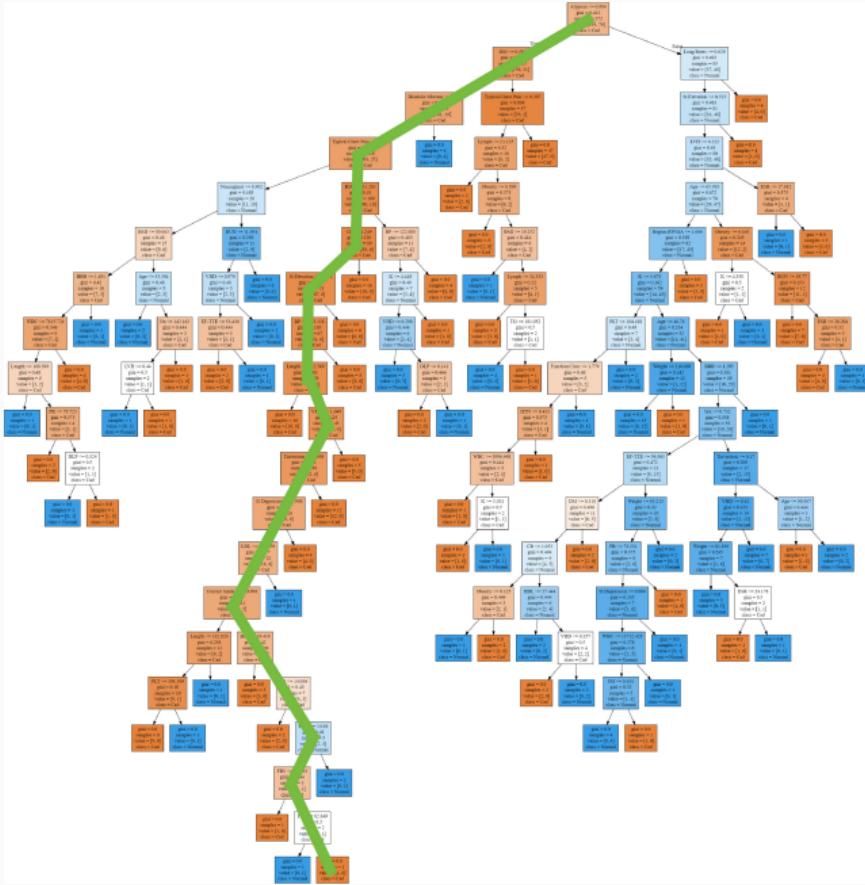


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1	1	1	0	0	1
1	1	1	0	1	1
1	1	1	1	0	1
1	1	1	1	1	1

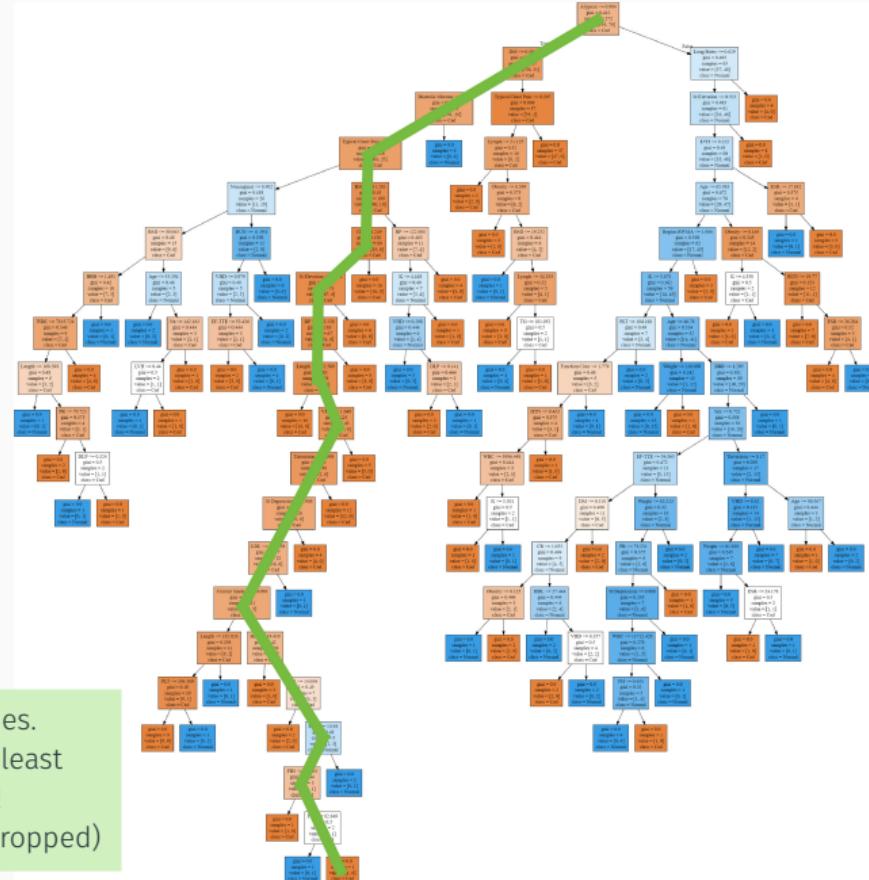
\therefore one AXp is {3, 5}
Compare with {1, 2, 3, 4, 5}...

Are *interpretable* models really interpretable? – large DTs



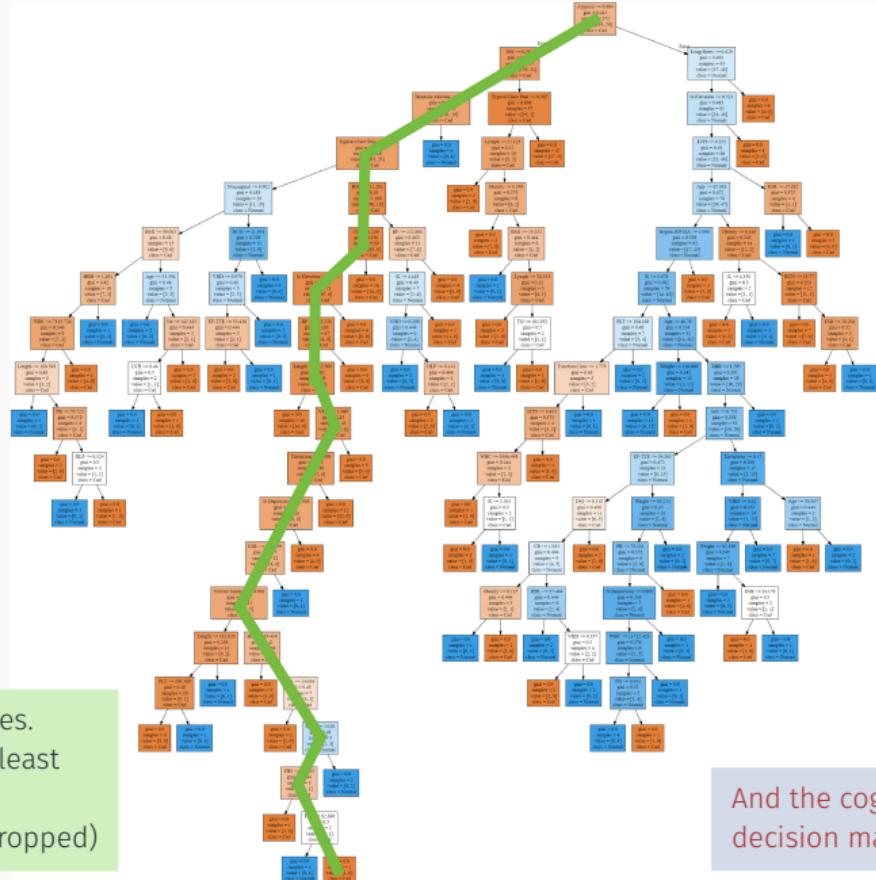
[GZM20]

Are *interpretable* models really interpretable? – large DTs



[GZM20]

Are *interpretable* models really interpretable? – large DTs

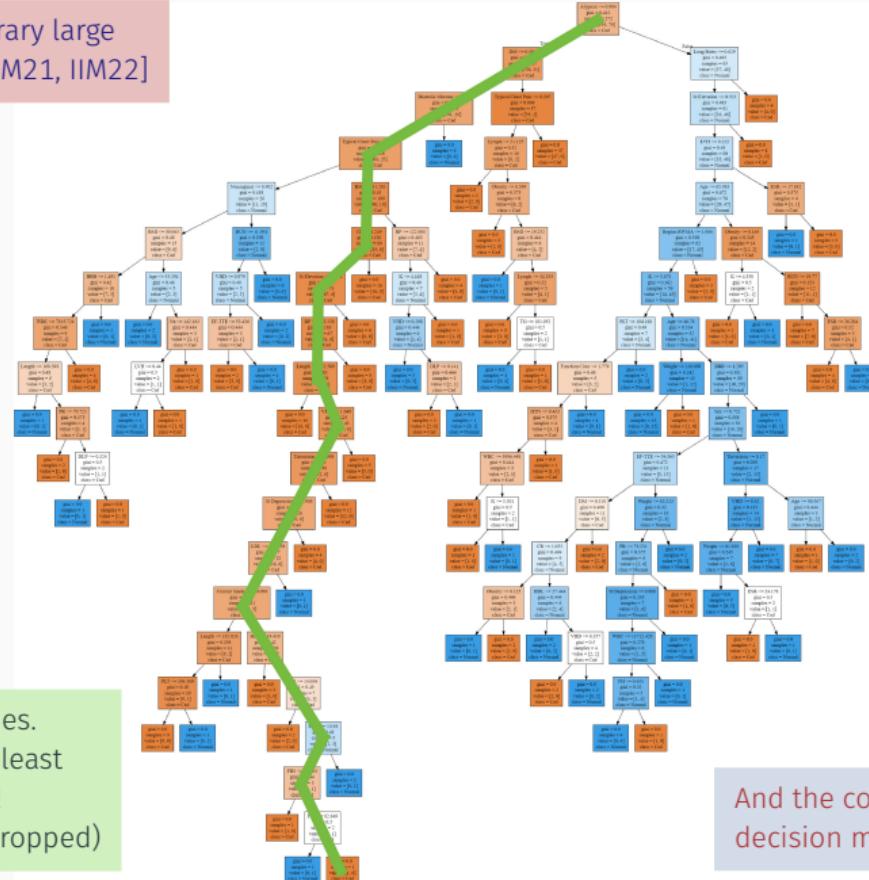


[GZM20]

Are *interpretable* models really interpretable? – large DTs

Redundancy can be arbitrary large
on path length [IIM20, HIIM21, IIM22]

[GZM20]



Path with 19 internal nodes.
By manual inspection, at least
10 literals are redundant!
(And at least 9 features dropped)

And the cognitive limits of human
decision makers are well-known [Mil56]

Are *interpretable* models really interpretable? – arbitrary redundancy [IIM20, HIIM21, IIM22]

- Classifier, with $x_1, \dots, x_m \in \{0, 1\}$:

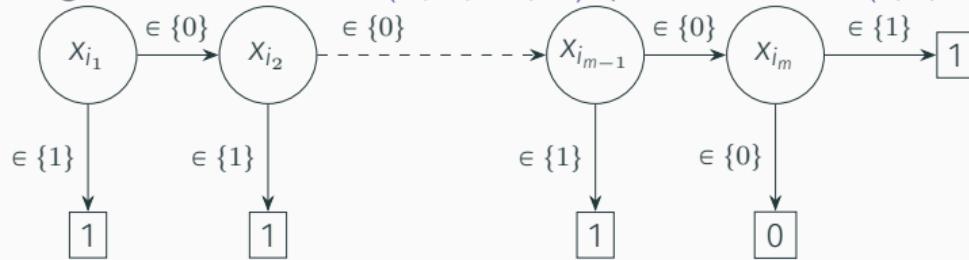
$$\kappa(x_1, x_2, \dots, x_{m-1}, x_m) = \bigvee_{i=1}^m x_i$$

Are *interpretable* models really interpretable? – arbitrary redundancy [IIM20, HIIM21, IIM22]

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- Build DT, by picking variables in order $\langle i_1, i_2, \dots, i_m \rangle$, permutation of $\langle 1, 2, \dots, m \rangle$:

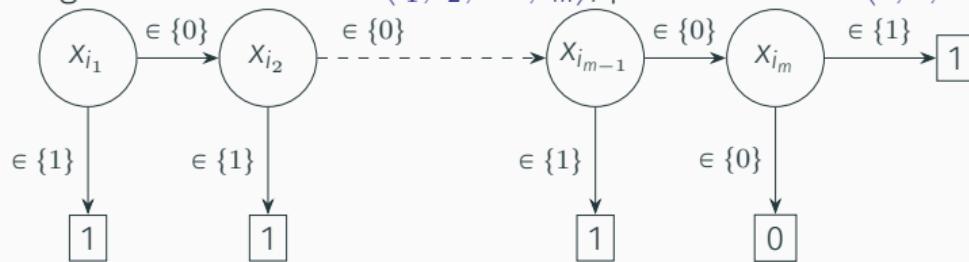


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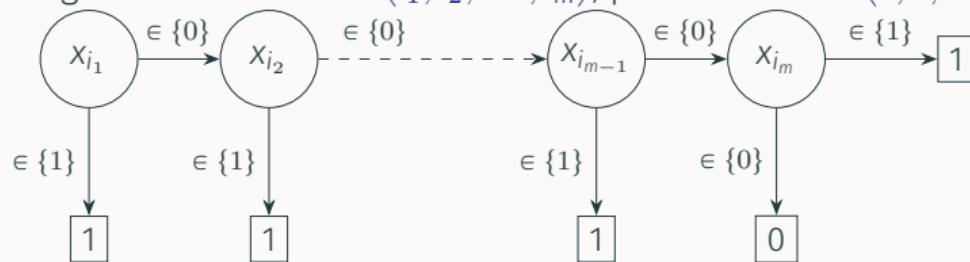
- Point: $(x_{i_1}, x_{i_2}, \dots, x_{i_{m-1}}, x_{i_m}) = (0, 0, \dots, 0, 1)$, and prediction 1

Are *interpretable* models really interpretable? – arbitrary redundancy [IIM20, HIIM21, IIM22]

- Classifier, with $x_1, \dots, x_m \in \{0, 1\}$:

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- Point: $(x_{i_1}, x_{i_2}, \dots, x_{i_{m-1}}, x_{i_m}) = (0, 0, \dots, 0, 1)$, and prediction 1
- Explanation using path in DT: $\{i_1, i_2, \dots, i_m\}$, i.e.

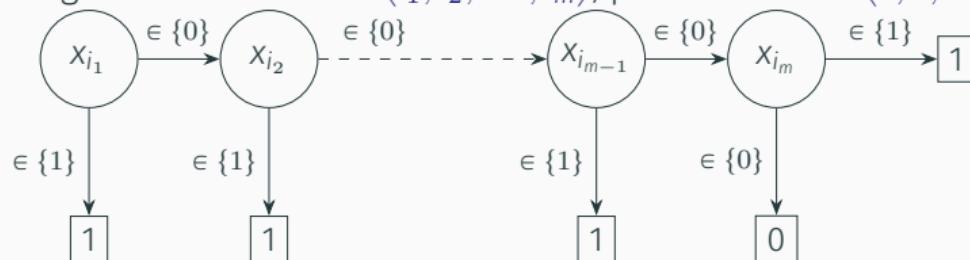
$$(x_{i_1} = 0) \wedge (x_{i_2} = 0) \wedge \dots \wedge (x_{i_{m-1}} = 0) \wedge (x_{i_m} = 1) \rightarrow \kappa(x_1, \dots, x_m)$$

Are *interpretable* models really interpretable? – arbitrary redundancy [IIM20, HIIM21, IIM22]

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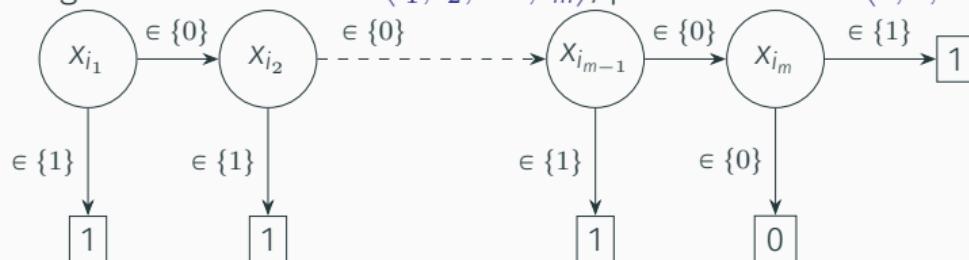
- But $\{i_m\}$ suffices for prediction, i.e. $\forall (\mathbf{x} \in \{0, 1\}^m). (x_{i_m}) \rightarrow \kappa(\mathbf{x})$

Are *interpretable* models really interpretable? – arbitrary redundancy [IIM20, IIM21, IIM22]

- Classifier, with $x_1, \dots, x_m \in \{0, 1\}$:

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- But $\{i_m\}$ suffices for prediction, i.e. $\forall (\mathbf{x} \in \{0, 1\}^m). (x_{i_m}) \rightarrow \kappa(\mathbf{x})$

- AXp's can be arbitrarily smaller than paths in (optimal) DTs!

[IIM20, IIM22]

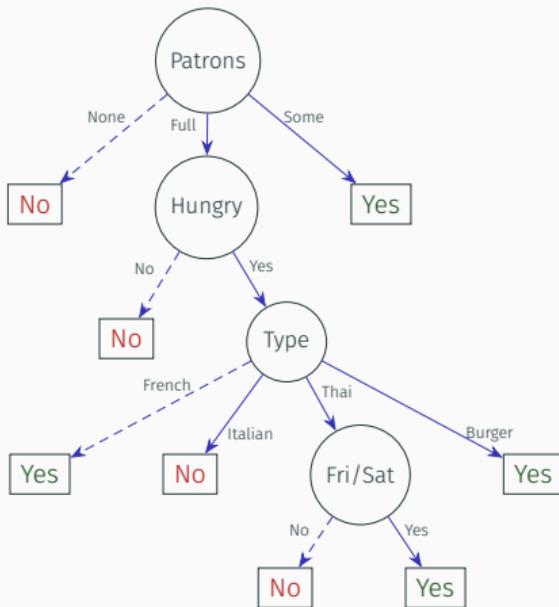
Explanation redundancy in DTs is ubiquitous – published DT examples

[IIM22]

DT Ref	D	#N	#P	%R	%C	%m	%M	%avg
[Alp14, Ch. 09, Fig. 9.1]	2	5	3	33	25	50	50	50
[Alp16, Ch. 03, Fig. 3.2]	2	5	3	33	25	50	50	50
[Bra20, Ch. 01, Fig. 1.3]	4	9	5	60	25	25	50	36
[BA97, Figure 1]	3	12	7	14	8	33	33	33
[BBHK10, Ch. 08, Fig. 8.2]	3	7	4	25	12	50	50	50
[BFOS84, Ch. 01, Fig. 1.1]	3	7	4	50	25	33	33	33
[DL01, Ch. 01, Fig. 1.2a]	2	5	3	33	25	33	33	33
[DL01, Ch. 01, Fig. 1.2b]	2	5	3	33	25	33	33	33
[KMND20, Ch. 04, Fig. 4.14]	3	7	4	25	12	50	50	50
[KMND20, Sec. 4.7, Ex. 4]	2	5	3	33	25	50	50	50
[Qui93, Ch. 01, Fig. 1.3]	3	12	7	28	17	33	50	41
[RM08, Ch. 01, Fig. 1.5]	3	9	5	20	12	33	33	33
[RM08, Ch. 01, Fig. 1.4]	3	7	4	50	25	33	33	33
[WFHP17, Ch. 01, Fig. 1.2]	3	7	4	25	12	50	50	50
[VLE ⁺ 16, Figure 4]	6	39	20	65	63	20	40	33
[Fla12, Ch. 02, Fig. 2.1(right)]	2	5	3	33	25	50	50	50
[Kot13, Figure 1]	3	10	6	33	11	33	33	33
[Mor82, Figure 1]	3	9	5	80	75	33	50	41
[PM17, Ch. 07, Fig. 7.4]	3	7	4	50	25	33	33	33
[RN10, Ch. 18, Fig. 18.6]	4	12	8	25	6	25	33	29
[SB14, Ch. 18, Page 212]	2	5	3	33	25	50	50	50
[Zho12, Ch. 01, Fig. 1.3]	2	5	3	33	25	33	33	33
[BHO09, Figure 1b]	4	13	7	71	50	33	50	36
[Zho21, Ch. 04, Fig. 4.3]	4	14	9	11	2	25	25	25

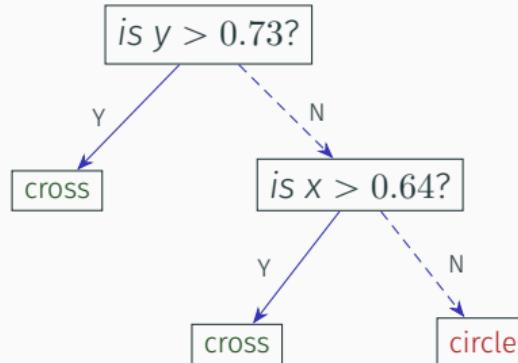
Many DTs have paths that are not minimal XPs – Russell&Norvig's book

[RN10]



- Explanation for $(P, H, T, W) = (\text{Full}, \text{Yes}, \text{Thai}, \text{No})$?

Many DTs have paths that are not minimal XPs – Zhou's book



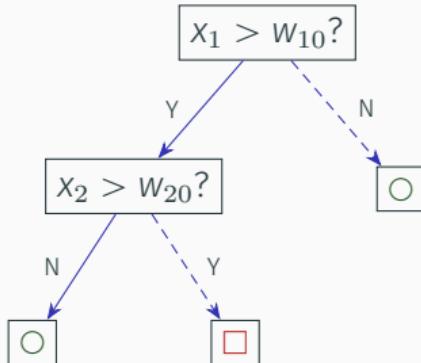
[Zho12]

- Explanation for $(x, y) = (1.25, -1.13)$?

Obs: True explanations can be computed for categorical, integer or real-valued features !

Many DTs have paths that are not minimal XPs – Alpaydin's book

[Alp14]

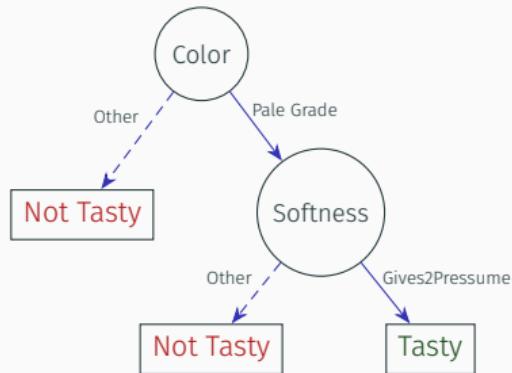


- Explanation for $(x_1, x_2) = (\alpha, \beta)$, with $\alpha > w_{10}$ and $\beta \leq w_{20}$?

Obs: True explanations can be computed for categorical, integer or real-valued features !

Many DTs have paths that are not minimal XPs – S.-S.&B.-D.'s book

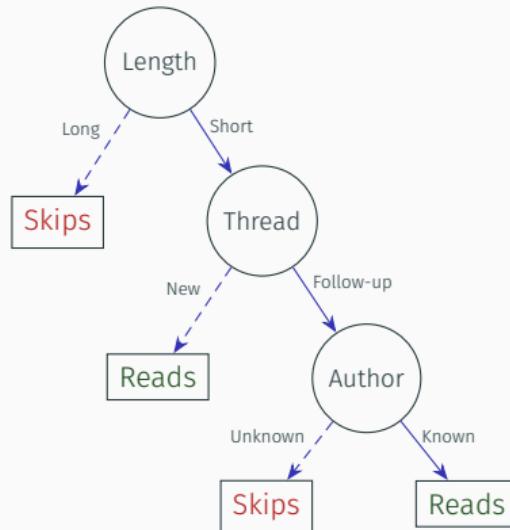
[SB14]



- Explanation for $(\text{color}, \text{softness}) = (\text{Pale Grade}, \text{Other})$?

Many DTs have paths that are not minimal XPs – Poole&Mackworth's book

[PM17]



- Explanation for $(L, T, A) = (\text{Short}, \text{Follow-Up}, \text{Unknown})$?
- Explanation for $(L, T, A) = (\text{Short}, \text{Follow-Up}, \text{Known})$?

Explanation redundancy in DTs is ubiquitous – DTs from datasets

[IIM20, HIIM21, IIM22]

Dataset	(#F #S)	IAI										ITI									
		D	#N	%A	#P	%R	%C	%m	%M	%avg	D	#N	%A	#P	%R	%C	%m	%M	%avg		
adult	(12 6061)	6	83	78	42	33	25	20	40	25	17	509	73	255	75	91	10	66	22		
anneal	(38 886)	6	29	99	15	26	16	16	33	21	9	31	100	16	25	4	12	20	16		
backache	(32 180)	4	17	72	9	33	39	25	33	30	3	9	91	5	80	87	50	66	54		
bank	(19 36293)	6	113	88	57	5	12	16	20	18	19	1467	86	734	69	64	7	63	27		
biodegradation	(41 1052)	5	19	65	10	30	1	25	50	33	8	71	76	36	50	8	14	40	21		
cancer	(9 449)	6	37	87	19	36	9	20	25	21	5	21	84	11	54	10	25	50	37		
car	(6 1728)	6	43	96	22	86	89	20	80	45	11	57	98	29	65	41	16	50	30		
colic	(22 357)	6	55	81	28	46	6	16	33	20	4	17	80	9	33	27	25	25	25		
compas	(11 1155)	6	77	34	39	17	8	16	20	17	15	183	37	92	66	43	12	60	27		
contraceptive	(9 1425)	6	99	49	50	8	2	20	60	37	17	385	48	193	27	32	12	66	21		
dermatology	(34 366)	6	33	90	17	23	3	16	33	21	7	17	95	9	22	0	14	20	17		
divorce	(54 150)	5	15	90	8	50	19	20	33	24	2	5	96	3	33	16	50	50	50		
german	(21 1000)	6	25	61	13	38	10	20	40	29	10	99	72	50	46	13	12	40	22		
heart-c	(13 302)	6	43	65	22	36	18	20	33	22	4	15	75	8	87	81	25	50	34		
heart-h	(13 293)	6	37	59	19	31	4	20	40	24	8	25	77	13	61	60	20	50	32		
kr-vs-kp	(36 3196)	6	49	96	25	80	75	16	60	33	13	67	99	34	79	43	7	70	35		
lending	(9 5082)	6	45	73	23	73	80	16	50	25	14	507	65	254	69	80	12	75	25		
letter	(16 18668)	6	127	58	64	1	0	20	20	20	46	4857	68	2429	6	7	6	25	9		
lymphography	(18 148)	6	61	76	31	35	25	16	33	21	6	21	86	11	9	0	16	16	16		
mortality	(118 13442)	6	111	74	56	8	14	16	20	17	26	865	76	433	61	61	7	54	19		
mushroom	(22 8124)	6	39	100	20	80	44	16	33	24	5	23	100	12	50	31	20	40	25		
pendigits	(16 10992)	6	121	88	61	0	0	—	—	—	38	937	85	469	25	86	6	25	11		
promoters	(58 106)	1	3	90	2	0	0	—	—	—	3	9	81	5	20	14	33	33	33		
recidivism	(15 3998)	6	105	61	53	28	22	16	33	18	15	611	51	306	53	38	9	44	16		
seismic_bumps	(18 2578)	6	37	89	19	42	19	20	33	24	8	39	93	20	60	79	20	60	42		
shuttle	(9 58000)	6	63	99	32	28	7	20	33	23	23	159	99	80	33	9	14	50	30		
soybean	(35 623)	6	63	88	32	9	5	25	25	25	16	71	89	36	22	1	9	12	10		
spambase	(57 4210)	6	63	75	32	37	12	16	33	19	15	143	91	72	76	98	7	58	25		
spect	(22 228)	6	45	82	23	60	51	20	50	35	6	15	86	8	87	98	50	83	65		
splice	(2 3178)	3	7	50	4	0	0	—	—	—	88	177	55	89	0	0	—	—	—		

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_2 :$	ELSE IF	$(x_2 \wedge x_4 \wedge x_6)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_3 :$	ELSE IF	$(\neg x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_4 :$	ELSE IF	$(x_4 \wedge x_6)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_5 :$	ELSE IF	$(\neg x_1 \wedge \neg x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_6 :$	ELSE IF	(x_6)	THEN	$\kappa(\mathbf{x}) = 0$
$R_{DEF} :$	ELSE			$\kappa(\mathbf{x}) = 1$

- Instance: $((0, 1, 0, 1, 0, 1), 0)$, i.e. rule R_2 fires

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
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$R_6 :$	ELSE IF	(x_6)	THEN	$\kappa(\mathbf{x}) = 0$
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- Instance: $((0, 1, 0, 1, 0, 1), 0)$, i.e. rule R_2 fires
- What is the abductive explanation?

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
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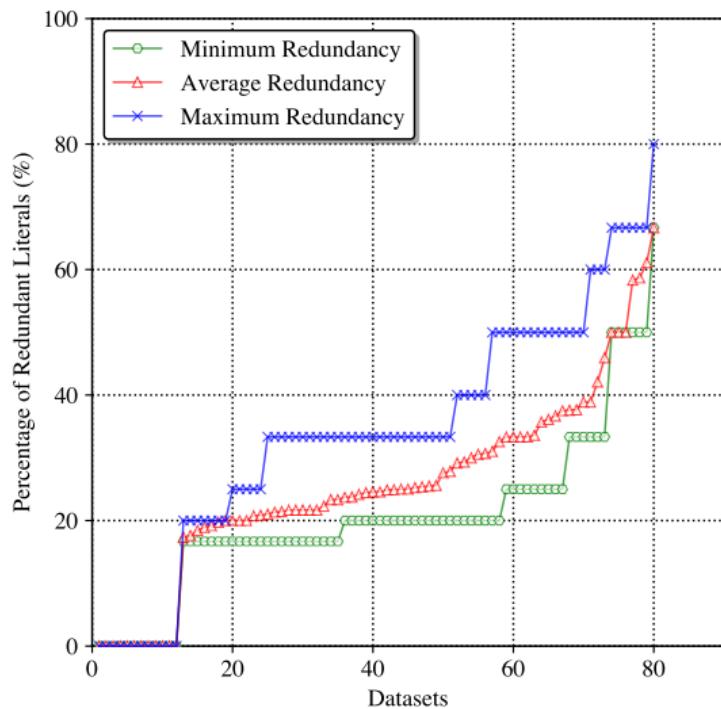
- Instance: $((0, 1, 0, 1, 0, 1), 0)$, i.e. rule R_2 fires
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- Recall: one AXp is $\{3, 4, 6\}$
 - Why?
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 - With 3, we do not need 2, since with 4 and 6 fixed, then R_4 is guaranteed to fire
 - Some questions:
 - Would average human decision maker be able to understand the AXp?
 - Would he/she be able to compute one AXp, by manual inspection?

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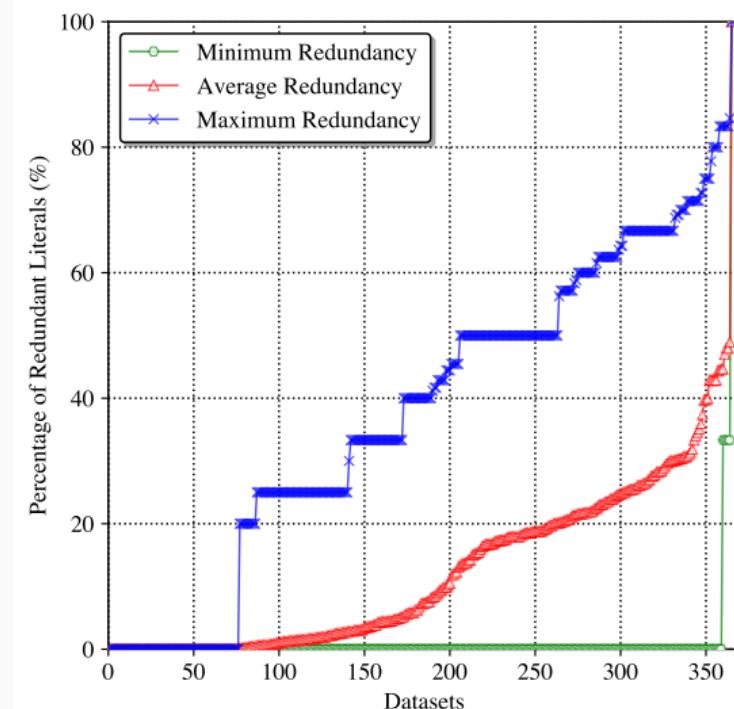
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 - Some questions:
 - Would average human decision maker be able to understand the AXp?
 - Would he/she be able to compute one AXp, by manual inspection?
- (BTW, we have proved that computing one AXp for DLs is computationally hard...)

Are *interpretable* models really interpretable? – DTs/DLs in practice

[MSI23]



DTs learned with Interpretable AI, max depth 6



DLs learned with CN2

Outline – Unit #03

Explanations for Decision Trees

XAI Queries for DTs

Myth #01: Intrinsic Interpretability

Detour: From Decision Trees to Explained Decision Sets

Explanations for Decision Graphs

Explanations for Monotonic Classifiers

Review examples

From DTs to explained DSs

[HM23a]

- Decision sets raise a number of issues:
 - **Overlap**: Two rules with different predictions can fire on the same input
 - **Incomplete coverage**: For some inputs, no rule may fire
 - A default rule defeats the purpose of unordered rules

From DTs to explained DSs

[HM23a]

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From DTs to explained DSs

[HM23a]

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From DTs to explained DSs

[HM23a]

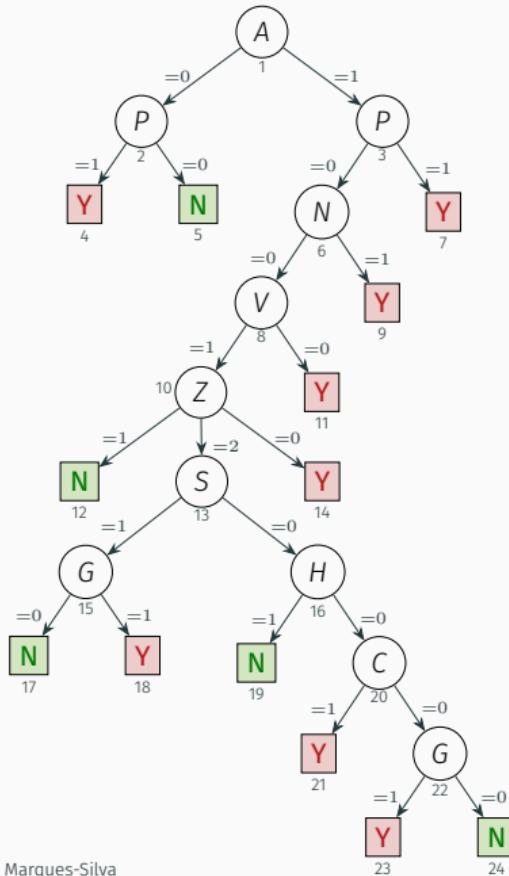
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- One can extract explained DSs from DTs

From DTs to explained DSs

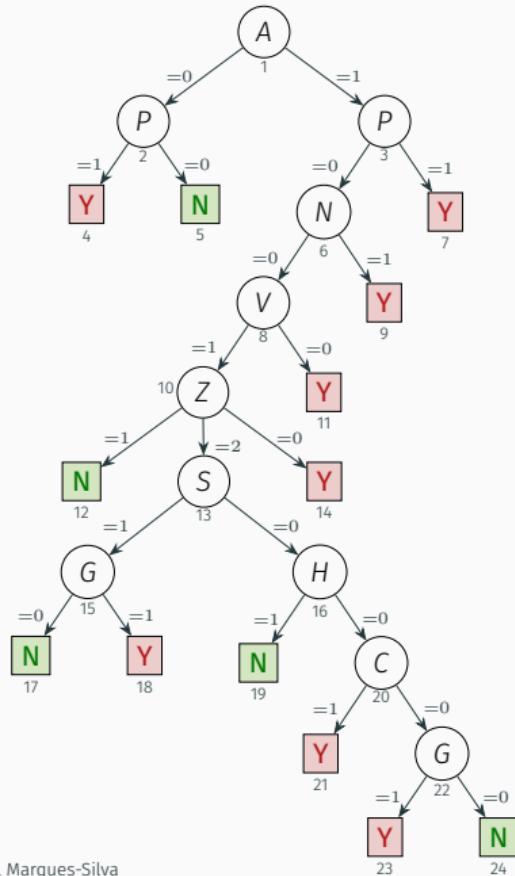
[HM23a]

- Decision sets raise a number of issues:
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 - A DS without overlap and complete coverage computes a classification function
- And explaining DSs is computationally hard...
- One can extract explained DSs from DTs
 - Extract one AXp (viewed as a logic rule) from each path in DT
 - Resulting rules are non-overlapping, and cover feature space

Example



Example



- R₀₁: IF [P] THEN $\kappa(\cdot) = \mathbf{Y}$
- R₀₂: IF [$\bar{A} \wedge \bar{P}$] THEN $\kappa(\cdot) = \mathbf{N}$
- R₀₃: IF [$\bar{P} \wedge \bar{N} \wedge V \wedge Z = 1$] THEN $\kappa(\cdot) = \mathbf{N}$
- R₀₄: IF [$\bar{P} \wedge \bar{N} \wedge V \wedge Z = 2 \wedge S \wedge \bar{G}$] THEN $\kappa(\cdot) = \mathbf{N}$
- R₀₅: IF [A \wedge Z = 2 \wedge S \wedge G] THEN $\kappa(\cdot) = \mathbf{Y}$
- R₀₆: IF [$\bar{P} \wedge \bar{N} \wedge V \wedge Z = 2 \wedge \bar{S} \wedge H$] THEN $\kappa(\cdot) = \mathbf{N}$
- R₀₇: IF [A \wedge Z = 2 \wedge \bar{S} \wedge \bar{H} \wedge C] THEN $\kappa(\cdot) = \mathbf{Y}$
- R₀₈: IF [A \wedge Z = 2 \wedge \bar{H} \wedge G] THEN $\kappa(\cdot) = \mathbf{Y}$
- R₀₉: IF [$\bar{P} \wedge \bar{N} \wedge V \wedge Z = 2 \wedge \bar{C} \wedge \bar{G}$] THEN $\kappa(\cdot) = \mathbf{N}$
- R₁₀: IF [A \wedge Z = 0] THEN $\kappa(\cdot) = \mathbf{Y}$
- R₁₁: IF [A \wedge \bar{V}] THEN $\kappa(\cdot) = \mathbf{Y}$
- R₁₂: IF [A \wedge N] THEN $\kappa(\cdot) = \mathbf{Y}$

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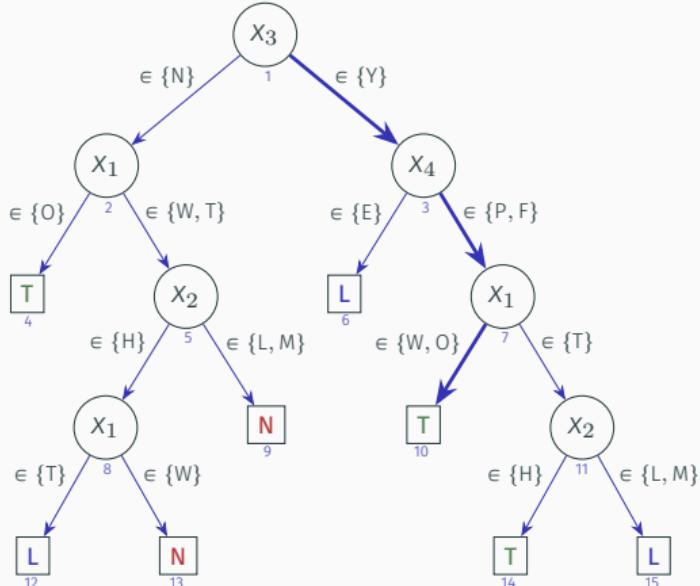
Explanation graphs – overview of results

[HIIM21]

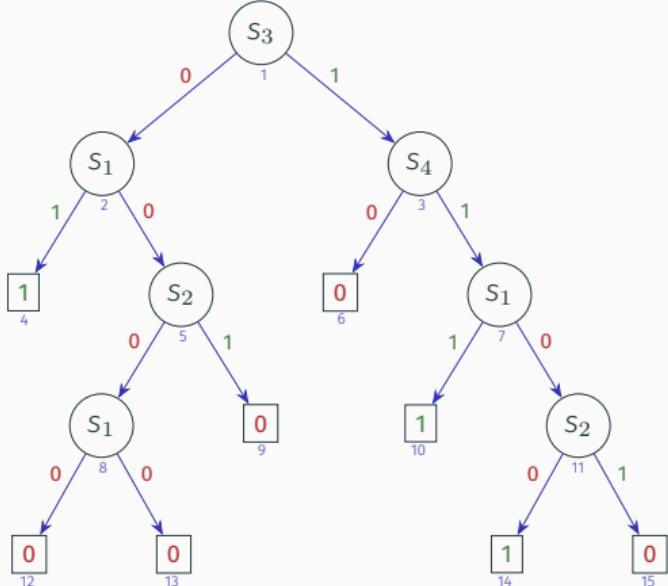
- Concept of explanation graph (XpG)
- Explanations of decision trees reducible to XpG's
- Explanations of decision graphs reducible to XpG's
- Explanations of OBDDs reducible to XpG's
- Explanations of OMDDs reducible to XpG's
- Explanations (AXp's and CXp's) of XpG's computed in polynomial time

Example of XpG – DTs

- DT; point: (O, L, Y, P) ; prediction T :

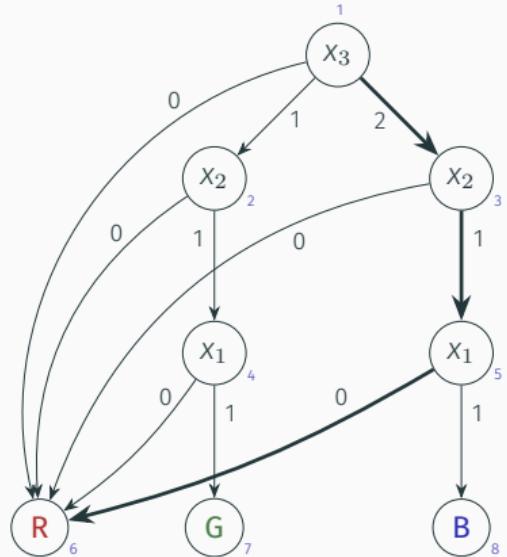


- **XpG:**

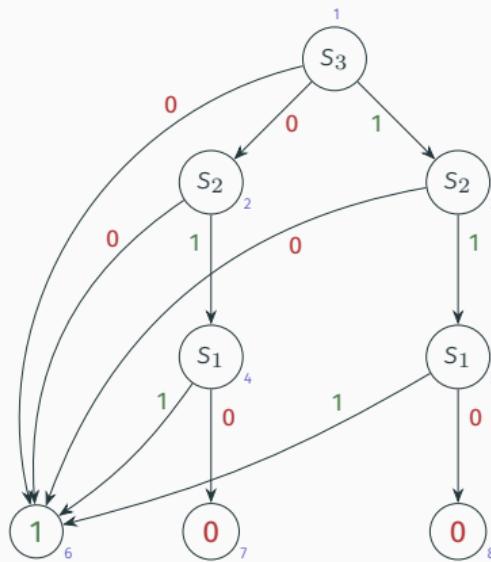


Example of XpG – OMDDs

- OMBBD; point: $(0, 1, 2)$; prediction R :



- **XpG:**



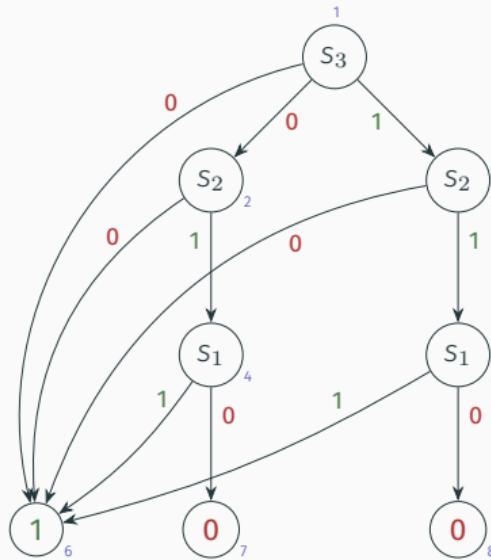
Finding one AXp for XpGs – polynomial time

- Algorithm (with no inconsistent paths):

$$S \leftarrow \mathcal{F}$$

For each feature i in \mathcal{F}

- XpG:



Finding one AXp for XpGs – polynomial time

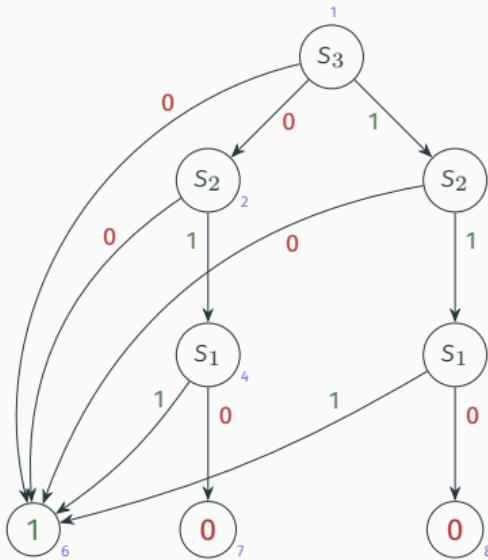
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For each feature i in \mathcal{F}

Drop feature i from \mathcal{S} , i.e. i is free

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Finding one AXp for XpGs – polynomial time

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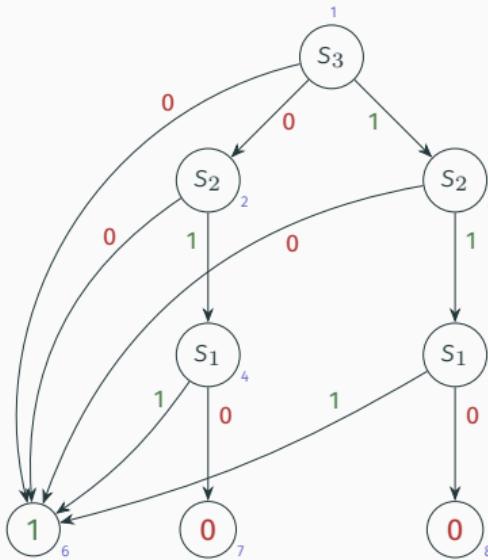
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Drop feature i from \mathcal{S} , i.e. i is free

If path to some **0** not blocked by 0-valued literals, then

Add feature i back to \mathcal{S}

- XpG:



Finding one AXp for XpGs – polynomial time

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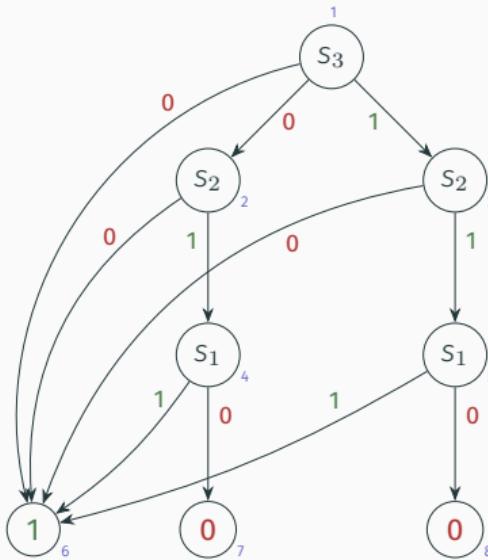
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Add feature i back to \mathcal{S}

Return \mathcal{S}

- XpG:



Finding one AXp for XpGs – polynomial time

- Algorithm (with no inconsistent paths):

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For each feature i in \mathcal{F}

Drop feature i from \mathcal{S} , i.e. i is free

If path to some **0** not blocked by 0-valued literals, then

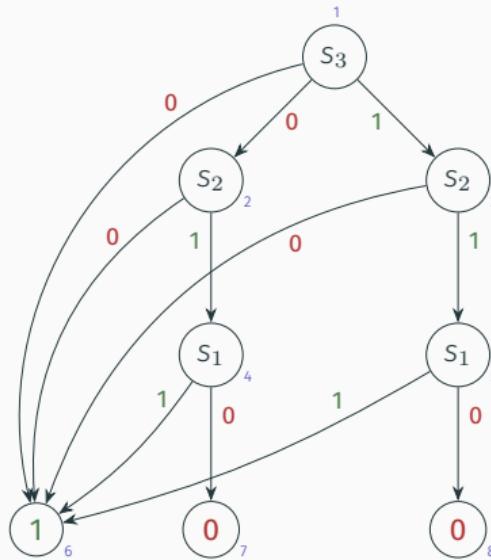
Add feature i back to \mathcal{S}

Return \mathcal{S}

- Example:

- $\mathcal{S} = \{1, 2, 3\}$

- XpG:



Finding one AXp for XpGs – polynomial time

- Algorithm (with no inconsistent paths):

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For each feature i in \mathcal{F}

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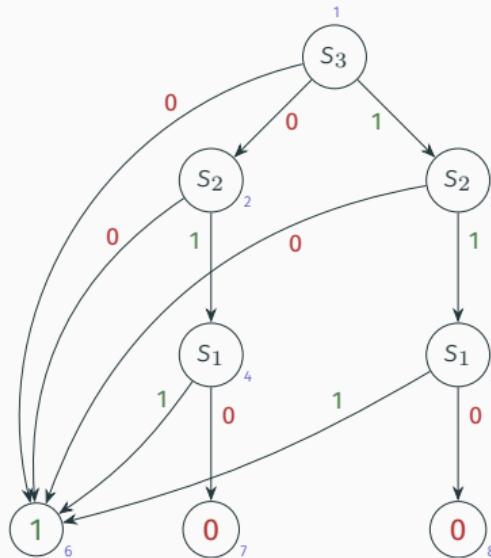
- Example:

- $\mathcal{S} = \{1, 2, 3\}$

- Feature 1 cannot be dropped, e.g.

$s_3 \rightarrow s_2 \rightarrow s_1 \rightarrow 0$

- XpG:



Finding one AXp for XpGs – polynomial time

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$\mathcal{S} \leftarrow \mathcal{F}$

For each feature i in \mathcal{F}

Drop feature i from \mathcal{S} , i.e. i is free
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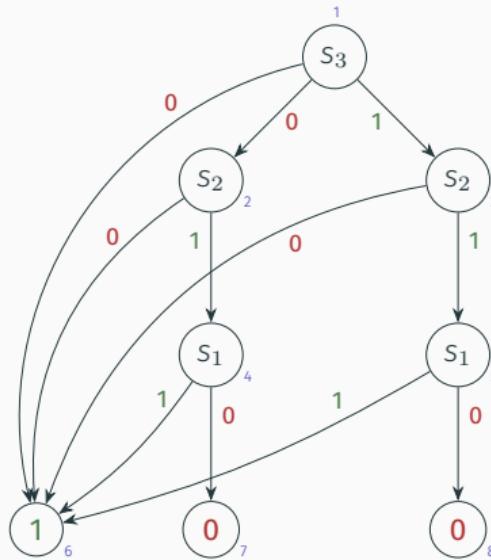
- $\mathcal{S} = \{1, 2, 3\}$

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Finding one AXp for XpGs – polynomial time

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Add feature i back to \mathcal{S}

Return \mathcal{S}

- Example:

- $\mathcal{S} = \{1, 2, 3\}$

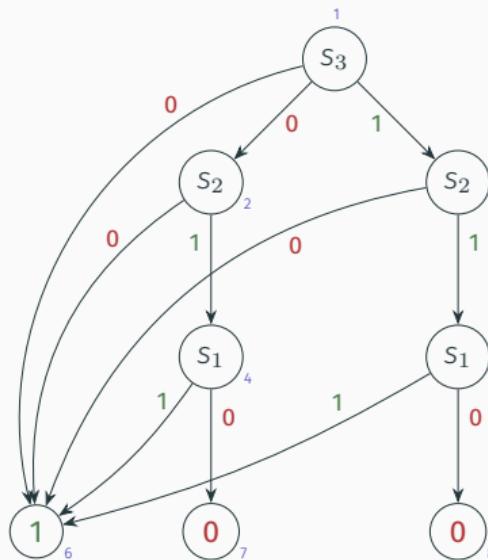
- Feature 1 cannot be dropped, e.g.

$s_3 \rightarrow s_2 \rightarrow s_1 \rightarrow 0$

- Both features 2 and 3 dropped from \mathcal{S}

- Return $\mathcal{S} = \{1\}$

- XpG:



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Review examples

Example monotonic classifier – $(\mathbf{v}, c) = ((10, 10, 5, 0), A)$

[MGC⁺21]

Variable	Meaning		Range
$\kappa(\cdot) \triangleq M$	Student grade		$\in \{A, B, C, D, E, F\}$
S	Final score		$\in \{0, \dots, 10\}$
Feat. id	Feat. var.	Feat. name	Domain
1	Q	Quiz	$\{0, \dots, 10\}$
2	X	Exam	$\{0, \dots, 10\}$
3	H	Homework	$\{0, \dots, 10\}$
4	R	Project	$\{0, \dots, 10\}$

$$M = \text{ITE}(S \geq 9, A, \text{ITE}(S \geq 7, B, \text{ITE}(S \geq 5, C, \text{ITE}(S \geq 4, D, \text{ite}(S \geq 2, E, F)))))$$

$$S = \max [0.3 \times Q + 0.6 \times X + 0.1 \times H, R]$$

$$\text{Also, } F \leq E \leq D \leq C \leq B \leq A$$

$$\text{And, } \kappa(\mathbf{x}_1) \leq \kappa(\mathbf{x}_2) \text{ if } \mathbf{x}_1 \leq \mathbf{x}_2$$

Explaining monotonic classifiers

- Instance (\mathbf{v}, c)
- Domain for $i \in \mathcal{F}$: $\lambda(i) \leq x_i \leq \mu(i)$
- Idea: refine lower and upper bounds on the prediction
 - \mathbf{v}_L and \mathbf{v}_U
- Utilities:
 - **FixAttr(i):**

```
 $\mathbf{v}_L \leftarrow (v_{L_1}, \dots, v_i, \dots, v_{L_N})$ 
 $\mathbf{v}_U \leftarrow (v_{U_1}, \dots, v_i, \dots, v_{U_N})$ 
 $(\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \setminus \{i\}, \mathcal{B} \cup \{i\})$ 
return ( $\mathbf{v}_L, \mathbf{v}_U, \mathcal{A}, \mathcal{B}$ )
```

- **FreeAttr(i):**

```
 $\mathbf{v}_L \leftarrow (v_{L_1}, \dots, \lambda(i), \dots, v_{L_N})$ 
 $\mathbf{v}_U \leftarrow (v_{U_1}, \dots, \mu(i), \dots, v_{U_N})$ 
 $(\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \setminus \{i\}, \mathcal{B} \cup \{i\})$ 
return ( $\mathbf{v}_L, \mathbf{v}_U, \mathcal{A}, \mathcal{B}$ )
```

Computing one AXp

```
1:  $\mathbf{v}_L \leftarrow (v_1, \dots, v_N)$ 
2:  $\mathbf{v}_U \leftarrow (v_1, \dots, v_N)$ 
3:  $(\mathcal{C}, \mathcal{D}, \mathcal{P}) \leftarrow (\mathcal{F}, \emptyset, \emptyset)$ 
4: for all  $i \in \mathcal{S}$  do
5:    $(\mathbf{v}_L, \mathbf{v}_U, \mathcal{C}, \mathcal{D}) \leftarrow \text{FreeAttr}(i, \mathbf{v}, \mathbf{v}_L, \mathbf{v}_U, \mathcal{C}, \mathcal{D})$ 
6: for all  $i \in \mathcal{F} \setminus \mathcal{S}$  do
7:    $(\mathbf{v}_L, \mathbf{v}_U, \mathcal{C}, \mathcal{D}) \leftarrow \text{FreeAttr}(i, \mathbf{v}, \mathbf{v}_L, \mathbf{v}_U, \mathcal{C}, \mathcal{D})$ 
8:   if  $\kappa(\mathbf{v}_L) \neq \kappa(\mathbf{v}_U)$  then
9:      $(\mathbf{v}_L, \mathbf{v}_U, \mathcal{D}, \mathcal{P}) \leftarrow \text{FixAttr}(i, \mathbf{v}, \mathbf{v}_L, \mathbf{v}_U, \mathcal{D}, \mathcal{P})$ 
10: return  $\mathcal{P}$ 
```

- ▷ Ensures: $\kappa(\mathbf{v}_L) = \kappa(\mathbf{v}_U)$
- ▷ \mathcal{S} : Some possible seed
- ▷ Require: $\kappa(\mathbf{v}_L) = \kappa(\mathbf{v}_U)$, given \mathcal{S}
- ▷ Loop inv.: $\kappa(\mathbf{v}_L) = \kappa(\mathbf{v}_U)$
- ▷ If invariant broken, fix it

- Obs: $\mathcal{S} = \emptyset$ for computing a single AXp/CXp

Computing one AXp – example

- $\lambda(i) = 0$ and $\mu(i) = 10$
- $\mathbf{v} = (10, 10, 5, 0)$, with $\kappa(\mathbf{v}) = A$
- **Q:** find one AXp (CXp is similar)

Feat.	Initial values		Changed values		Predictions		Dec.	Resulting values	
	\mathbf{v}_L	\mathbf{v}_U	\mathbf{v}_L	\mathbf{v}_U	$\kappa(\mathbf{v}_L)$	$\kappa(\mathbf{v}_U)$		\mathbf{v}_L	\mathbf{v}_U
1	(10,10,5,0)	(10,10,5,0)	(0,10,5,0)	(10,10,5,0)	C	A	✓	(10,10,5,0)	(10,10,5,0)
2	(10,10,5,0)	(10,10,5,0)	(10,0,5,0)	(10,10,5,0)	E	A	✓	(10,10,5,0)	(10,10,5,0)
3	(10,10,5,0)	(10,10,5,0)	(10,10,0,0)	(10,10,10,0)	A	A	✗	(10,10,0,0)	(10,10,10,0)
4	(10,10,0,0)	(10,10,10,0)	(10,10,0,0)	(10,10,10,10)	A	A	✗	(10,10,0,0)	(10,10,10,10)

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Recap computation of (W)AXps/(W)CXps

$$\begin{aligned} \text{WAXp}(\mathcal{X}) &:= \forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (x_j = v_j) \rightarrow (\sigma(\mathbf{x})) \\ \text{WCXp}(\mathcal{Y}) &:= \exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (x_j = v_j) \wedge (\neg \sigma(\mathbf{x})) \end{aligned}$$

Recap computation of $(W)AXps/(W)CXps$

$$\begin{aligned} WAXp(\mathcal{X}) &:= \forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (x_j = v_j) \rightarrow (\sigma(\mathbf{x})) \\ WCXp(\mathcal{Y}) &:= \exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (x_j = v_j) \wedge (\neg \sigma(\mathbf{x})) \end{aligned}$$

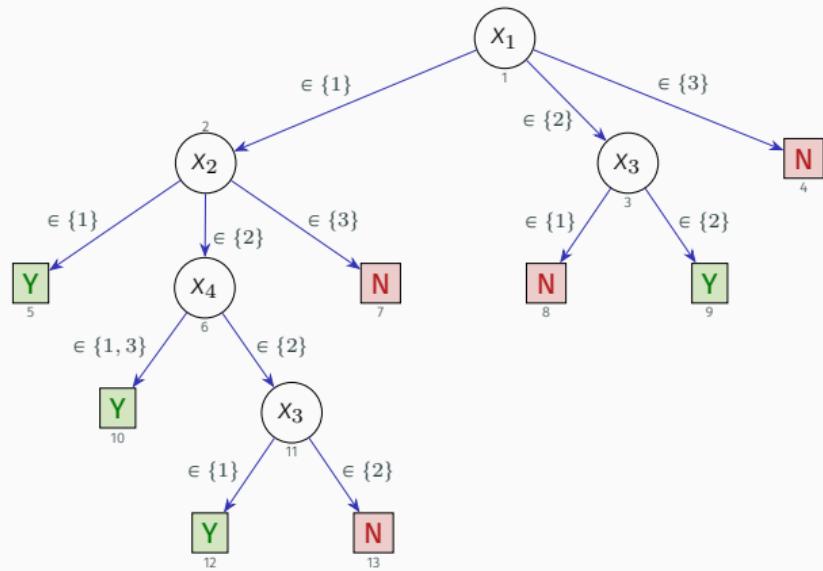
Input: Predicate \mathbb{P} , parameterized by \mathcal{T}, \mathcal{M}

Output: One XP \mathcal{S}

```
1: procedure oneXP( $\mathbb{P}$ )
2:    $\mathcal{S} \leftarrow \mathcal{F}$                                  $\triangleright$  Initialization:  $\mathbb{P}(\mathcal{S})$  holds
3:   for  $i \in \mathcal{F}$  do
4:     if  $\mathbb{P}(\mathcal{S} \setminus \{i\})$  then                 $\triangleright$  Loop invariant:  $\mathbb{P}(\mathcal{S})$  holds
5:        $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$ 
6:   return  $\mathcal{S}$                                  $\triangleright$  Update  $\mathcal{S}$  only if  $\mathbb{P}(\mathcal{S} \setminus \{i\})$  holds
                                                  $\triangleright$  Returned set  $\mathcal{S}$ :  $\mathbb{P}(\mathcal{S})$  holds
```

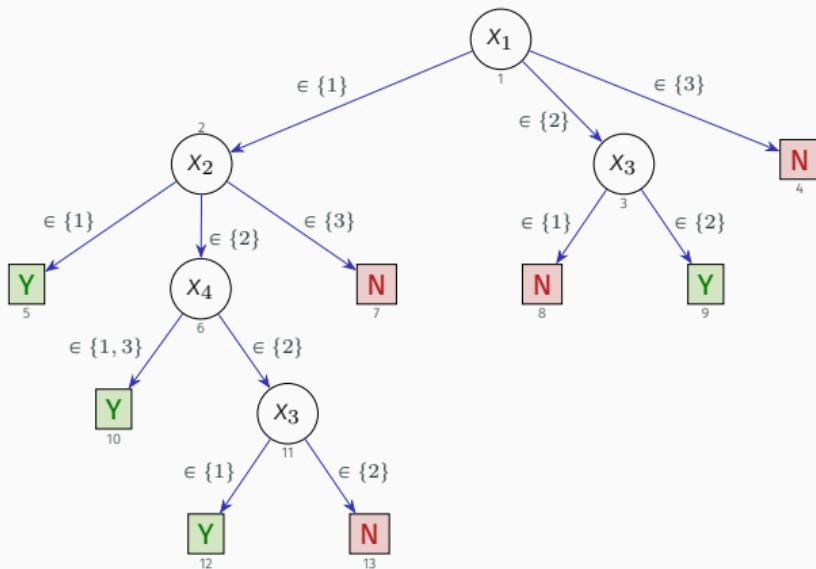
Review exercise – one AXp for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$



Review exercise – one AXp for example DT

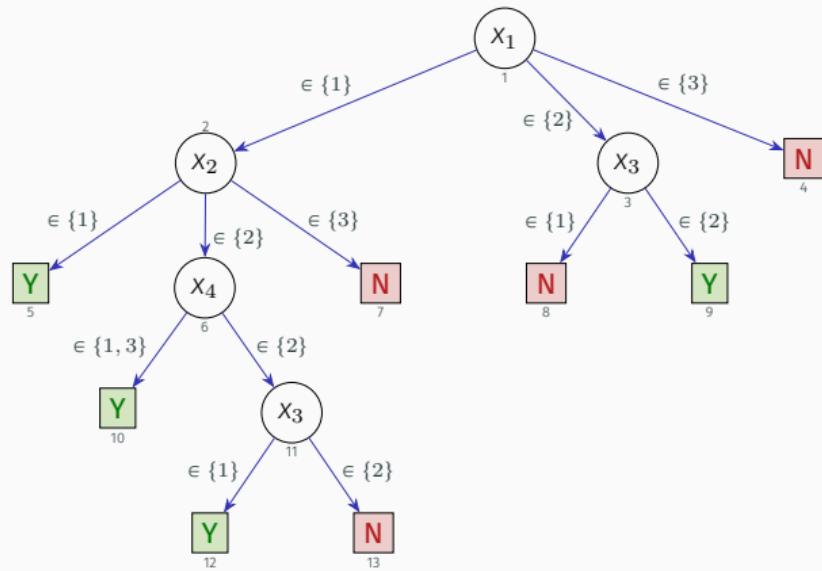
- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$



- Finding on AXp:

Review exercise – one AXp for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$

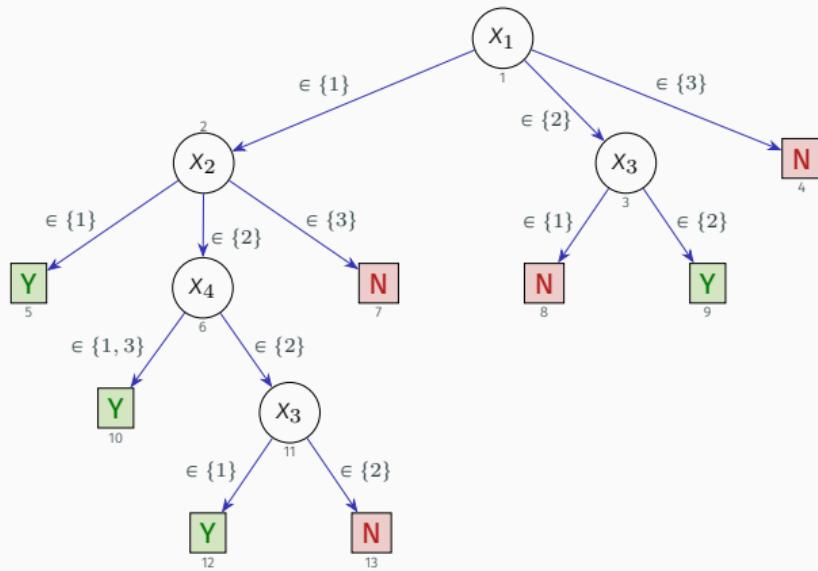


- Finding on AXp:

- 1st path inconsistent: $H_1 = \{3\}$

Review exercise – one AXp for example DT

- Instance: $(v, c) = ((1, 2, 1, 2), \text{Y})$

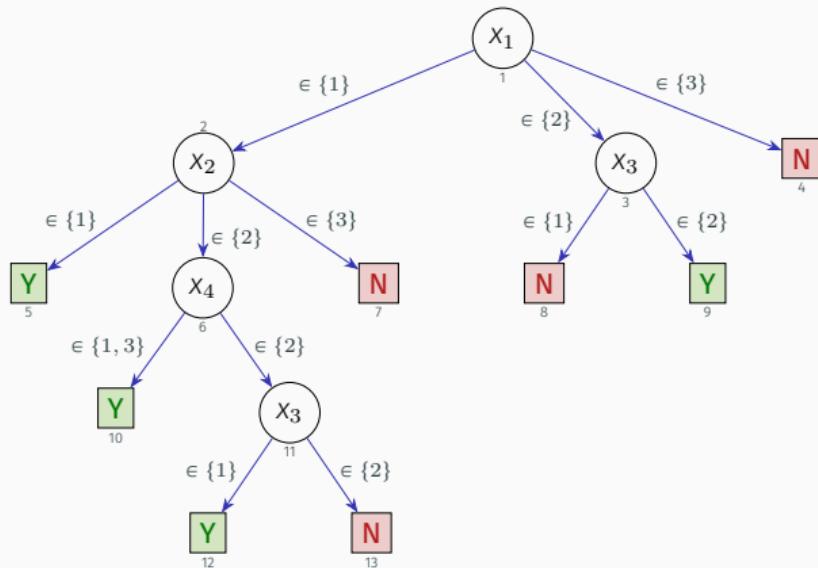


- Finding on AXp:

- 1st path inconsistent: $H_1 = \{3\}$
- 2nd path inconsistent: $H_2 = \{2\}$

Review exercise – one AXp for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$

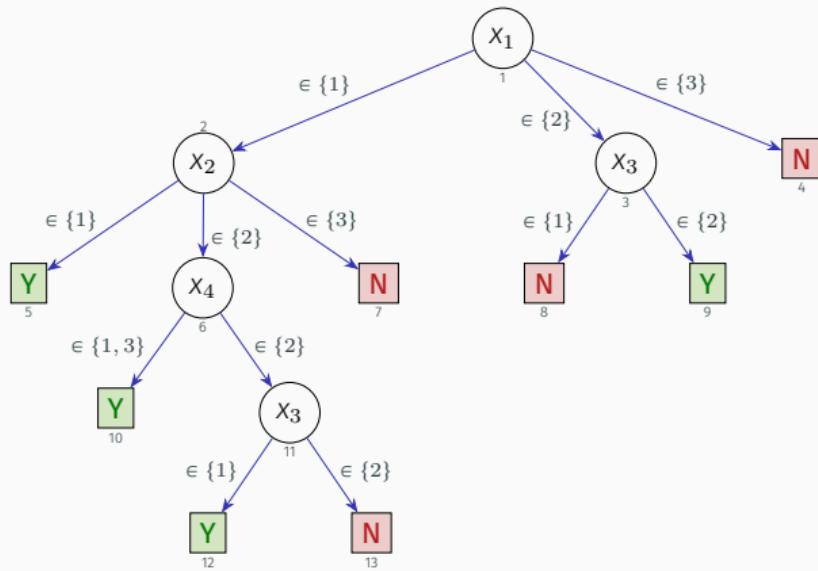


- Finding on AXp:

- 1st path inconsistent: $H_1 = \{3\}$
- 2nd path inconsistent: $H_2 = \{2\}$
- 3rd path inconsistent: $H_3 = \{1\}$

Review exercise – one AXp for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$

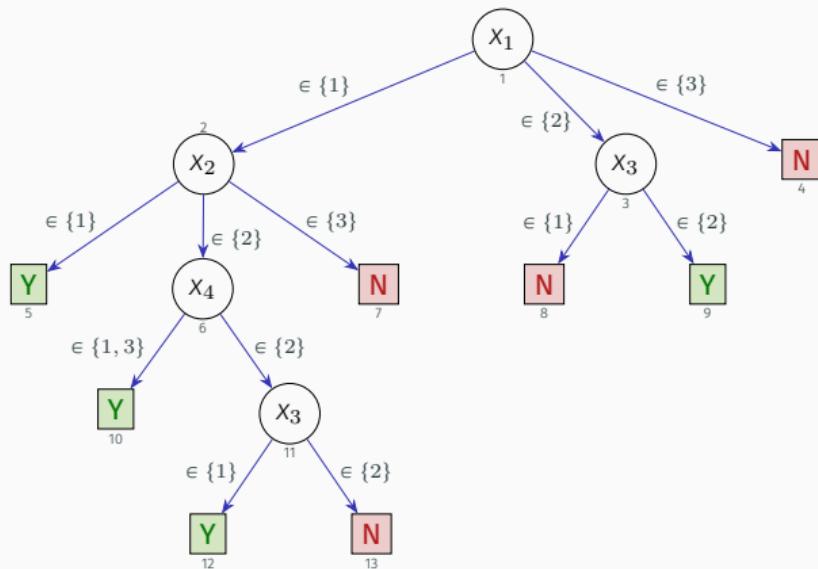


- Finding on AXp:

- 1st path inconsistent: $H_1 = \{3\}$
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- 4th path inconsistent: $H_4 = \{1\}$

Review exercise – one AXp for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$



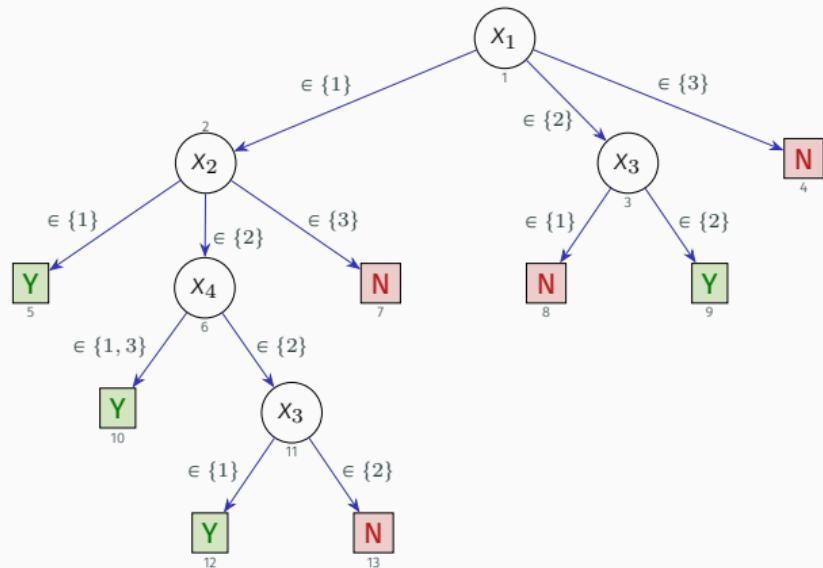
- Finding on AXp:

- 1st path inconsistent: $H_1 = \{3\}$
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- 4th path inconsistent: $H_4 = \{1\}$

- AXp is MHS of H_j sets: $\{1, 2, 3\}$

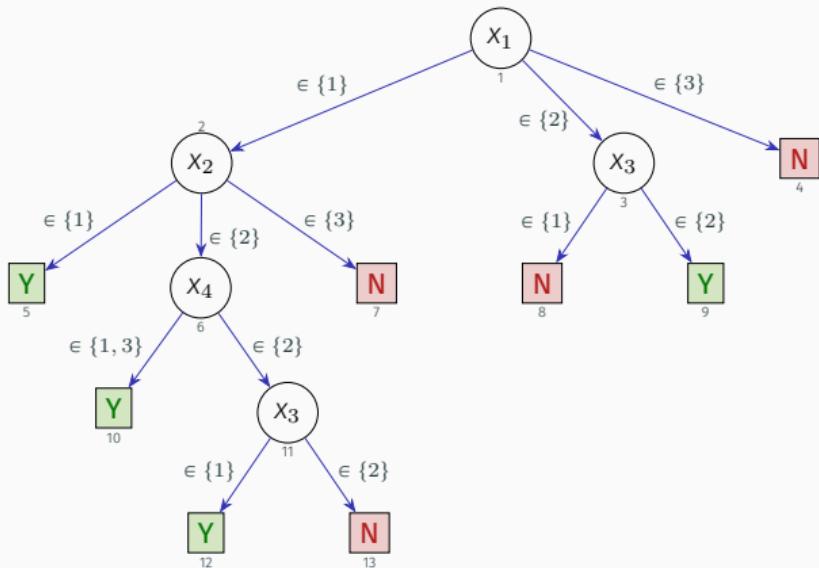
Review exercise – all CXps & AXps for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$



Review exercise – all CXps & AXps for example DT

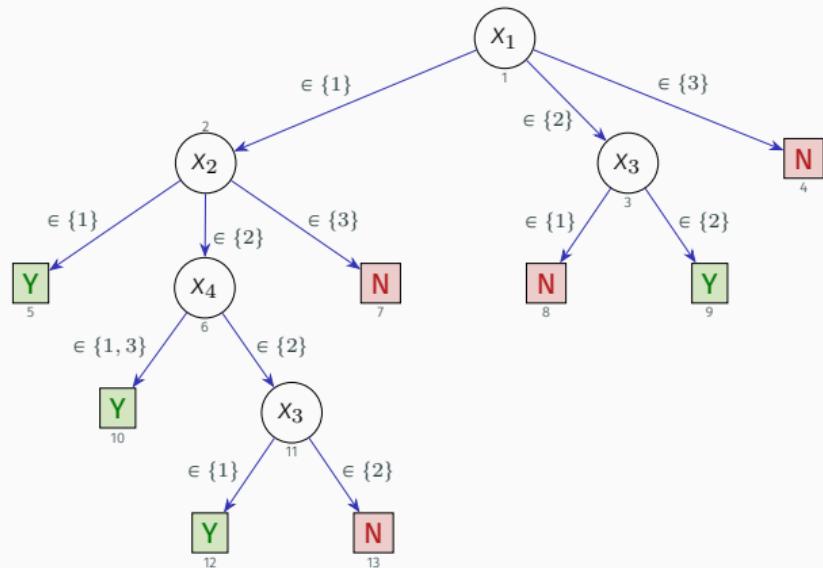
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- Finding CXps:

Review exercise – all CXps & AXps for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$

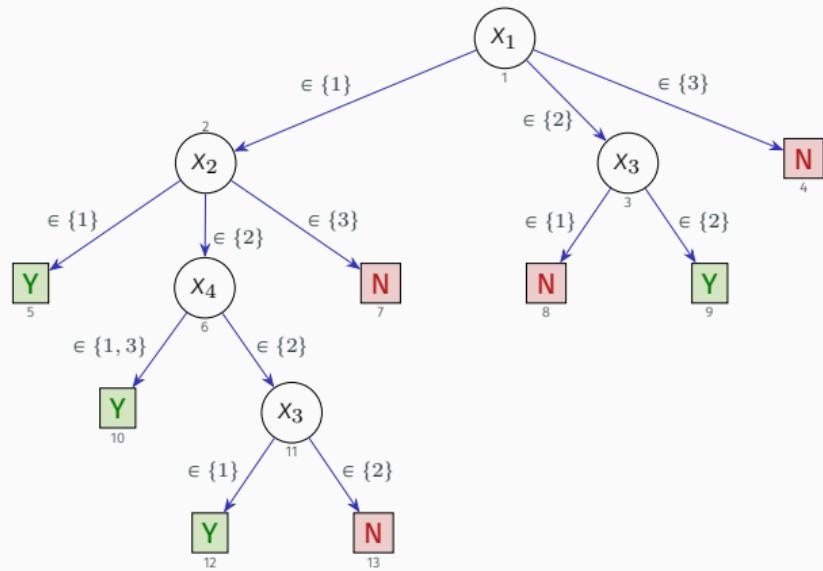


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Review exercise – all CXps & AXps for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$

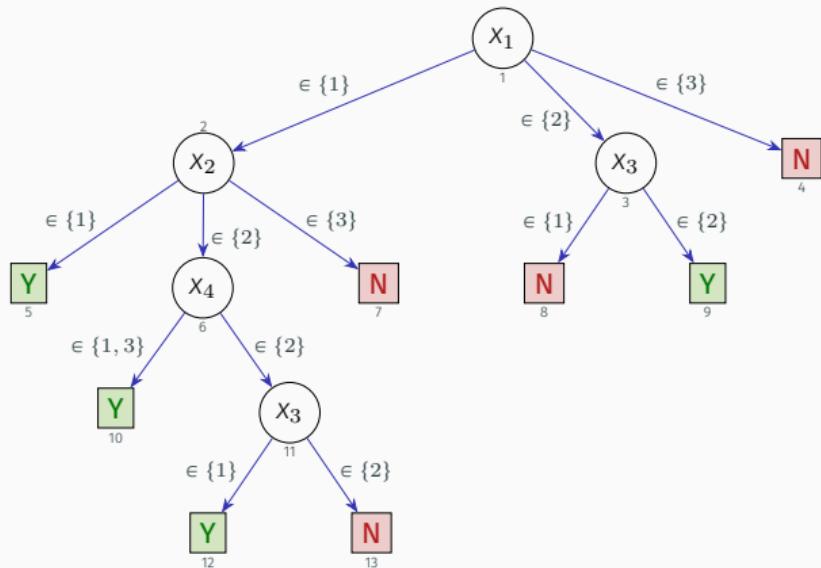


Finding CXps:

- 1st path: $I_1 = \{3\}$
- 2nd path: $I_2 = \{2\}$

Review exercise – all CXps & AXps for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$

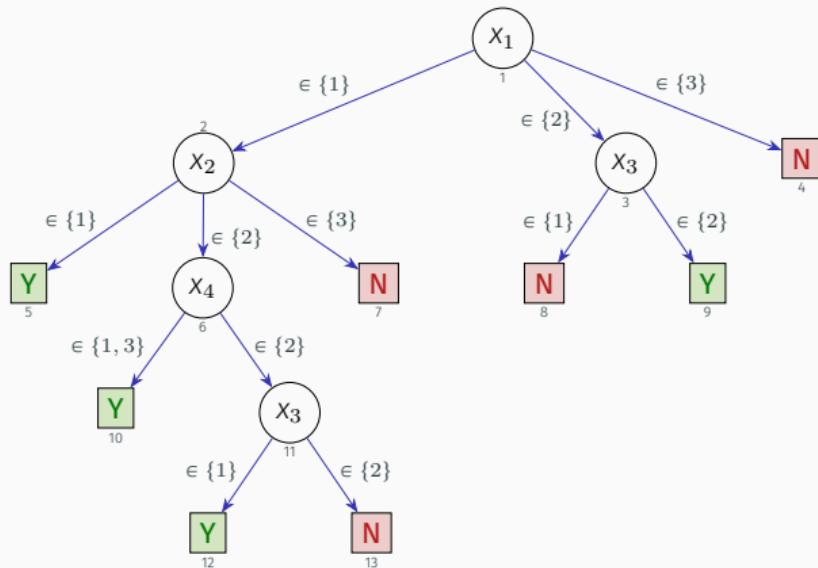


Finding CXps:

- 1st path: $I_1 = \{3\}$
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Review exercise – all CXps & AXps for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$

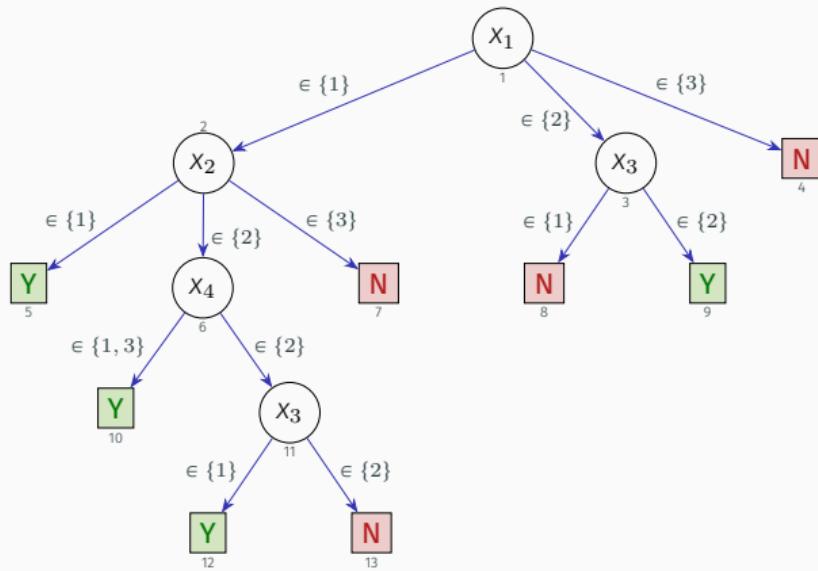


Finding CXps:

- 1st path: $I_1 = \{3\}$
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Review exercise – all CXps & AXps for example DT

- Instance: $(v, c) = ((1, 2, 1, 2), \text{Y})$

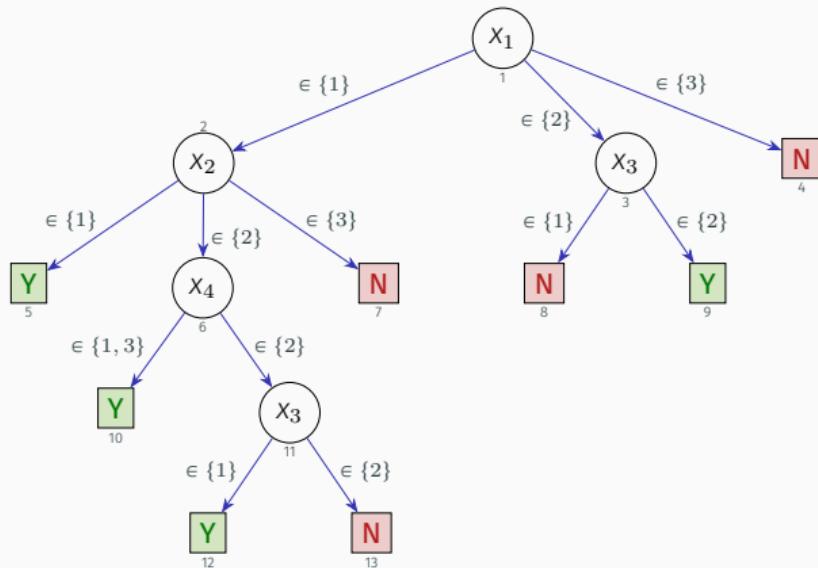


Finding CXps:

- 1st path: $I_1 = \{3\}$
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- $\mathcal{L} = \{\{1\}, \{2\}, \{3\}\} = \mathbb{C}$

Review exercise – all CXps & AXps for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \text{Y})$



- Finding CXps:

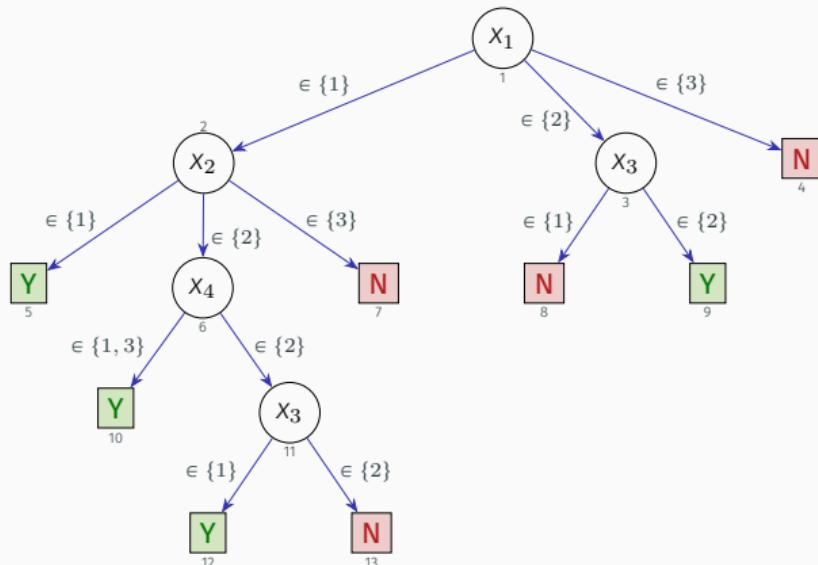
- 1st path: $I_1 = \{3\}$
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- 3rd path: $I_3 = \{1\}$
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- $\mathcal{L} = \{\{1\}, \{2\}, \{3\}\} = \mathbb{C}$

- Finding AXps:

(i.e. all MHSes of sets in \mathbb{C})

Review exercise – all CXps & AXps for example DT

- Instance: $(\mathbf{v}, c) = ((1, 2, 1, 2), \mathbf{Y})$



- Finding CXps:

- 1st path: $I_1 = \{3\}$
- 2nd path: $I_2 = \{2\}$
- 3rd path: $I_3 = \{1\}$
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- $\mathcal{L} = \{\{1\}, \{2\}, \{3\}\} = \mathbb{C}$

- Finding AXps:

(i.e. all MHSes of sets in \mathbb{C})

- $\mathbb{A} = \{\{1, 2, 3\}\}$

Another review exercise – one AXp for example DL

- DL:

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_2 :$	ELSE IF	$(x_1 \wedge x_5)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_3 :$	ELSE IF	$(x_2 \wedge x_4)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_4 :$	ELSE IF	$(x_1 \wedge x_7)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_5 :$	ELSE IF	$(\neg x_4 \wedge x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_6 :$	ELSE IF	$(\neg x_4 \wedge \neg x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_7 :$	ELSE IF	$(\neg x_2 \wedge x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_{DEF} :$	ELSE			$\kappa(\mathbf{x}) = 0$

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$R_{DEF} :$	ELSE			$\kappa(\mathbf{x}) = 0$

- Instance: $\mathbf{v} = (0, 1, 0, 1, 0, 1, 0)$
 - The prediction is 1, due to R_3

Another review exercise – one AXp for example DL

- DL:

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_2 :$	ELSE IF	$(x_1 \wedge x_5)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_3 :$	ELSE IF	$(x_2 \wedge x_4)$	THEN	$\kappa(\mathbf{x}) = 1$
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$R_5 :$	ELSE IF	$(\neg x_4 \wedge x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
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- Instance: $\mathbf{v} = (0, 1, 0, 1, 0, 1, 0)$
 - The prediction is 1, due to R_3
- AXp:

Another review exercise – one AXp for example DL

- DL:

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_2 :$	ELSE IF	$(x_1 \wedge x_5)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_3 :$	ELSE IF	$(x_2 \wedge x_4)$	THEN	$\kappa(\mathbf{x}) = 1$
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$R_7 :$	ELSE IF	$(\neg x_2 \wedge x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_{DEF} :$	ELSE			$\kappa(\mathbf{x}) = 0$

- Instance: $\mathbf{v} = (0, 1, 0, 1, 0, 1, 0)$
 - The prediction is 1, due to R_3
 - AXp: {1, 2}

Another review exercise – one AXp for example DL

- DL:

$R_1 :$	IF	$(x_1 \wedge x_3)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_2 :$	ELSE IF	$(x_1 \wedge x_5)$	THEN	$\kappa(\mathbf{x}) = 0$
$R_3 :$	ELSE IF	$(x_2 \wedge x_4)$	THEN	$\kappa(\mathbf{x}) = 1$
$R_4 :$	ELSE IF	$(x_1 \wedge x_7)$	THEN	$\kappa(\mathbf{x}) = 0$
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$R_{DEF} :$	ELSE			$\kappa(\mathbf{x}) = 0$

- Instance: $\mathbf{v} = (0, 1, 0, 1, 0, 1, 0)$
 - The prediction is 1, due to R_3
- AXp: {1, 2}
- Quiz: write down the constraints and confirm AXp with SAT solver

Questions?

Lecture 03

Recapitulate second lecture

- Rigorous definitions of abductive and contrastive explanations

Recapitulate second lecture

- Rigorous definitions of abductive and contrastive explanations
- Example algorithm for finding one AXp/CXp

Recapitulate second lecture

- Rigorous definitions of abductive and contrastive explanations
- Example algorithm for finding one AXp/CXp
- Explanations for DTs

Recapitulate second lecture

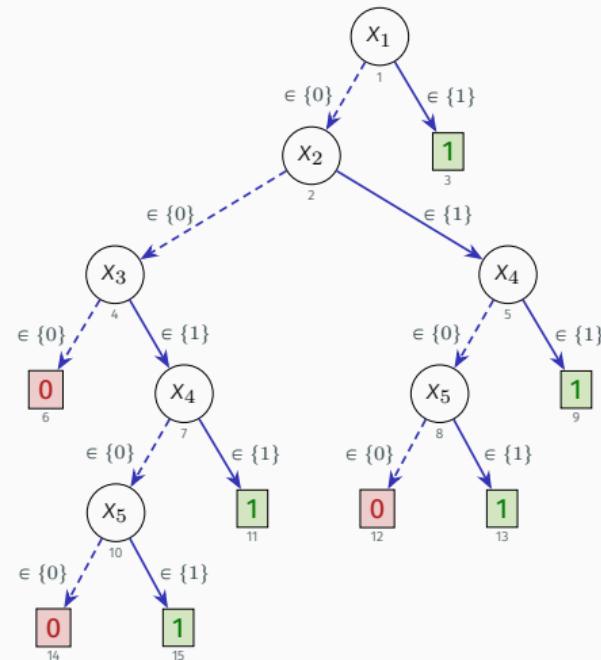
- Rigorous definitions of abductive and contrastive explanations
- Example algorithm for finding one AXp/CXp
- Explanations for DTs
- Explanations for XpGs

Recapitulate second lecture

- Rigorous definitions of abductive and contrastive explanations
- Example algorithm for finding one AXp/CXp
- Explanations for DTs
- Explanations for XpGs
- Explanations for monotonic classifiers

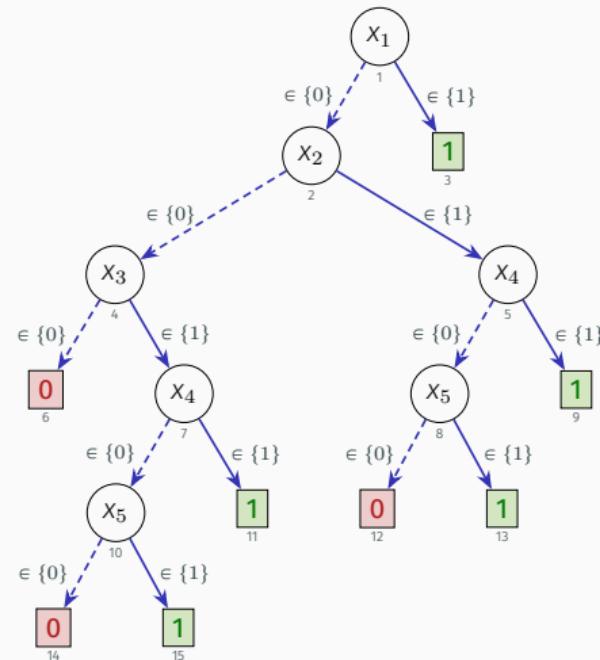
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$



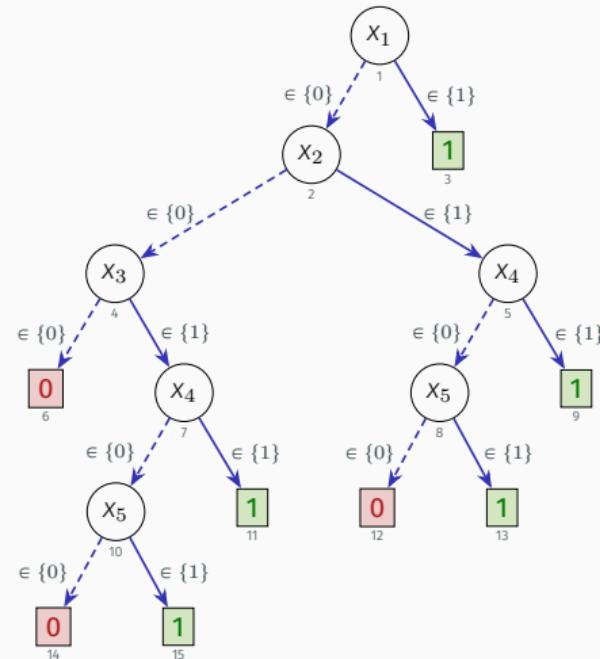
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$



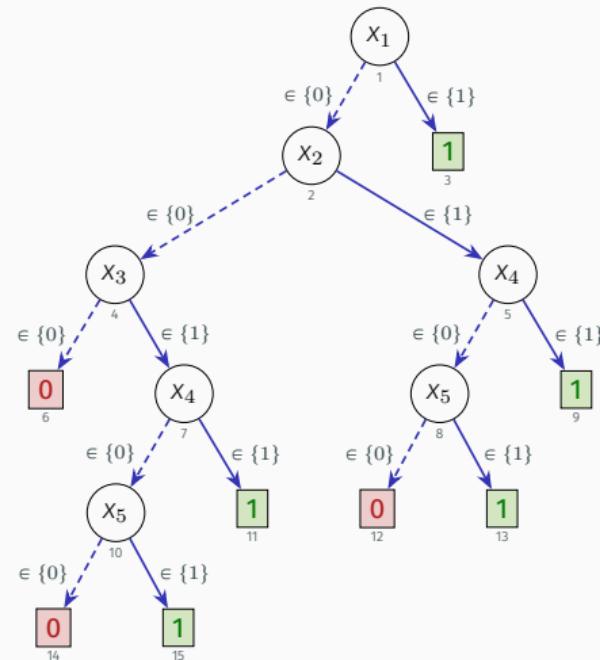
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$
- All CXps:



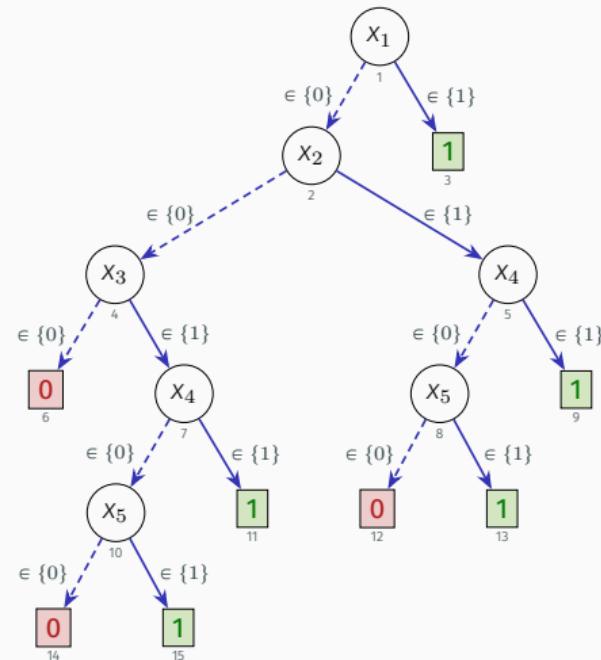
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$
- All CXps:
 - $I_1: \{5\}$



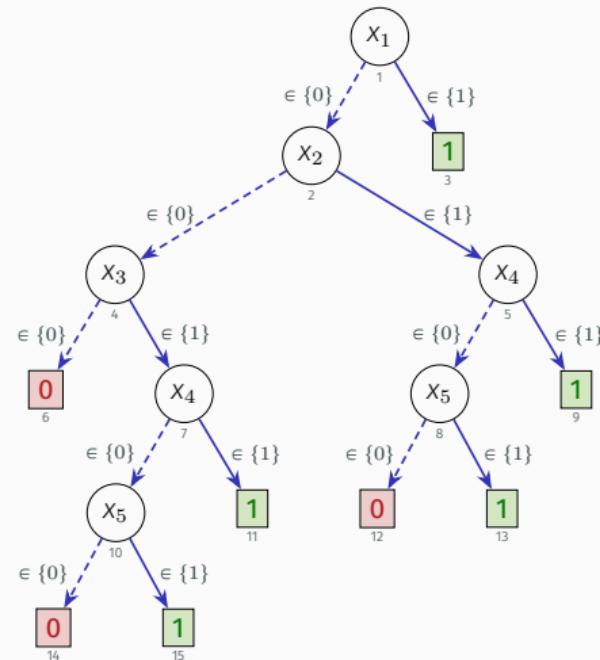
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$
- All CXps:
 - $I_1: \{5\}$
 - $I_2: \{4\}$



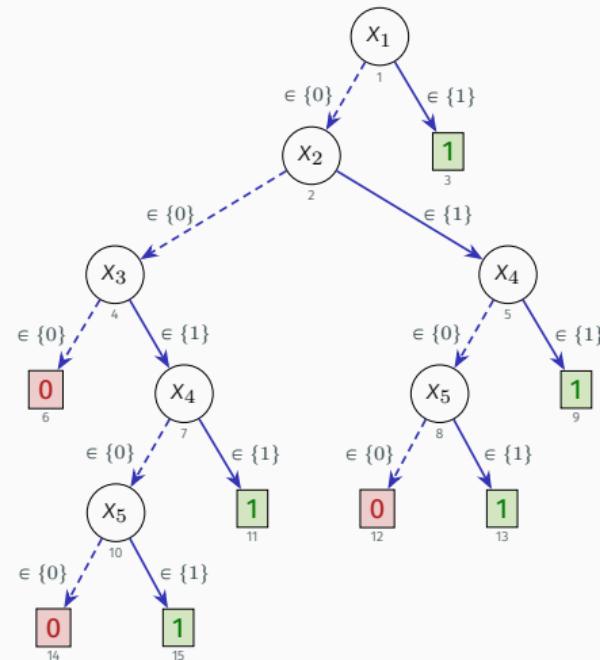
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$
- All CXps:
 - $l_1: \{5\}$
 - $l_2: \{4\}$
 - $l_3: \{2, 5\}$



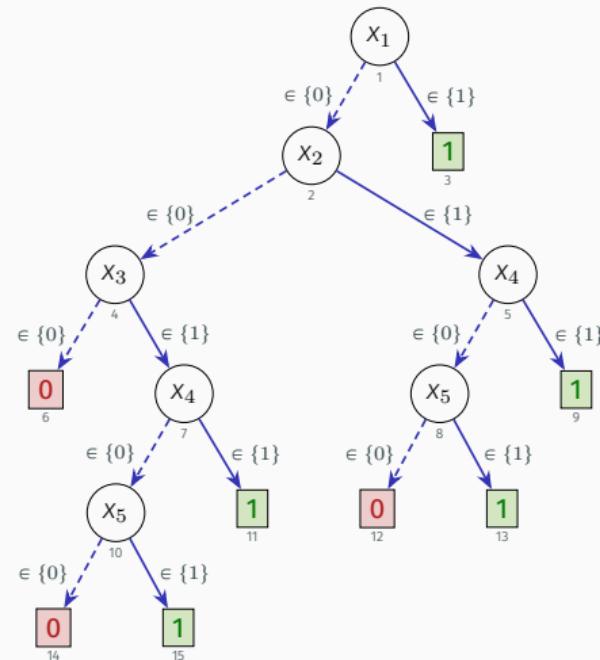
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$
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 - $l_1: \{5\}$
 - $l_2: \{4\}$
 - $l_3: \{2, 5\}$
 - $l_4: \{2, 4\}$



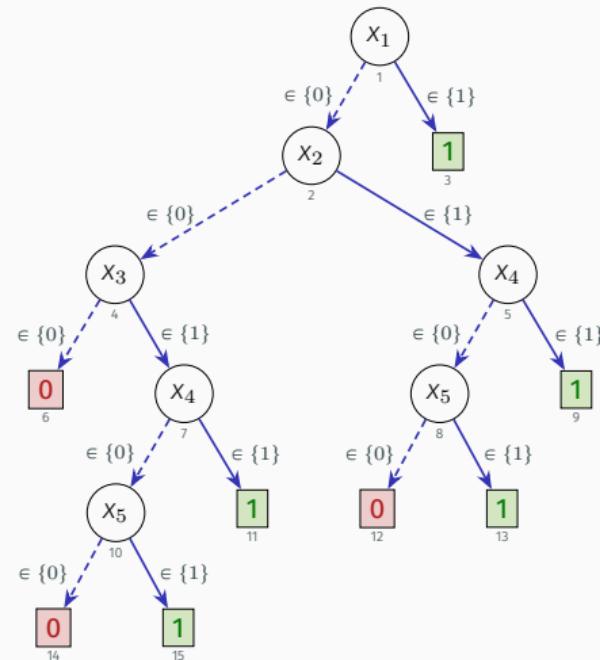
Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$
- All CXps:
 - $l_1: \{5\}$
 - $l_2: \{4\}$
 - $l_3: \{2, 5\}$
 - $l_4: \{2, 4\}$
 - $l_5: \{1\}$



Recap AXps/CXps: DT example

- Instance: $((0, 0, 1, 0, 0), 0)$
- One AXp: $\{1, 4, 5\}$
- All CXps:
 - $l_1: \{5\}$
 - $l_2: \{4\}$
 - $l_3: \{2, 5\}$
 - $l_4: \{2, 4\}$
 - $l_5: \{1\}$
 - $\mathcal{L} = \{\{1\}, \{4\}, \{5\}\}$



Recap AXps/CXps: DL example

- R₁: IF $(x_1 = 1)$ THEN 0
 R₂: ELSE IF $(x_2 = 1)$ THEN 1
 R₃: ELSE IF $(x_4 = 1)$ THEN 0
 R_{DEF}: ELSE THEN 1

Entry	x_1	x_2	x_3	x_4	Rule	$\kappa_1(\mathbf{x})$
00	0	0	0	0	R _{DEF}	1
01	0	0	0	1	R ₃	0
02	0	0	0	2	R _{DEF}	1
03	0	0	1	0	R _{DEF}	1
04	0	0	1	1	R ₃	0
05	0	0	1	2	R _{DEF}	1
06	0	1	0	0	R ₂	1
07	0	1	0	1	R ₂	1
08	0	1	0	2	R ₂	1
09	0	1	1	0	R ₂	1
10	0	1	1	1	R ₂	1
11	0	1	1	2	R ₂	1
12	1	0	0	0	R ₁	0
13	1	0	0	1	R ₁	0
14	1	0	0	2	R ₁	0
15	1	0	1	0	R ₁	0
16	1	0	1	1	R ₁	0
17	1	0	1	2	R ₁	0
18	1	1	0	0	R ₁	0
19	1	1	0	1	R ₁	0
20	1	1	0	2	R ₁	0
21	1	1	1	0	R ₁	0
22	1	1	1	1	R ₁	0
23	1	1	1	2	R ₁	0

Recap AXps/CXps: DL example

- $R_1:$ IF $(x_1 = 1)$ THEN 0
- $R_2:$ ELSE IF $(x_2 = 1)$ THEN 1
- $R_3:$ ELSE IF $(x_4 = 1)$ THEN 0
- $R_{DEF}:$ ELSE THEN 1

- Instance: $(\mathbf{v}, c) = ((0, 0, 1, 2), 1)$
- AXp's: $\{1, 4\}$ (prediction unchanged)
- CXp's:
 - $\{1\}$, by flipping the value of feature 1
 - $\{4\}$, by flipping the value of feature 4
 - But also, $\{\{1\}, \{4\}\}$ by MHS duality

Entry	x_1	x_2	x_3	x_4	Rule	$\kappa_1(\mathbf{x})$
00	0	0	0	0	R_{DEF}	1
01	0	0	0	1	R_3	0
02	0	0	0	2	R_{DEF}	1
03	0	0	1	0	R_{DEF}	1
04	0	0	1	1	R_3	0
05	0	0	1	2	R_{DEF}	1
06	0	1	0	0	R_2	1
07	0	1	0	1	R_2	1
08	0	1	0	2	R_2	1
09	0	1	1	0	R_2	1
10	0	1	1	1	R_2	1
11	0	1	1	2	R_2	1
12	1	0	0	0	R_1	0
13	1	0	0	1	R_1	0
14	1	0	0	2	R_1	0
15	1	0	1	0	R_1	0
16	1	0	1	1	R_1	0
17	1	0	1	2	R_1	0
18	1	1	0	0	R_1	0
19	1	1	0	1	R_1	0
20	1	1	0	2	R_1	0
21	1	1	1	0	R_1	0
22	1	1	1	1	R_1	0
23	1	1	1	2	R_1	0

Plan for this course

- Lecture 01 – unit(s):
 - #01: Foundations
- Lecture 02 – unit(s):
 - #02: Principles of symbolic XAI – **feature selection**
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 – unit(s):
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 – unit(s):
 - #06: Recent, emerging & advanced topics
- Lecture 05 – unit(s):
 - #07: Principles of symbolic XAI – **feature attribution** (& myth of Shapley values in XAI)
 - #08: Corrected feature attribution – nuSHAP
 - #09: Conclusions & research directions

Some necessary comments...

- Std question: Can we apply symbolic XAI to this highly complex ML model XYZ?

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 - Most likely answer: **No!**

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 - Most likely answer: No! But ...

Some necessary comments...

- Std question: Can we apply symbolic XAI to this highly complex ML model XYZ?
 - Most likely answer: No! But ...
- Would you...
 - ride in a car that fails to break 10% of the time, or that fails to turn 20% of the time?

Some necessary comments...

- Std question: Can we apply symbolic XAI to this highly complex ML model XYZ?
 - Most likely answer: No! But ...
- Would you...
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 - fly with a airliner whose planes crash in about 1% of its flights?

Some necessary comments...

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 - Most likely answer: No! But ...
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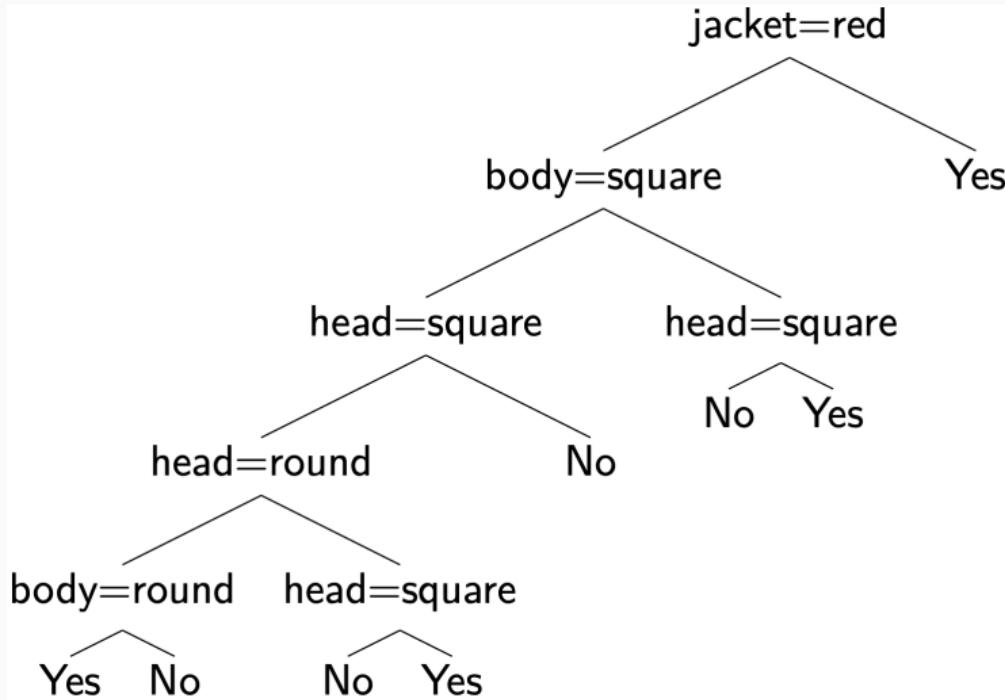
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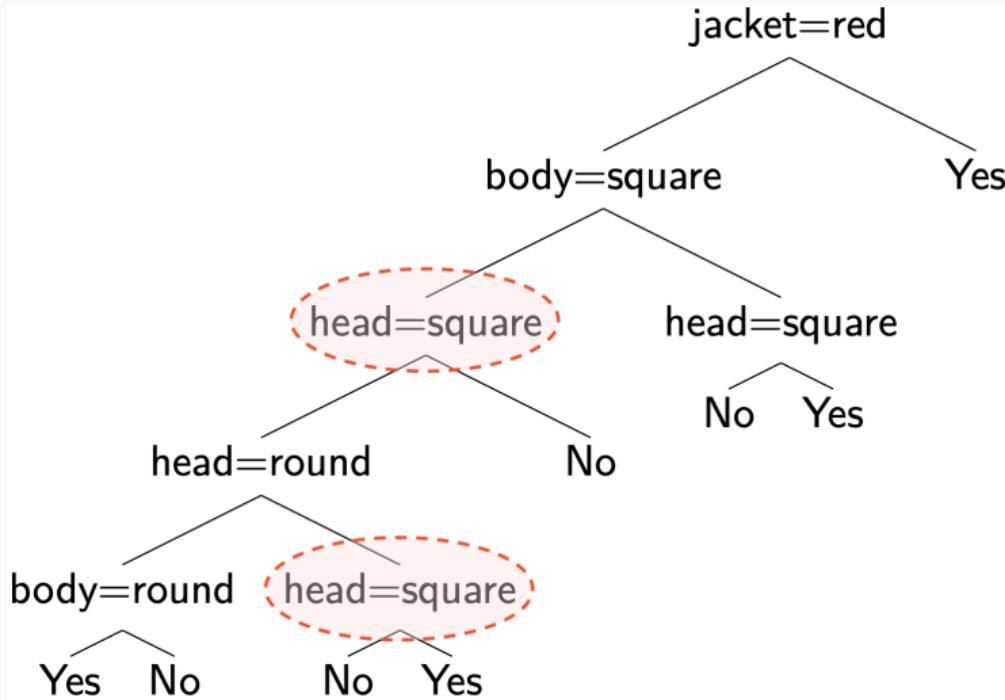
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 - More examples next...



Source: Xiyang Hu, Cynthia Rudin, Margo I. Seltzer:

Optimal Sparse Decision Trees.

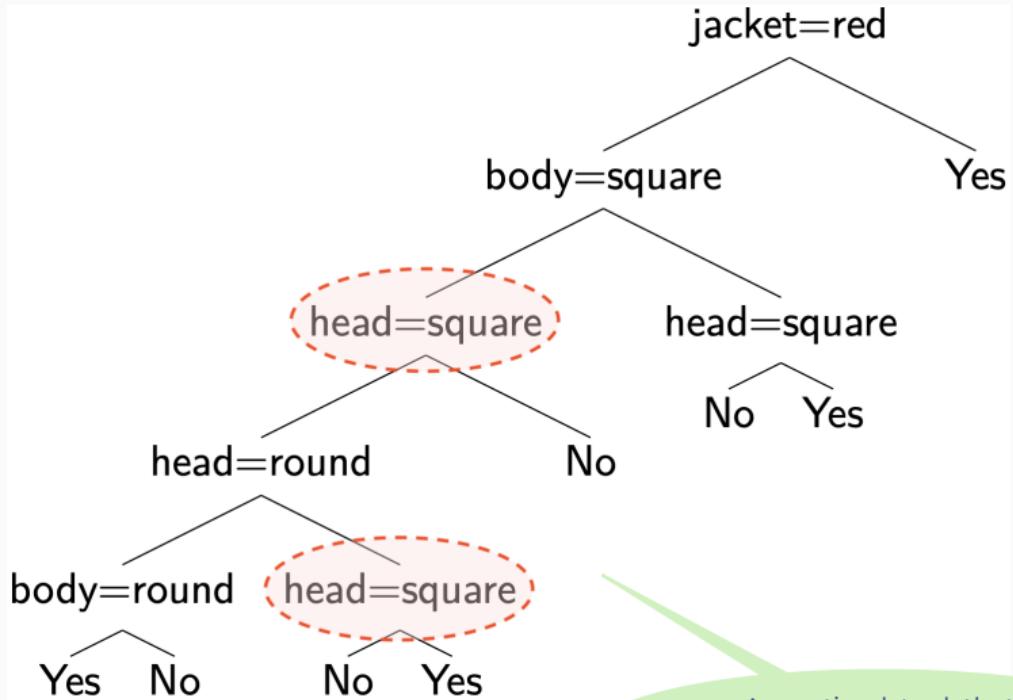
NeurIPS 2019: 7265-7273



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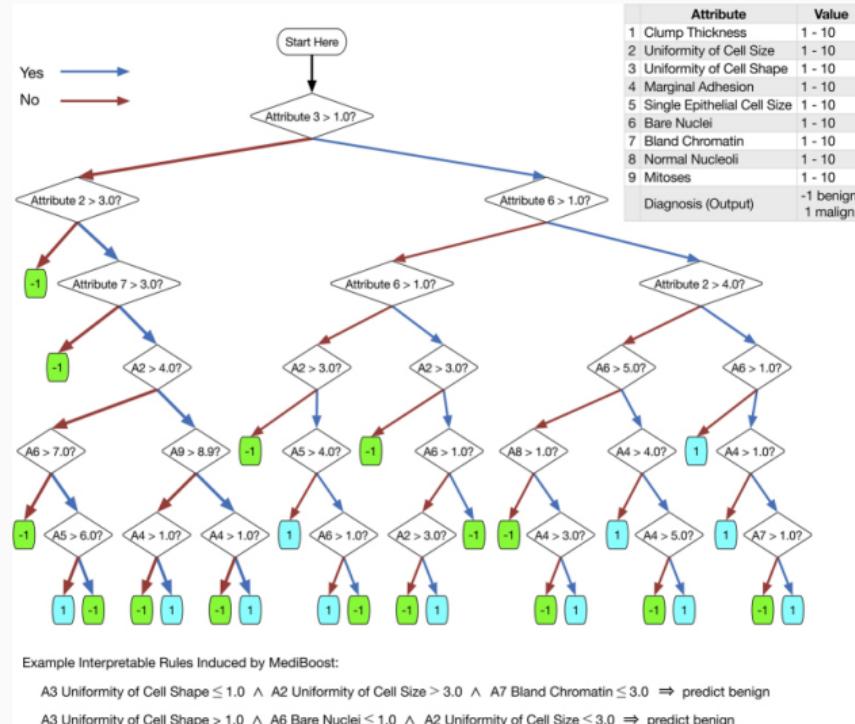
An optimal tool that
produces non-optimal DTs...!?

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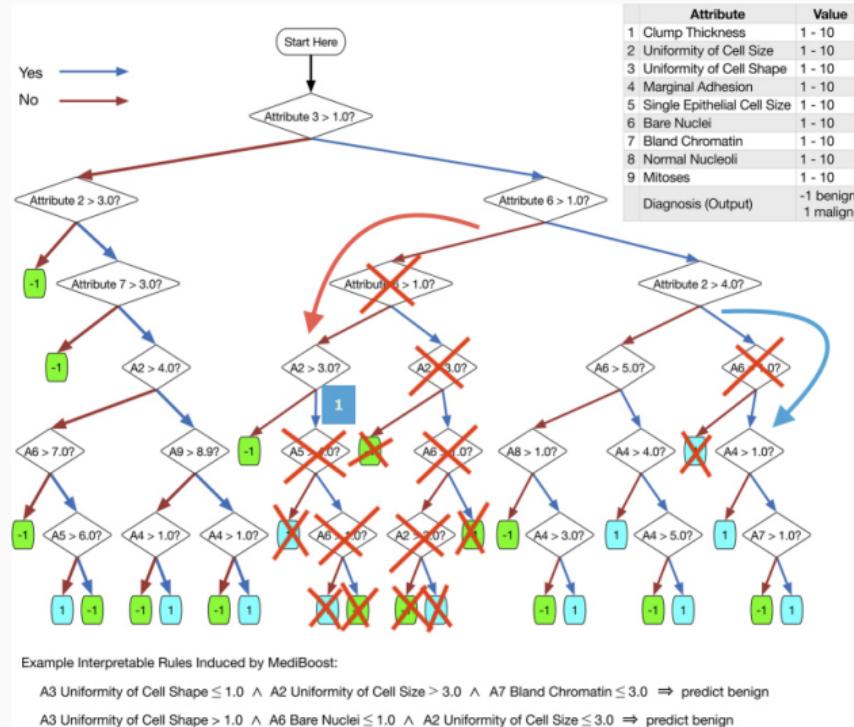
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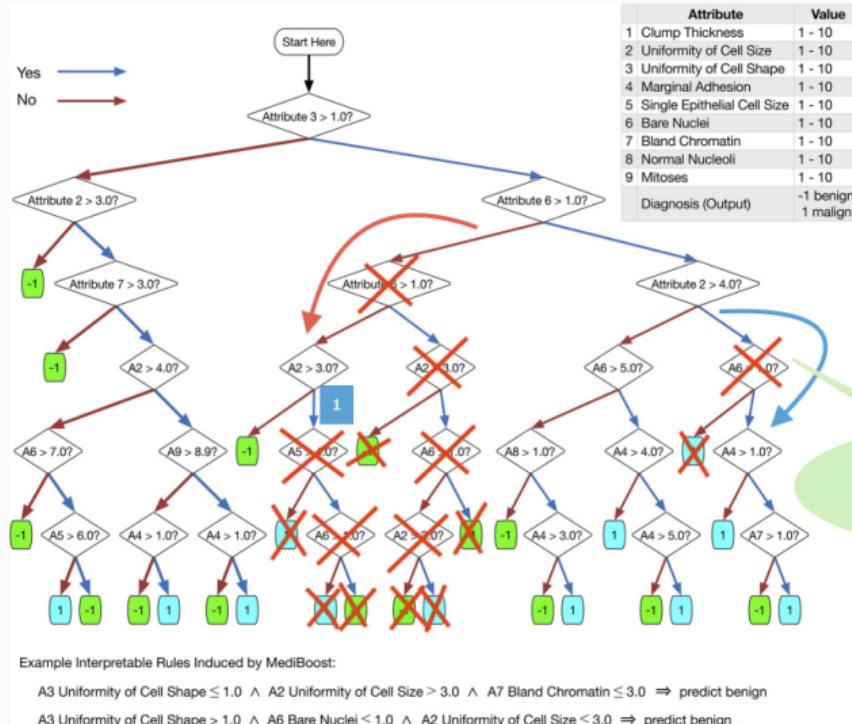
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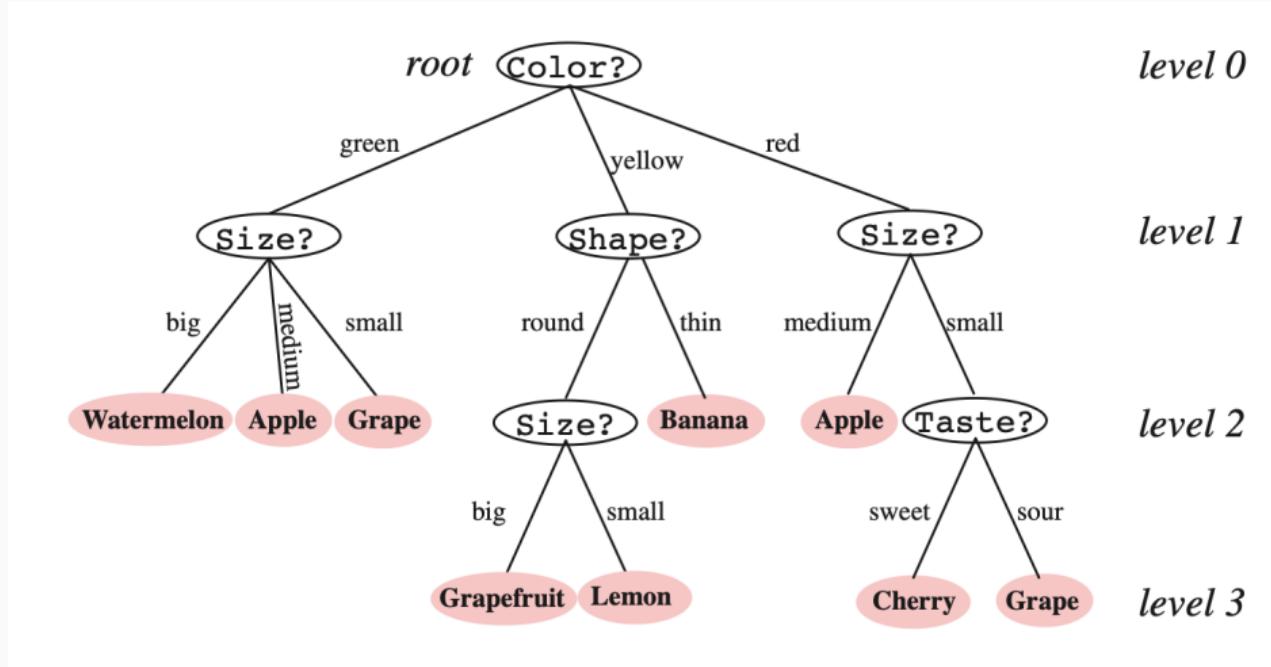
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- **For trustworthy AI, there exists no alternative to rigorous logic-based explanations!**

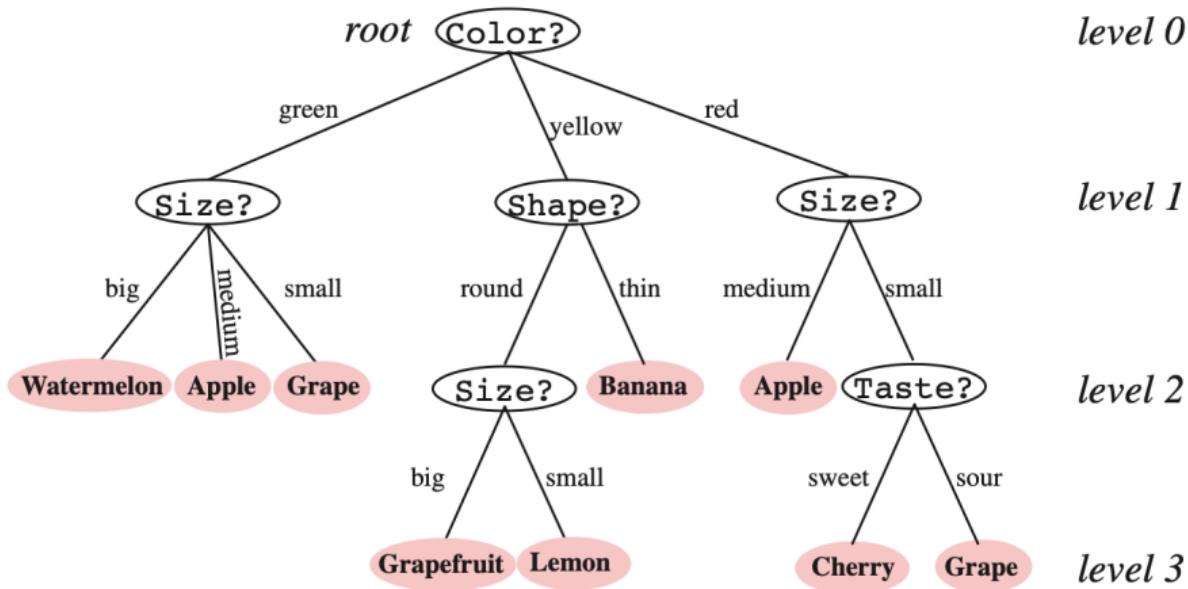
BTW, problematic DTs even in books...

[dud01]



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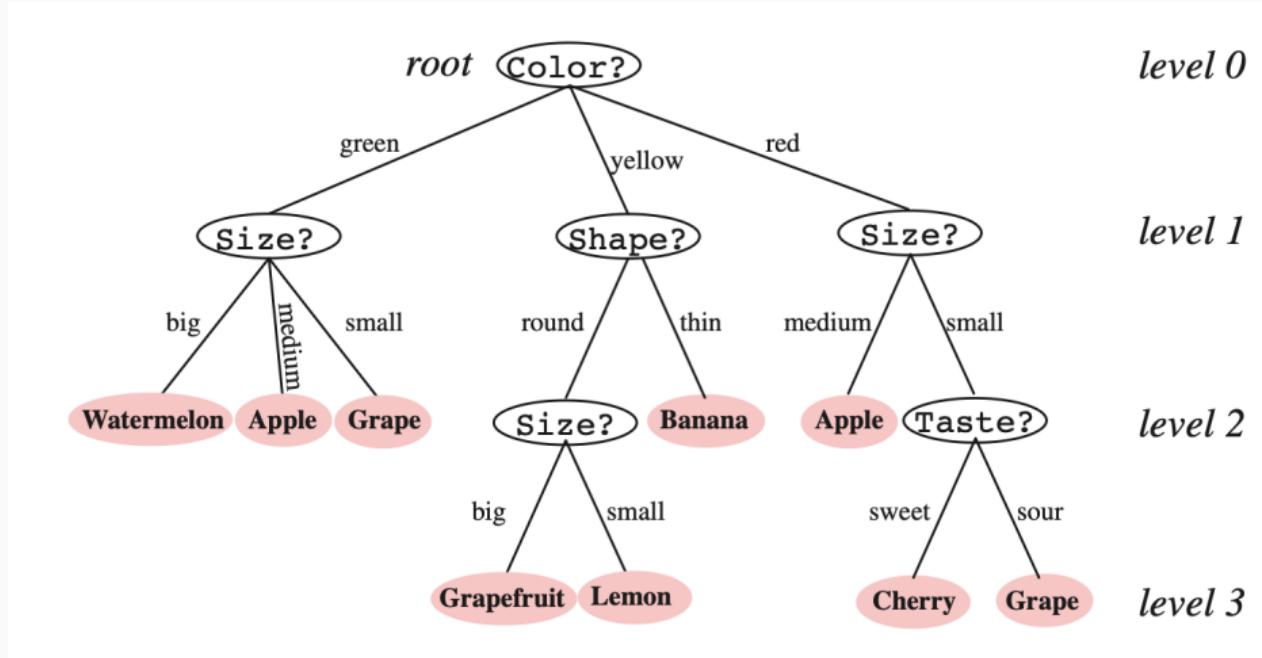
[dud01]



- What if $\text{Color} = \text{yellow} \wedge \text{Shape} = \text{round} \wedge \text{Size} = \text{medium}??$

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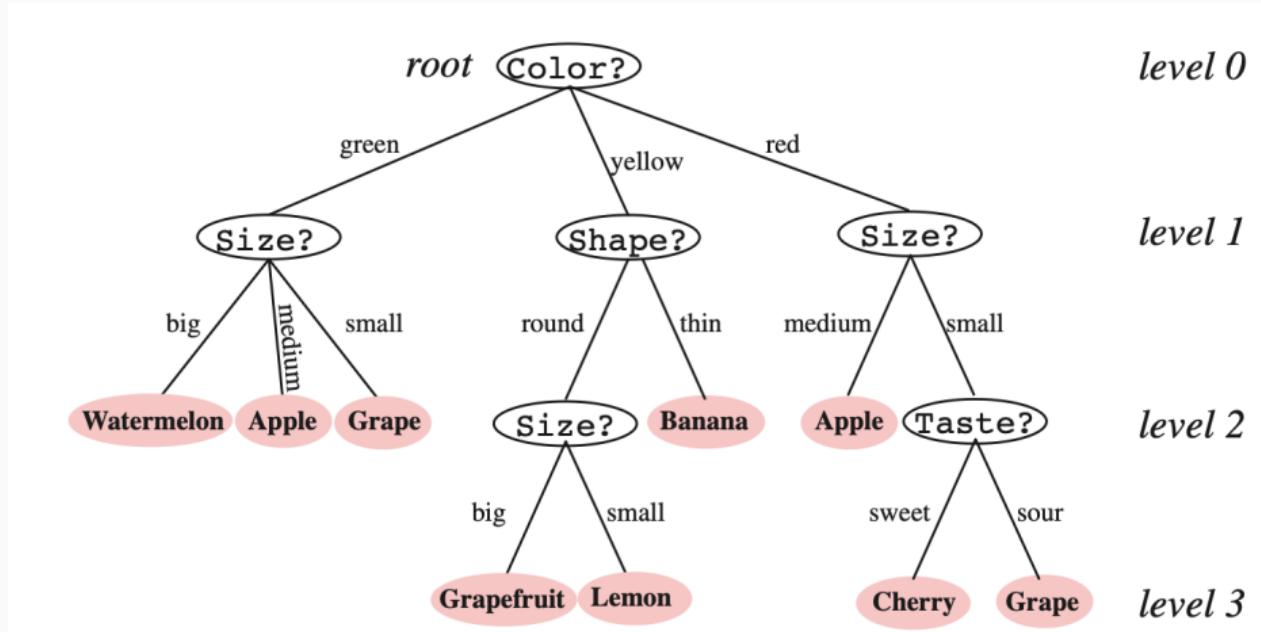
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- Or, what if $\text{Color} = \text{red} \wedge \text{Size} = \text{big}$??
- Easy to envision more serious use-cases...

Unit #04

(Efficient) Intractability in Symbolic XAI

Outline – Unit #04

Explaining Decision Lists

Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI

An encoding for DLs – components

R₁: IF (τ_1) THEN d_1
R₂: ELSE IF (τ_2) THEN d_2
...
R_j: ELSE IF (τ_j) THEN d_j
...
R_n: ELSE IF (τ_n) THEN d_n
R_{DEF}: ELSE THEN d_{n+1}

An encoding for DLs – components

R ₁ :	IF	(τ_1)	THEN	d_1
R ₂ :	ELSE IF	(τ_2)	THEN	d_2
...				
R _j :	ELSE IF	(τ_j)	THEN	d_j
...				
R _n :	ELSE IF	(τ_n)	THEN	d_n
R _{DEF} :	ELSE		THEN	d_{n+1}

- Clauses for encoding ϕ : $\mathfrak{E}_\phi(z_1, \dots)$, such that $z_1 = 1$ iff $\phi = 1$
- For τ_j : $\mathfrak{E}_{\tau_j}(t_j, \dots)$
- For $x_i = v_i$: $\mathfrak{E}_{x_i=v_i}(l_i, \dots)$
- Let $e_j = 1$ iff d_j matches c
- Prediction change with rule up to R_j (with $d_j \neq c$), if $\tau_j \not\models \perp$ and $\tau_k \models \perp$, for $1 \leq k < j$, with $e_k = 1$:

$$\left[f_j \leftrightarrow \left(t_j \wedge \bigwedge_{1 \leq k < j, e_k=1} \neg t_k \right) \right]$$

An encoding for DLs – components

R ₁ :	IF	(τ_1)	THEN	d_1
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...				
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- For $x_i = v_i$: $\mathfrak{E}_{x_i=v_i}(l_i, \dots)$
- Let $e_j = 1$ iff d_j matches c
- Require that at least one f_j , with $e_j = 0$ and $1 \leq j \leq n$, to be consistent (i.e. some rule up to j with prediction other than c to fire):

$$\left(\bigvee_{1 \leq j \leq n, e_j=0} f_j \right)$$

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- The set of soft clauses is given by: $\mathcal{S} \triangleq \{(l_i), i = 1, \dots, m\}$
- The set of hard clauses is given by:

$$\begin{aligned}\mathcal{B} \triangleq & \bigwedge\nolimits_{1 \leqslant i \leqslant m} \mathfrak{E}_{x_i=v_i}(l_i, \dots) \wedge \bigwedge\nolimits_{1 \leqslant j \leqslant n} \mathfrak{E}_{\tau_j}(t_j, \dots) \wedge \\ & \bigwedge\nolimits_{1 \leqslant j \leqslant n, e_j=0} \left(f_j \leftrightarrow \left(t_j \wedge \bigwedge\nolimits_{1 \leqslant k < j, e_k=1} \neg t_k \right) \right) \wedge \left(\bigvee\nolimits_{1 \leqslant j \leqslant n, e_j=0} f_j \right)\end{aligned}$$

- $\mathcal{B} \cup \mathcal{S} \models \perp$
 - MUSes are AXp's & MCSes are CXp's

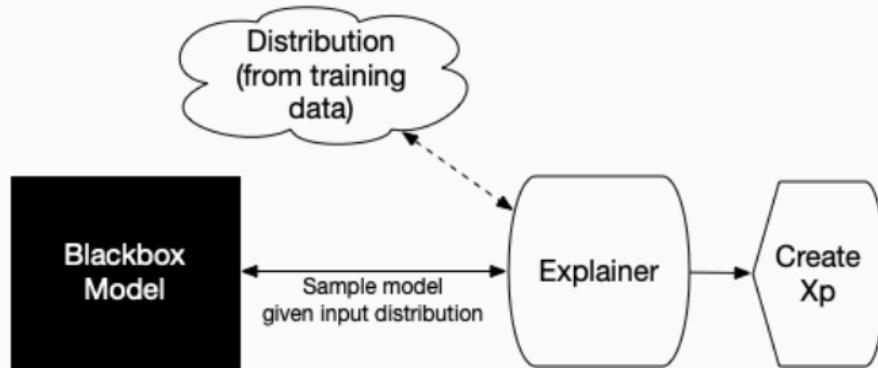
Outline – Unit #04

Explaining Decision Lists

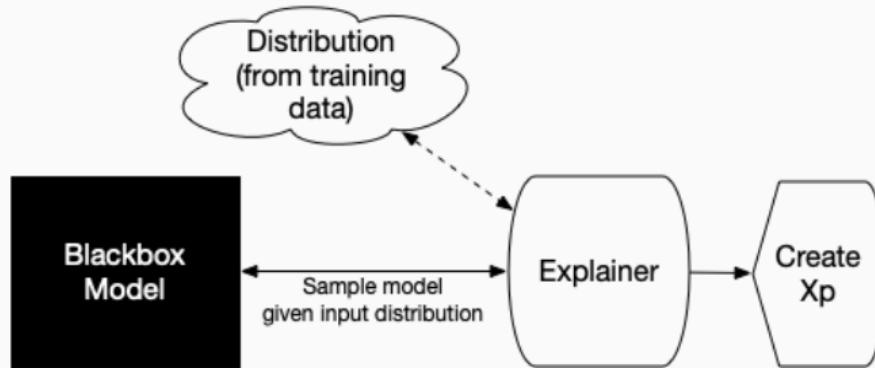
Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI

What is model-agnostic explainability?



What is model-agnostic explainability?



- Wildly popular XAI approach

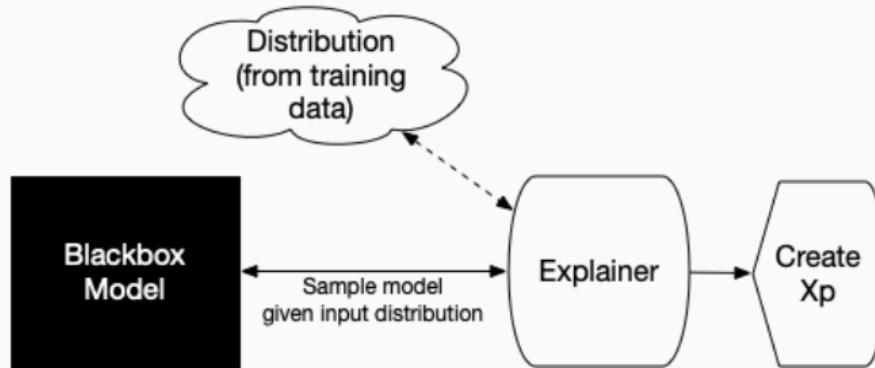
[RSG16, LL17, RSG18]

- **Feature attribution:** LIME, SHAP, ...
- **Feature selection:** Anchors, ...

[RSG16, LL17]

[RSG18]

What is model-agnostic explainability?



- Wildly popular XAI approach
 - **Feature attribution:** LIME, SHAP, ...
 - **Feature selection:** Anchors, ...
- **Q:** Are model-agnostic explanations rigorous?

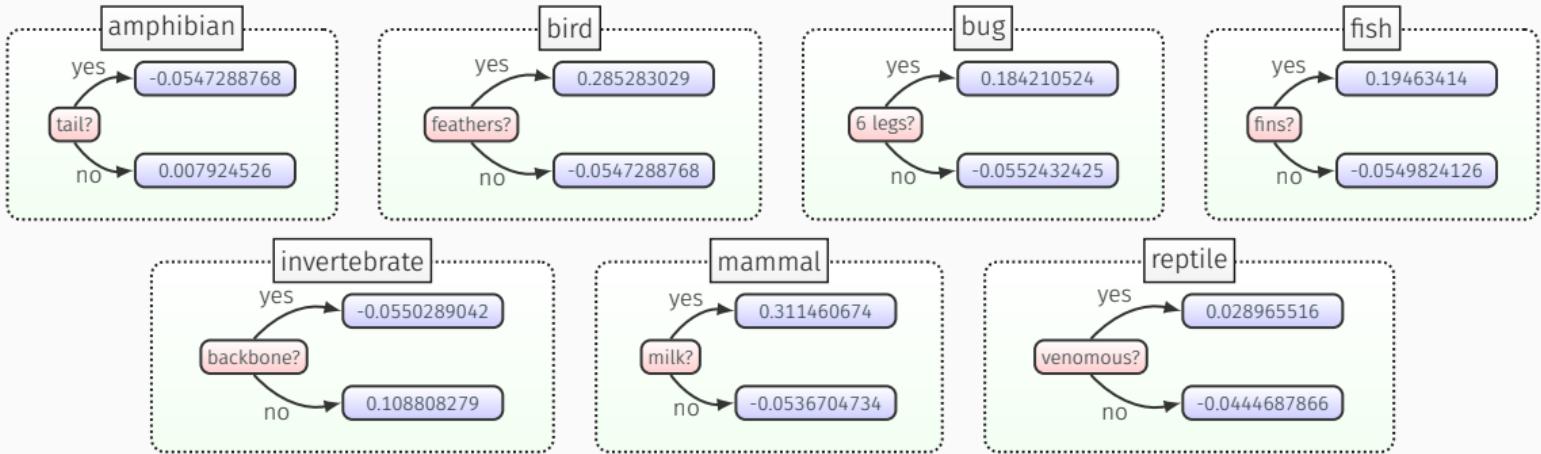
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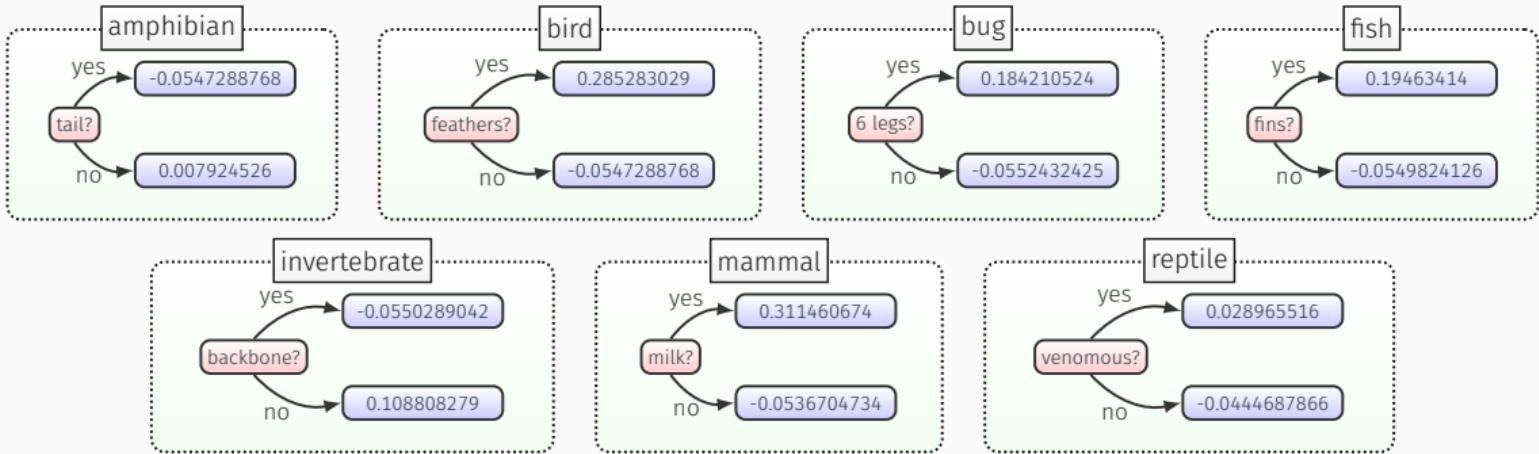
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[INM19c, Ign20]



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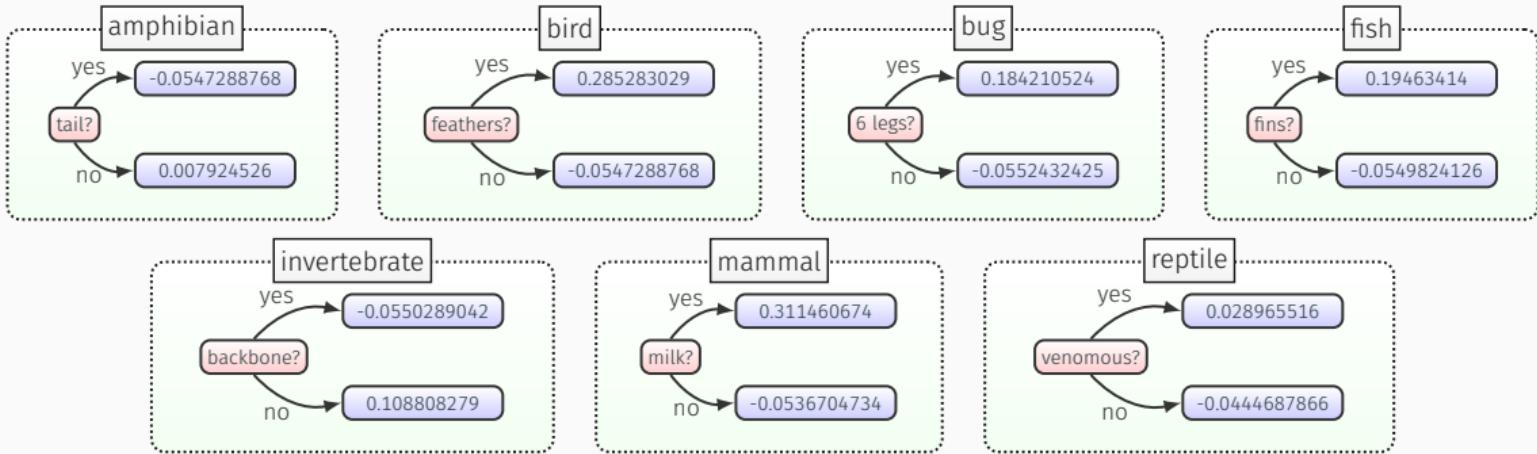


- Example instance:

IF $(\text{animal_name} = \text{pitviper}) \wedge \neg \text{hair} \wedge \neg \text{feathers} \wedge \text{eggs} \wedge \neg \text{milk} \wedge \neg \text{airborne} \wedge \neg \text{aquatic} \wedge \text{predator} \wedge \neg \text{toothed} \wedge \text{backbone} \wedge \text{breathes} \wedge \text{venomous} \wedge \neg \text{fins} \wedge (\text{legs} = 0) \wedge \text{tail} \wedge \neg \text{domestic} \wedge \neg \text{catsize}$
THEN $(\text{class} = \text{reptile})$

Easy to spot problems – BT for zoo dataset & Anchor

[INM19c, Ign20]



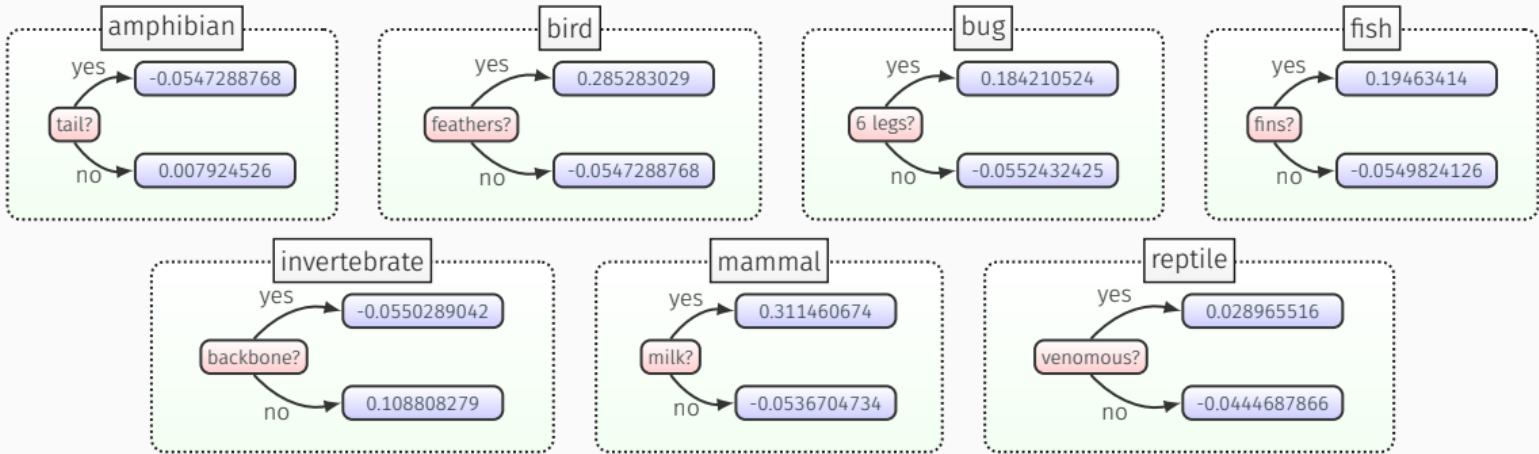
- Example instance (& Anchor picks):

[RSG18]

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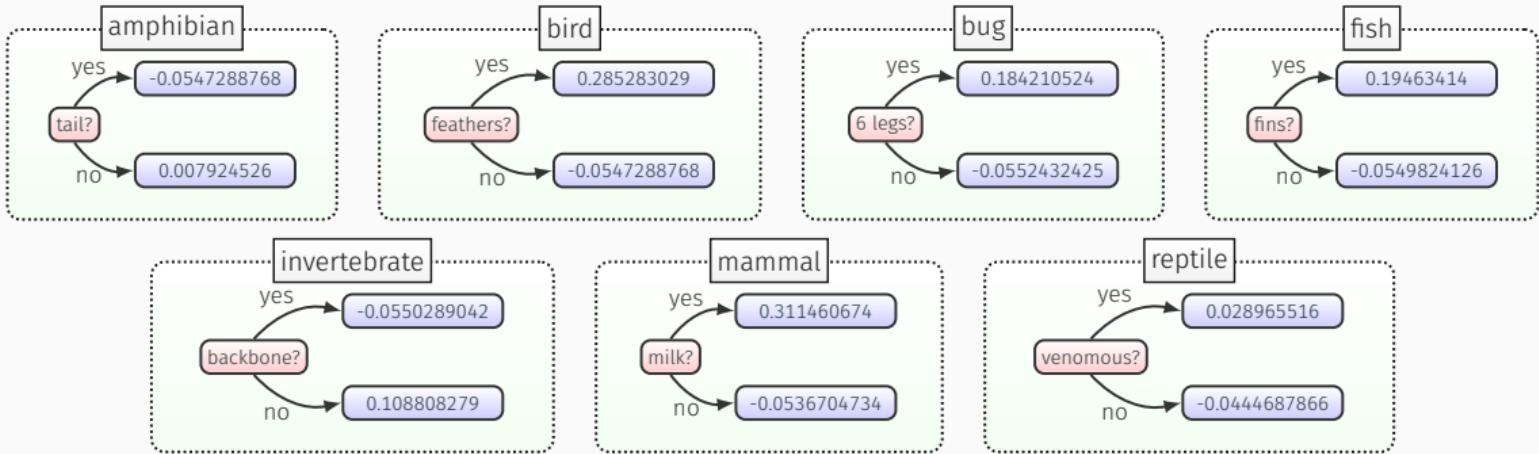
- Explanation obtained with Anchor:

[RSG18]

IF $\neg \text{hair} \wedge \neg \text{milk} \wedge \neg \text{toothed} \wedge \neg \text{fins}$
THEN (class = reptile)

Easy to spot problems – BT for zoo dataset & Anchor

[INM19c, Ign20]



- But, explanation **incorrectly “explains”** another instance (from training data!)

IF $(\text{animal_name} = \text{toad}) \wedge \neg \text{hair} \wedge \neg \text{feathers} \wedge \text{eggs} \wedge \neg \text{milk} \wedge \neg \text{airborne} \wedge \neg \text{aquatic} \wedge \neg \text{predator} \wedge \neg \text{toothed} \wedge \text{backbone} \wedge \text{breathes} \wedge \neg \text{venomous} \wedge \neg \text{fins} \wedge (\text{legs} = 4) \wedge \neg \text{tail} \wedge \neg \text{domestic} \wedge \neg \text{catsize}$

THEN $(\text{class} = \text{amphibian})$

Incorrect explanations:

Classifier for deciding bank loans

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Explanation X: age = 45, salary = 50K

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X is consistent with Bessie $\coloneqq (v_1, \text{Y})$

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∴ different outcomes & same explanation !?

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2. And, \mathcal{X} is subset-minimal:

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Depending on logic encoding used for classifier, different automated reasoners can be employed

- Approach is bounded by scalability of rigorous explanations...

How serious is the lack of rigor of model-agnostic explanations?

- Obs: Lack of rigor of model-agnostic explanations known since 2019

[INM19c, Ign20, YIS⁺23]

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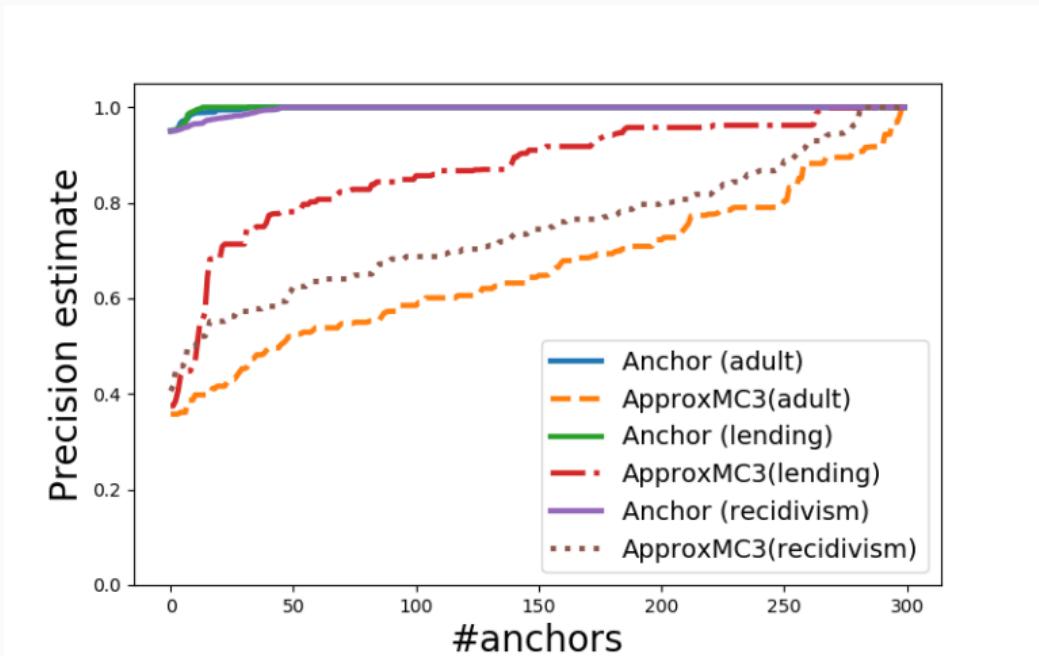
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[NSM⁺19]

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- For feature attribution we proposed different ways of assessing rigor

[INM19c, NSM⁺19, Ign20, YIS⁺23]

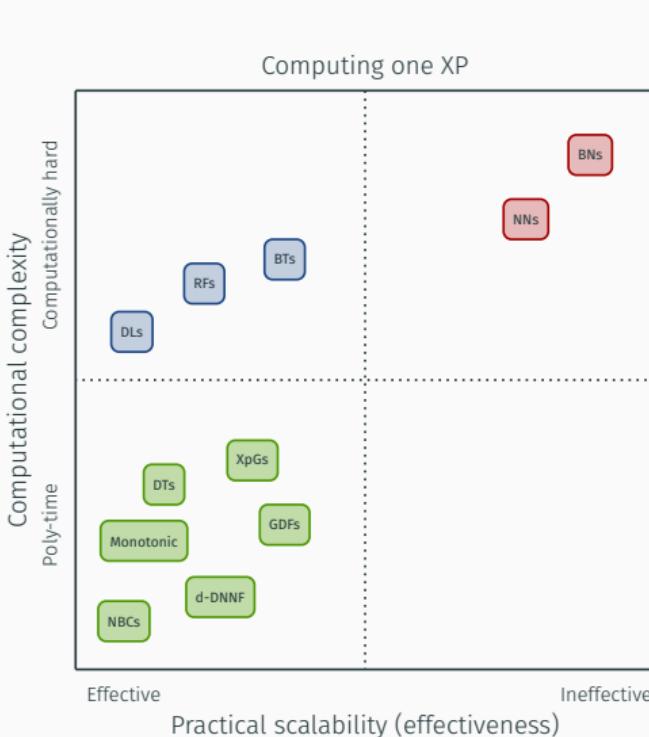


Outline – Unit #04

Explaining Decision Lists

Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI



[INM19c, Ign20, IIM20, MGC⁺20, MGC⁺21, HIIM21, IMS21, IM21, CM21, HII⁺22, IISMS22]

• Formal explanations efficient for several families of classifiers

• Polynomial-time:

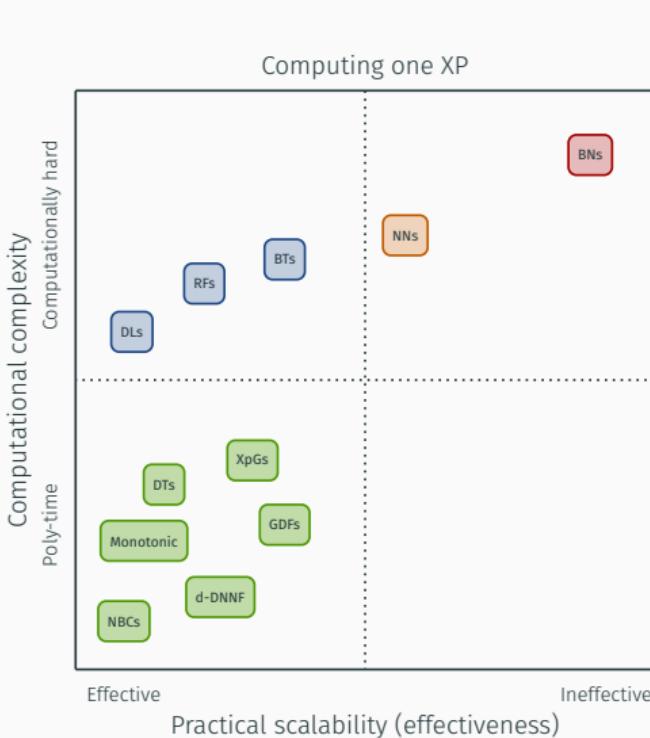
- Naive-Bayes classifiers (**NBCs**) [MGC⁺20]
- Decision trees (**DTs**) [IIM20, HIIM21]
- **XpG's:** DTs, OBDDs, OMDDs, etc. [HIIM21]
- **Monotonic** classifiers [MGC⁺21]
- Propositional languages (e.g. d-DNNF, ...) [HII⁺22]
- Additional results [CM21, HII⁺22]

• Comp. hard, but **effective** (efficient in practice):

- Random forests (**RFs**) [IMS21]
- Decision lists (**DLS**) [IM21]
- Boosted trees (**BTs**) [INM19c, Ign20, IISMS22]

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- Neural networks (**NNs**) [INM19a]
- Bayesian networks (**BNs**) [SCD18]



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- Random forests (**RFs**) [IMS21]
- Decision lists (**DLS**) [IM21]
- Boosted trees (**BTs**) [INM19c, Ign20, IISMS22]

• Comp. hard, but some practical **scalability**:

- Neural networks (**NNs**) [HM23b]

• Comp. hard, and **ineffective** (hard in practice):

- Bayesian networks (**BNs**) [SCD18]

Results for RFs in 2021 (with SAT)

[IMS21]

Dataset	#F #C #I			RF			CNF		SAT oracle				AXp (RFexpl)				Anchor	
	D	#N	%A	#var	#cl	MxS	MxU	#S	#U	Mx	m	avg	%w	avg	%w	avg	%w	
ann-thyroid	(21 3 718) 4	2192	98	17854	29230	0.12	0.15	2	18	0.36	0.05	0.13	96	0.32	4			
appendicitis	(7 2 43) 6	1920	90	5181	10085	0.02	0.02	4	3	0.05	0.01	0.03	100	0.48	0			
banknote	(4 2 138) 5	2772	97	8068	16776	0.01	0.01	2	2	0.03	0.02	0.02	100	0.19	0			
biodegradation	(41 2 106 5	4420	88	11007	23842	0.31	1.05	17	22	2.27	0.04	0.29	97	4.07	3			
heart-c	(13 2 61) 5	3910	85	5594	11963	0.04	0.02	6	7	0.07	0.01	0.04	100	0.85	0			
ionosphere	(34 2 71) 5	2096	87	7174	14406	0.02	0.02	22	11	0.11	0.02	0.03	100	12.43	0			
karhunen	(64 10 200) 5	6198	91	36708	70224	1.06	1.41	35	29	14.64	0.65	2.78	100	28.15	0			
letter	(16 26 398 8	44304	82	28991	68148	1.97	3.31	8	8	6.91	0.24	1.61	70	2.48	30			
magic	(10 2 381) 6	9840	84	29530	66776	0.51	1.84	6	4	2.13	0.07	0.14	99	0.91	1			
new-thyroid	(5 3 43) 5	1766	100	17443	28134	0.03	0.01	3	2	0.08	0.03	0.05	100	0.36	0			
pendigits	(16 10 220) 6	12004	95	30522	59922	2.40	1.32	10	6	4.11	0.14	0.94	96	3.68	4			
ring	(20 2 740 6	6188	89	19114	42362	0.27	0.44	11	9	1.25	0.05	0.25	92	7.25	8			
segmentation	(19 7 42) 4	1966	90	21288	35381	0.11	0.17	8	10	0.53	0.11	0.31	100	4.13	0			
shuttle	(9 7 116 3	1460	99	18669	29478	0.11	0.08	2	7	0.34	0.05	0.14	99	0.42	1			
sonar	(60 2 42) 5	2614	88	9938	20537	0.04	0.06	36	24	0.43	0.04	0.09	100	23.02	0			
spectf	(44 2 54) 5	2306	88	6707	13449	0.07	0.06	20	24	0.34	0.02	0.07	100	8.12	0			
texture	(40 11 550) 5	5724	87	34293	64187	0.79	0.63	23	17	3.24	0.19	0.93	100	28.13	0			
twonorm	(20 2 740 5	6266	94	21198	46901	0.08	0.08	12	8	0.28	0.06	0.10	100	5.73	0			
vowel	(13 11 198) 6	10176	90	44523	88696	1.66	2.11	8	5	4.52	0.15	1.15	66	1.67	34			
waveform-40	(40 3 500 5	6232	83	30438	58380	0.50	0.86	15	25	7.07	0.11	0.88	100	11.93	0			
wpbc	(33 2 78) 5	2432	76	9078	18675	1.00	1.53	20	13	5.33	0.03	0.65	79	3.91	21			

Results for NNs in 2019 (with SMT/MILP)

[INM19a]

Dataset		Minimal explanation			Minimum explanation		
		size	SMT (s)	MILP (s)	size	SMT (s)	MILP (s)
australian	(14)	m	1	0.03	0.05	—	—
		a	8.79	1.38	0.33	—	—
		M	14	17.00	1.43	—	—
backache	(32)	m	13	0.13	0.14	—	—
		a	19.28	5.08	0.85	—	—
		M	26	22.21	2.75	—	—
breast-cancer	(9)	m	3	0.02	0.04	3	0.02
		a	5.15	0.65	0.20	4.86	0.41
		M	9	6.11	0.41	9	24.80
cleve	(13)	m	4	0.05	0.07	4	0.07
		a	8.62	3.32	0.32	7.89	5.14
		M	13	60.74	0.60	13	39.06
hepatitis	(19)	m	6	0.02	0.04	4	0.04
		a	11.42	0.07	0.06	9.39	2.89
		M	19	0.26	0.20	19	22.23
voting	(16)	m	3	0.01	0.02	3	0.02
		a	4.56	0.04	0.13	3.46	0.25
		M	11	0.10	0.37	11	1.77
spect	(22)	m	3	0.02	0.02	3	0.04
		a	7.31	0.13	0.07	6.44	0.67
		M	20	0.88	0.29	20	10.73

Results for NNs in 2019 (with SMT/MILP)

[INM19a]

First rigorous approach
for explaining NNs !

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		M	14	17.00	1.43	—	—	—
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		a	19.28	5.08	0.85	—	—	—
		M	26	22.21	2.75	—	—	—
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		M	9	6.11	0.41	9	24.80	1.81
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Scales to (a few)
tens of neurons...

Results for NNs in 2023 (using Marabou [KHI⁺19])

[HM23b]

DNN	points	AXp	#Calls	Time	#TO	AXp	#Calls	Time	#TO
$\epsilon = 0.1$					$\epsilon = 0.05$				
ACASXU_1_5	#1	3	5	185.9	0	2	5	113.8	0
	#2	2	5	273.8	0	1	5	33.2	0
	#3	0	5	714.2	0	0	5	4.3	0
ACASXU_3_1	#1	0	5	2219.3	0	0	5	14.2	0
	#2	2	5	4263.5	1	0	5	1853.1	0
	#3	1	5	581.8	0	0	5	355.9	0
ACASXU_3_2	#1	3	5	13739.3	2	1	5	6890.1	1
	#2	3	5	226.4	0	2	5	125.1	0
	#3	2	5	1740.6	0	2	5	173.6	0
ACASXU_3_5	#1	4	5	43.6	0	2	5	59.4	0
	#2	3	5	5039.4	0	2	5	4303.8	1
	#3	2	5	5574.9	1	2	5	2660.3	0
ACASXU_3_6	#1	1	5	6225.0	1	0	5	51.0	0
	#2	3	5	4957.2	1	2	5	1897.3	0
	#3	1	5	196.1	0	1	5	919.2	0
ACASXU_3_7	#1	3	5	6256.2	0	4	5	26.9	0
	#2	4	5	311.3	0	1	5	6958.6	1
	#3	2	5	7756.5	1	1	5	7807.6	1
ACASXU_4_1	#1	2	5	12413.0	2	1	5	5090.5	1
	#2	1	5	5035.1	1	0	5	2335.6	0
	#3	4	5	1237.3	0	4	5	1143.4	0
ACASXU_4_2	#1	4	5	15.9	0	4	5	12.1	0
	#2	3	5	1507.6	0	1	5	111.3	0
	#3	2	5	5641.6	2	0	5	1639.1	0

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ACASXU_3_6	#1	1	5	6225.0	1	0	5	51.0	0
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Scales to a few hundred neurons

More recent results (from 2024)...

[IHM⁺24a]

Model	Deletion							SwiftXplain						
	avgC	nCalls	Len	Mn	Mx	avg	TO	avgC	nCalls	Len	FD%	Mn	Mx	avg
gtsrb-dense	0.06	1024	448	52.0	76.3	63.1	0	0.23	54	447	77.4	10.8	14.0	12.2
gtsrb-convSmall	0.06	1024	309	59.2	82.6	65.1	0	0.22	74	313	39.7	15.1	19.5	16.2
gtsrb-conv	—	—	—	—	—	—	100	96.49	45	174	33.2	3858.7	6427.7	4449.4
mnist-denseSmall	0.28	784	177	190.9	420.3	220.4	0	0.77	111	180	15.5	77.6	104.4	85.1
mnist-dense	0.19	784	231	138.1	179.9	150.6	0	0.75	183	229	11.5	130.1	145.5	136.8
mnist-convSmall	—	—	—	—	—	—	100	98.56	52	116	21.3	4115.2	6858.3	5132.8

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Scales to **tens of thousands** of neurons!

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Scales to **tens of thousands** of neurons!

Largest for MNIST: 10142 neurons
Largest for GSTRB: 94308 neurons

Unit #05

Queries in Symbolic XAI

Outline – Unit #05

Enumeration of Explanations

Feature Necessity & Relevancy

How to navigate the space of XPs?

- **Goal:** iteratively list yet unlisted XPs (either AXp's or CXp's)

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 - For NBCs: enumeration with polynomial delay [MGC⁺20]
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[MGC⁺20]

[MGC⁺21]

[HIIM21, IIM22]

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- No known algorithms for **direct** enumeration of AXp's
 - Akin to enumerating MUSes

[MGC⁺20]

[MGC⁺21]

[HIIM21, IIM22]

[MM20]

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- There are algorithms for direct enumeration of CXp's
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- No known algorithms for **direct** enumeration of AXp's
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- No known algorithms for **direct** enumeration of AXp's [MM20]
 - Akin to enumerating MUSes
- Enumeration of MCSes + dualization often not realistic [LS08, FK96]
 - There can be too many CXp's...
- Best solution is a MARCO-like algorithm (for enumerating MUSes) [LPMM16]
 - On-demand enumeration of AXp's/CXp's

Recall computing one AXp/CXp – oneXP

Input: Predicate \mathbb{P} , parameterized by \mathcal{T}, \mathcal{M}

Output: One XP \mathcal{S}

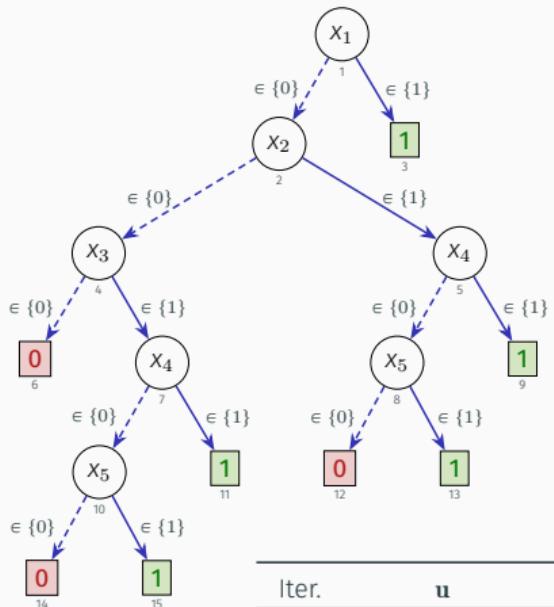
```
1: procedure oneXP( $\mathbb{P}$ )
2:    $\mathcal{S} \leftarrow \mathcal{F}$                                  $\triangleright$  Initialization:  $\mathbb{P}(\mathcal{S})$  holds
3:   for  $i \in \mathcal{F}$  do
4:     if  $\mathbb{P}(\mathcal{S} \setminus \{i\})$  then            $\triangleright$  Loop invariant:  $\mathbb{P}(\mathcal{S})$  holds
5:        $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$ 
6:   return  $\mathcal{S}$                                  $\triangleright$  Update  $\mathcal{S}$  only if  $\mathbb{P}(\mathcal{S} \setminus \{i\})$  holds
                                                 $\triangleright$  Returned set  $\mathcal{S}$ :  $\mathbb{P}(\mathcal{S})$  holds
```

Generic oracle-based enumeration algorithm

Input: Parameters $\mathbb{P}_{\text{axp}}, \mathbb{P}_{\text{cxp}}, \mathcal{T}, \mathcal{F}, \kappa, \mathbf{v}$

```
1:  $\mathcal{H} \leftarrow \emptyset$                                  $\triangleright \mathcal{H}$  defined on set  $U = \{u_1, \dots, u_m\}$ ; initially no constraints
2: repeat
3:    $(\text{outc}, \mathbf{u}) \leftarrow \text{SAT}(\mathcal{H})$            $\triangleright$  Use SAT oracle to pick assignment s.t. known constraints in  $\mathcal{H}$ 
4:   if  $\text{outc} = \text{true}$  then
5:      $\mathcal{S} \leftarrow \{i \in \mathcal{F} \mid u_i = 0\}$             $\triangleright \mathcal{S}$ : fixed features
6:      $\mathcal{U} \leftarrow \{i \in \mathcal{F} \mid u_i = 1\}$             $\triangleright \mathcal{U}$ : universal features;  $\mathcal{F} = \mathcal{S} \cup \mathcal{U}$ 
7:     if  $\mathbb{P}_{\text{cxp}}(\mathcal{U}; \mathcal{T}, \mathcal{F}, \kappa, \mathbf{v})$  then       $\triangleright \mathcal{U} = \mathcal{F} \setminus \mathcal{S} \supseteq$  some Cxp
8:        $\mathcal{P} \leftarrow \text{oneXP}(\mathcal{U}; \mathbb{P}_{\text{cxp}}, \mathcal{T}, \mathcal{F}, \kappa, \mathbf{v})$ 
9:       reportCxp( $\mathcal{P}$ )
10:       $\mathcal{H} \leftarrow \mathcal{H} \cup \{(\vee_{i \in \mathcal{P}} \neg u_i)\}$          $\triangleright \mathcal{P} \subseteq \mathcal{U}$ : one 1-value variable must be 0 in future iterations
11:    else                                               $\triangleright \mathcal{S} \supseteq$  some Axp
12:       $\mathcal{P} \leftarrow \text{oneXP}(\mathcal{S}; \mathbb{P}_{\text{axp}}, \mathcal{T}, \mathcal{F}, \kappa, \mathbf{v})$ 
13:      reportAxp( $\mathcal{P}$ )
14:       $\mathcal{H} \leftarrow \mathcal{H} \cup \{(\vee_{i \in \mathcal{P}} u_i)\}$          $\triangleright \mathcal{P} \subseteq \mathcal{S}$ : one 0-value variable must be 1 in future iterations
15: until  $\text{outc} = \text{false}$ 
```

DT classifier – example run of enumerator



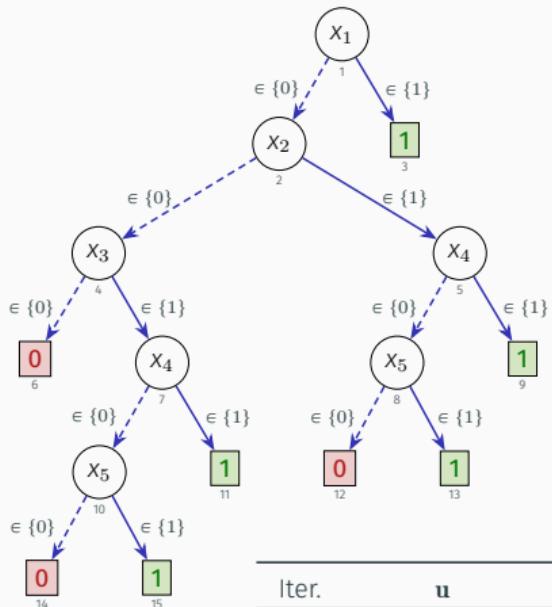
- Instance: $(\mathbf{v}, c) = ((0, 0, 1, 0, 1), 1)$

x_3	x_5	x_1	x_2	x_4	$\kappa_2(\mathbf{x})$
1	1	0	0	0	1
1	1	0	0	1	1
1	1	0	1	0	1
1	1	0	1	1	1
1	1	1	0	0	1
1	1	1	0	1	1
1	1	1	1	0	1
1	1	1	1	1	1

x_3	x_5	x_1	x_2	x_4	$\kappa_2(\mathbf{x})$
0	0	0	0	0	0
0	1	0	0	0	0
1	0	0	0	0	0
1	1	0	0	0	1

Iter.	\mathbf{u}	\mathcal{S}	$\mathbb{P}_{\text{exp}}(\cdot)$	AXp	CXp	Clause	Resulting \mathcal{H}
1	(1, 1, 1, 1, 1)	\emptyset	1	-	{3}	$(\neg u_3)$	$\{(\neg u_3)\}$
2	(1, 1, 0, 1, 1)	{3}	1	-	{5}	$(\neg u_5)$	$\{(\neg u_3), (\neg u_5)\}$
3	(1, 1, 0, 1, 0)	{3, 5}	0	{3, 5}	-	$(u_3 \vee u_5)$	$\{(\neg u_3), (\neg u_5), (u_3 \vee u_5)\}$
5	[outc = false]	-	-	-	-	-	$\{(\neg u_3), (\neg u_5), (u_3 \vee u_5)\}$

DT classifier – another example run of enumerator



• Instance: $(\mathbf{v}, c) = ((0, 0, 1, 0, 1), 1)$

x_3	x_5	x_1	x_2	x_4	$\kappa_2(\mathbf{x})$
1	1	0	0	0	1
1	1	0	0	1	1
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1	(0, 0, 0, 0, 0)	{1, 2, 3, 4, 5}	0	{3, 5}	-	$(u_3 \vee u_5)$	$\{(u_3 \vee u_5)\}$
2	(0, 0, 1, 0, 0)	{1, 2, 4, 5}	1	-	{3}	$(\neg u_3)$	$\{(u_3 \vee u_5), (\neg u_3)\}$
3	(0, 0, 0, 0, 1)	{1, 2, 3, 4}	1	-	{5}	$(\neg u_5)$	$\{(u_3 \vee u_5), (\neg u_3), (\neg u_5)\}$
5	[outc = false]	-	-	-	-	-	$\{(u_3 \vee u_5), (\neg u_3), (\neg u_5)\}$

DTs admit more efficient algorithms

- Recall:
 - Given instance (\mathbf{v}, c) , create set \mathcal{I}
 - For each path P_k with prediction $d \neq c$:
 - Let I_k denote the features with literals inconsistent with \mathbf{v}
 - Add I_k to \mathcal{I}
 - Remove from \mathcal{I} the sets that have a proper subset in \mathcal{I} , and duplicates
- \mathcal{I} is the set of CXp's – algorithm runs in poly-time

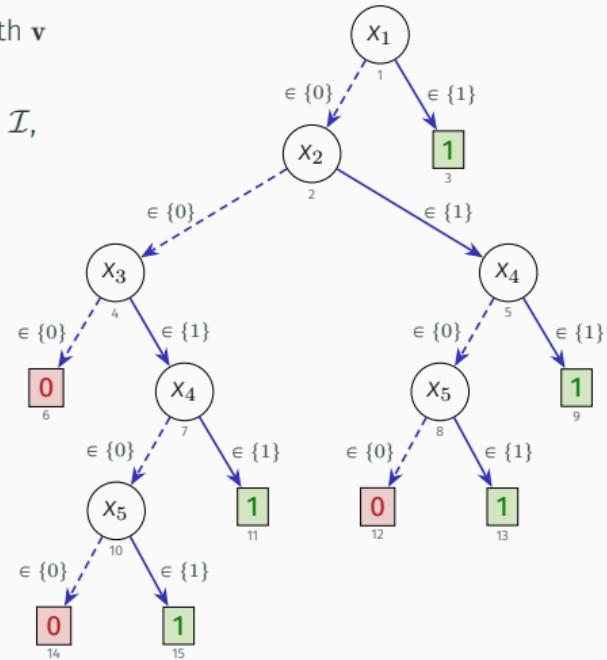
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 - Obs: starting hypergraph is poly-size!
 - And each MHS is an AXp**
- Example:
 - $I_1 = \{3\}$
 - $I_2 = \{5\}$
 - $I_3 = \{2, 5\}$
 - \therefore keep I_1 and I_2
 - AXp's: MHSes yield $\{\{3, 5\}\}$



Outline – Unit #05

Enumeration of Explanations

Feature Necessity & Relevancy

(Conditioned) Classifier Decision Problem ((C)CDP)

[HCM + 23]

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[HCM⁺23]

- Given $c \in \mathcal{K}$, CDP is to decide whether the following statement holds:

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- Claim:** (C)CDP is in NP-complete for DLs, RFs, BTs, boolean NNs and BNNs

Feature necessity

- Consider instance (\mathbf{v}, c)
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 - **This holds for any classifier!**

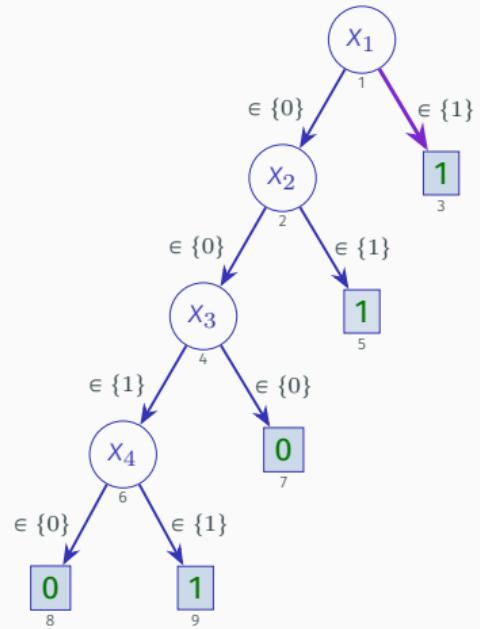
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- **Claim #04:** AXp-necessity of $t \in \mathcal{F}$ is in P if t has a domain size which is polynomially-bounded on instance size
 - **This holds for any classifier!**
 - Let \mathbf{u} be obtained from \mathbf{v} by replacing the constant v_t by some variable $u_t \in \mathcal{D}_t$
 - Feature t is AXp-necessary if $\kappa(\mathbf{u}) \neq \kappa(\mathbf{v})$ for some value $u_t \in \mathcal{D}_t$

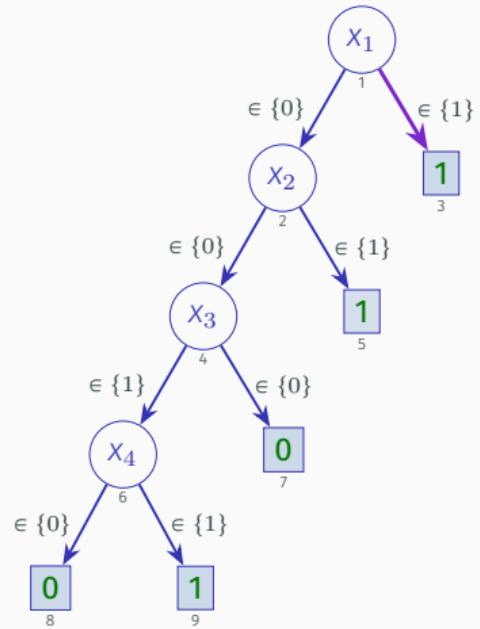
An example

- Instance $(\mathbf{v}, c) = ((0, 0, 0, 0), 0)$



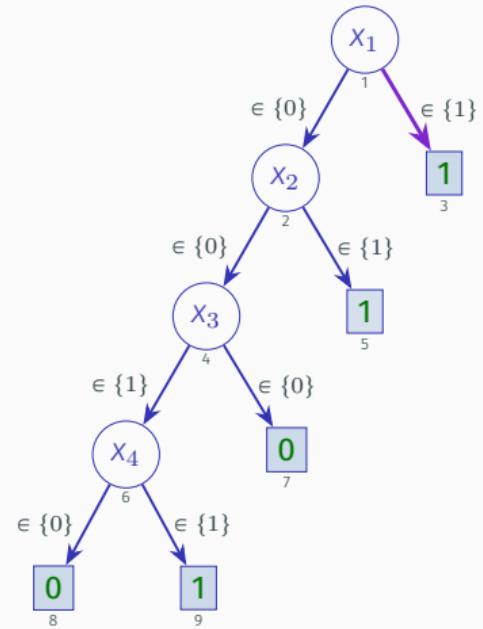
An example

- Instance $(\mathbf{v}, c) = ((0, 0, 0, 0), 0)$
- Is feature 1 AXp-necessary?



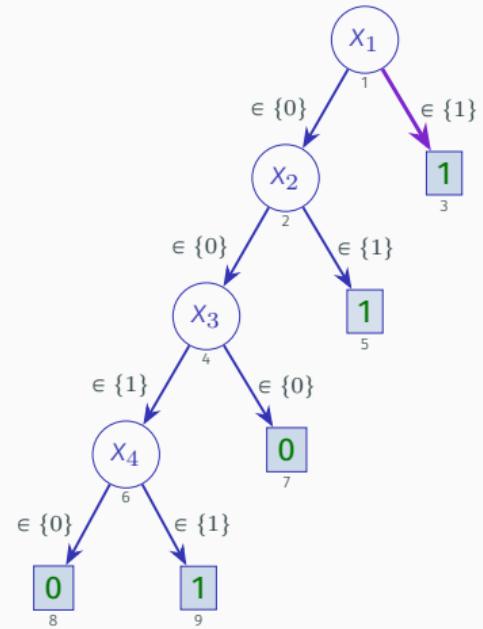
An example

- Instance $(\mathbf{v}, c) = ((0, 0, 0, 0), 0)$
- Is feature 1 AXp-necessary?
 - Does there exist u_1 , such that $\kappa(u_1, 0, 0, 0) \neq \kappa(0, 0, 0, 0)$?



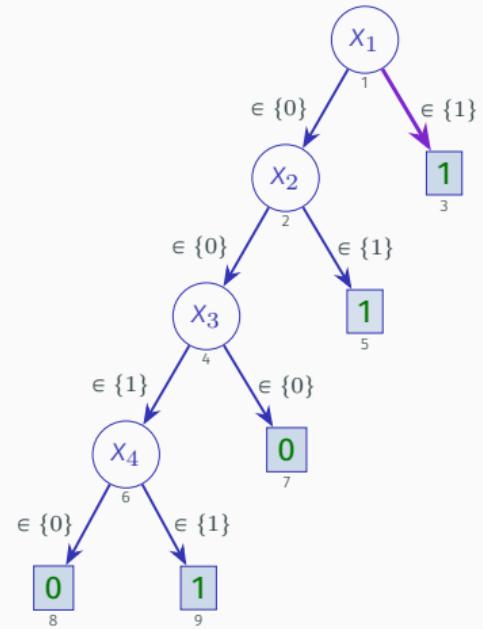
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 - **Yes!** Thus, feature 1 is AXp-necessary



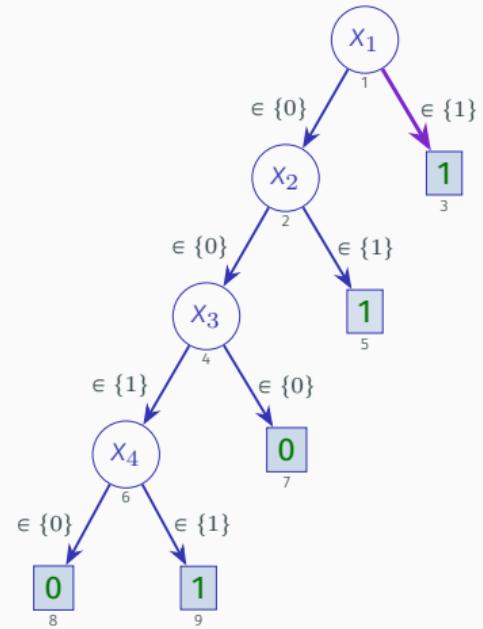
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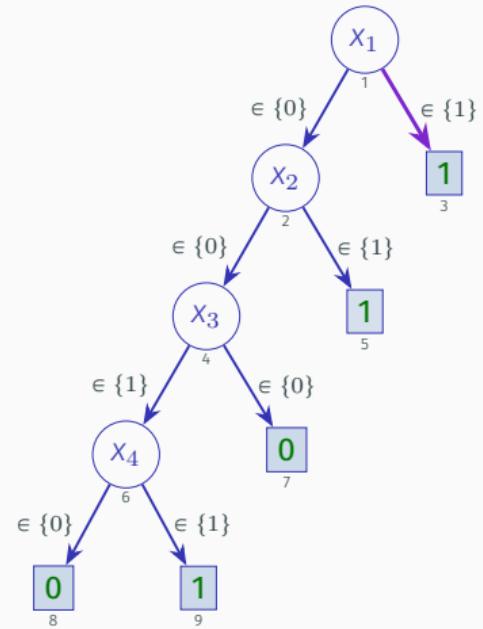
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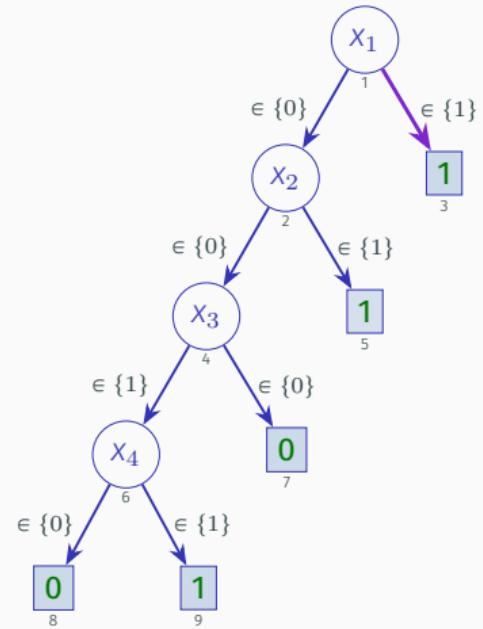
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- Is feature 3 AXp-necessary?
 - Does there exist u_3 , such that $\kappa(0, 0, u_3, 0) \neq \kappa(0, 0, 0, 0)$?
 - **No!** Thus, feature 3 is **not** AXp-necessary



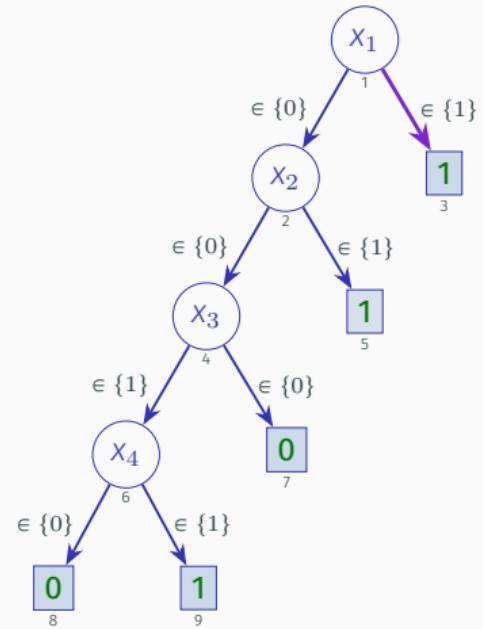
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- Confirmation:
 - CXps:
 - AXps:



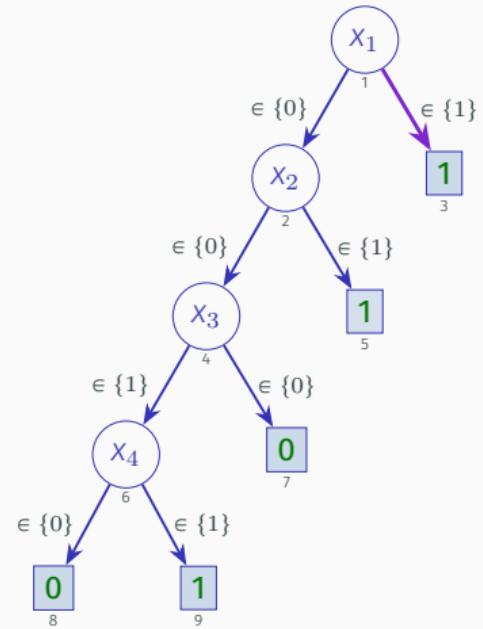
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- A feature $i \in \mathcal{F}$ is **irrelevant** if $i \notin F_{\mathbb{A}}$ (and so, if $i \notin F_{\mathbb{C}}$)
 - A feature is **irrelevant** if it is **not** included in **any** AXp (or CXp)

An example

- Consider the classifier:

$$\kappa(x_1, x_2, x_3, x_4) = \bigvee_{i=1}^4 x_i$$

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- Feature 4 is **relevant**, since it is included in one (and the only) AXp/CXp
- Features 1, 2, 3 are **irrelevant**, since there are not included in any AXp/CXp
- Obs: **irrelevant features are absolutely unimportant!**

We could propose some other explanation by adding features 1, 2 or 3 to AXp $\{4\}$, but prediction would remain unchanged for **any** value assigned to those features

- And we aim for **irreducibility** (**Occam's razor is a mainstay of AI/ML**)

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- General case: best solution is to exploit **abstraction refinement**

Abstraction refinement for feature relevancy

- Claim: $\mathcal{X} \subseteq \mathcal{F}$ and $t \in \mathcal{X}$. If $\text{WAXp}(\mathcal{X})$ holds and $\text{WAXp}(\mathcal{X} \setminus \{t\})$ does not hold, then **any AXp** $\mathcal{Z} \subseteq \mathcal{X} \subseteq \mathcal{F}$ must contain feature t .

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- Repeatedly guess weak WAXp candidates \mathcal{X} , with $t \in \mathcal{X}$ [e.g. use SAT oracle]
- Check that WAXp condition holds for \mathcal{X} : $\text{WAXp}(\mathcal{X})$; and [e.g. use WAXp oracle]

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- Block counterexamples in both cases

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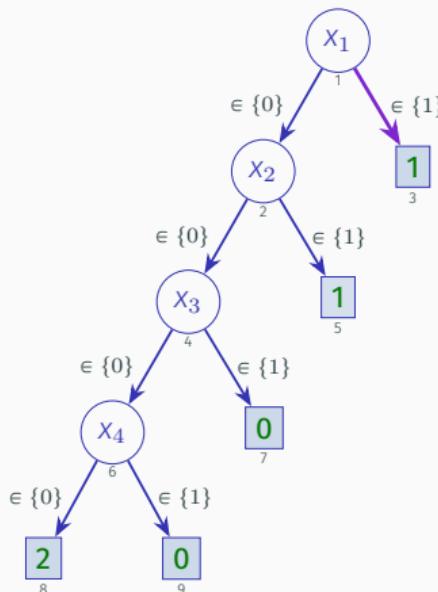
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A general abstraction refinement algorithm

Input: Instance \mathbf{v} , Target Feature t ; Feature Set \mathcal{F} , Classifier κ

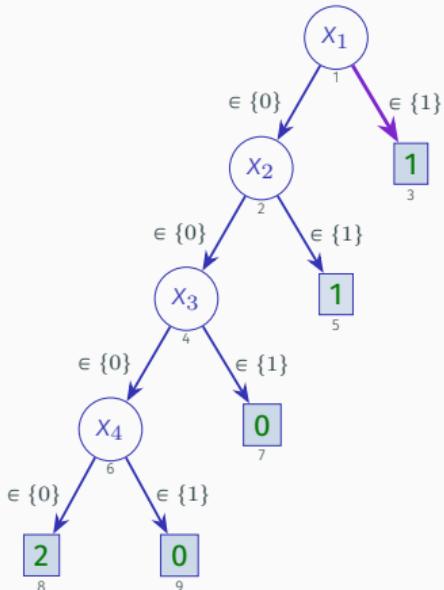
```
1: function FRPCGR( $\mathbf{v}, t; \mathcal{F}, \kappa$ )
2:    $\mathcal{H} \leftarrow \emptyset$                                  $\triangleright \mathcal{H}$  overapproximates the subsets of  $\mathcal{F}$  that do not contain an AXp containing  $t$ 
3:   repeat
4:     ( $\text{outc}, s$ )  $\leftarrow \text{SAT}(\mathcal{H}, s_t)$            $\triangleright$  Use SAT oracle to pick candidate WAXp containing  $t$ 
5:     if  $\text{outc} = \text{true}$  then
6:        $\mathcal{P} \leftarrow \{i \in \mathcal{F} \mid s_i = 1\}$             $\triangleright$  Set  $\mathcal{P}$  is the candidate WAXp, and  $t \in \mathcal{P}$ 
7:        $\mathcal{D} \leftarrow \{i \in \mathcal{F} \mid s_i = 0\}$             $\triangleright$  Set  $\mathcal{D}$  contains the features not included in  $\mathcal{P}$ 
8:       if  $\neg \text{WAXp}(\mathcal{P})$  then                   $\triangleright$  Is  $\mathcal{P}$  not a WAXp?
9:          $\mathcal{H} \leftarrow \mathcal{H} \cup \text{newPosCl}(\mathcal{D}; t, \kappa)$      $\triangleright \mathcal{P}$  is not a WAXp; must pick some non-picked feature
10:        else                                          $\triangleright \mathcal{P}$  is a WAXp
11:          if  $\neg \text{WAXp}(\mathcal{P} \setminus \{t\})$  then       $\triangleright \mathcal{P}$  without  $t$  not a WAXp?
12:            reportWeakAXp( $\mathcal{P}$ )                     $\triangleright$  Feature  $t$  is included in any AXp  $\mathcal{X} \subseteq \mathcal{P}$ 
13:            return true
14:           $\mathcal{H} \leftarrow \mathcal{H} \cup \text{newNegCl}(\mathcal{P}; t, \kappa)$      $\triangleright \text{WAXp}(\mathcal{P} \setminus \{t\})$  holds; some feature in  $\mathcal{P}$  must not be picked
15:        until  $\text{outc} = \text{false}$ 
16:      return false                                      $\triangleright$  If  $\mathcal{H}$  becomes inconsistent, then there is no AXp that contains  $t$ 
```

An example: feature relevancy for DT, using abstraction refinement



- Instance: $(\mathbf{v}, c) = ((1, 1, 1, 1), 1)$
- Is $t = 1$ relevant?

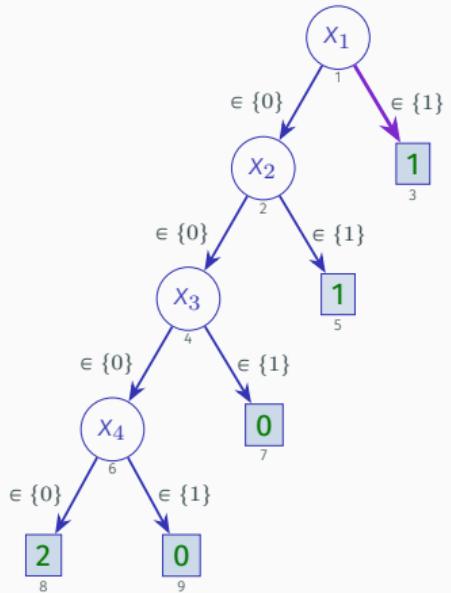
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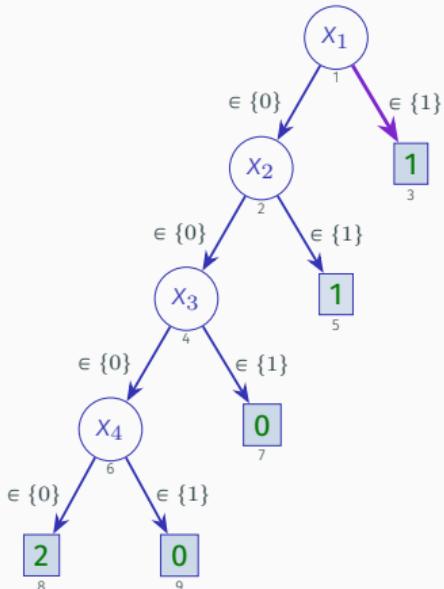
$t = 1$					
s	\mathcal{P}	WAXp(\mathcal{P})	WAXp($\mathcal{P} \setminus \{t\}$)	Return?	Clause
(1, 1, 1, 1)	{1, 2, 3, 4}	✓	✓	—	$(\neg u_2 \vee \neg u_3 \vee \neg u_4)$
(1, 1, 0, 1)	{1, 2, 4}	✓	✓	—	$(\neg u_2 \vee \neg u_4)$
(1, 1, 0, 0)	{1, 2}	✓	✓	—	$(\neg u_2)$
(1, 0, 0, 0)	{1}	✓	✗	true	—

Another example



- Instance: $(\mathbf{v}, c) = ((1, 1, 1, 1), 1)$
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(1, 1, 0, 1)	{1, 2, 4}	✓	✓	—	$(\neg u_1 \vee \neg u_2)$
(1, 0, 0, 1)	{1, 4}	✓	✓	—	$(\neg u_1)$
(0, 1, 0, 1)	{2, 4}	✓	✓	—	$(\neg u_2)$
(0, 0, 0, 1)	{4}	✗	—	—	$(u_1 \vee u_2 \vee u_3)$
(0, 0, 1, 1)	{3, 4}	✗	—	—	$(u_1 \vee u_2)$
[outc = false]	—	—	—	false	—

Questions?

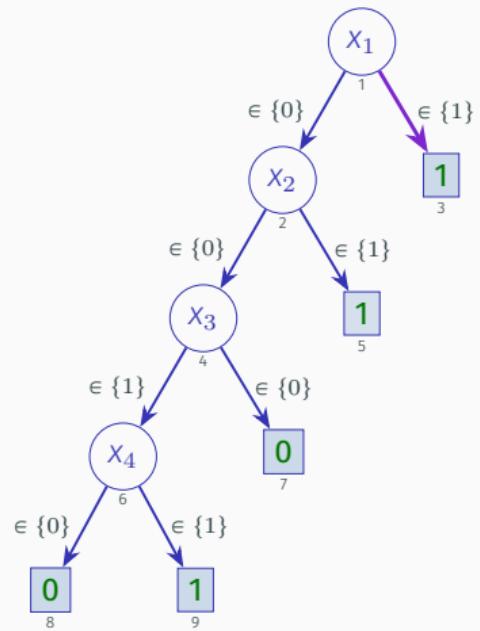
Lecture 04

Recapitulate third lecture

- Logic encoding for explaining DLs
 - And status of (in)tractability in logic-based XAI
- Query: enumeration of explanations
- Query: feature necessity, AXp & CXp
- Query: feature relevancy

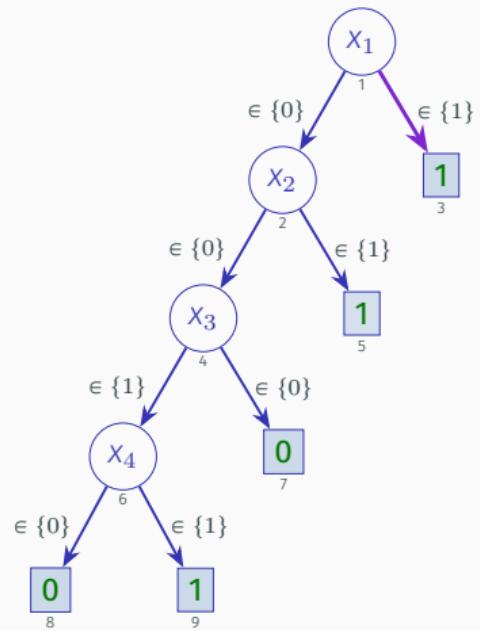
Recap example

- Instance $(\mathbf{v}, c) = ((0, 0, 0, 0), 0)$



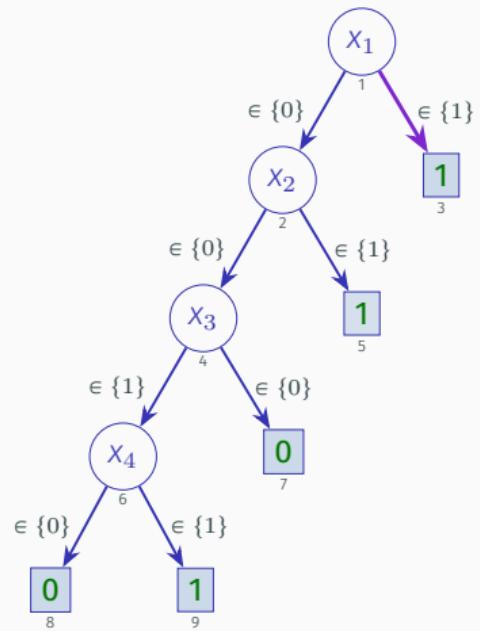
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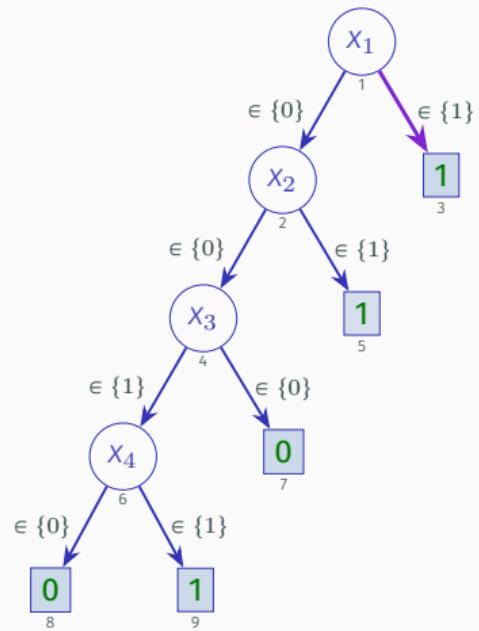
Recap example

- Instance $(\mathbf{v}, c) = ((0, 0, 0, 0), 0)$
- Is feature 1 AXp-necessary?
 - Does there exist u_1 , such that $\kappa(u_1, 0, 0, 0) \neq \kappa(0, 0, 0, 0)$?



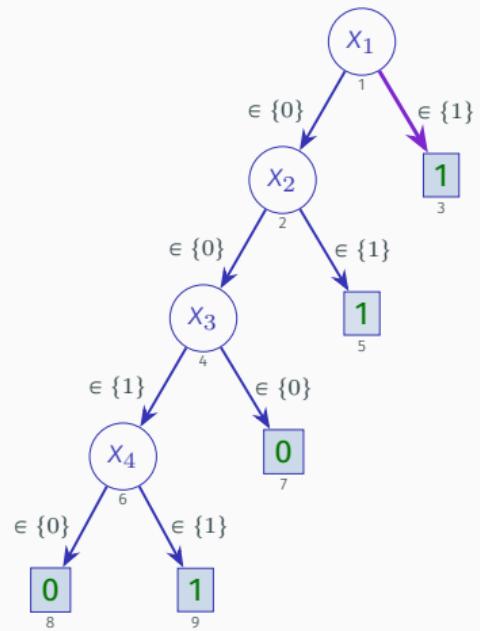
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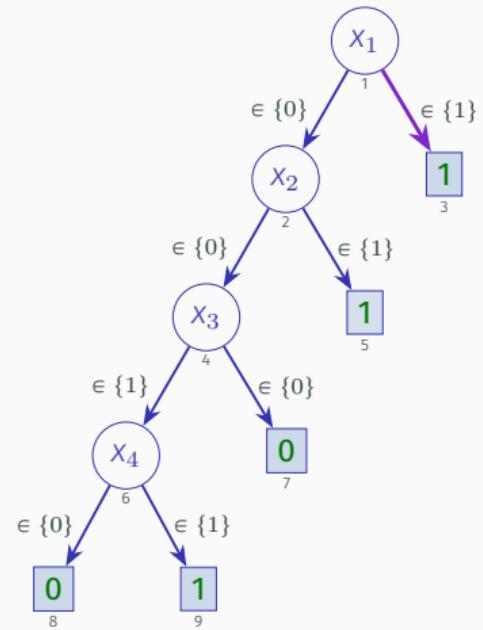
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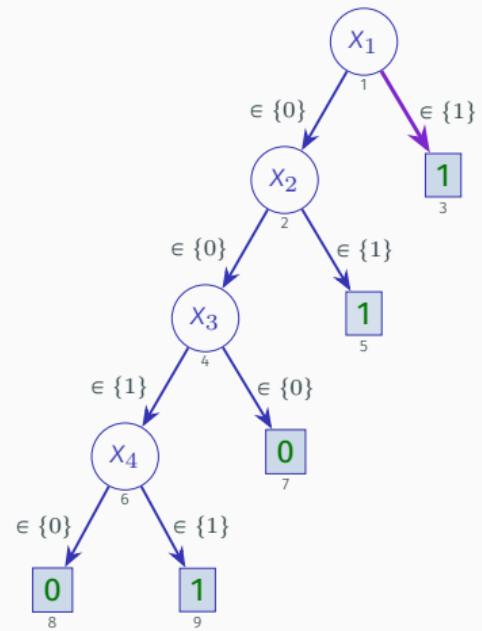
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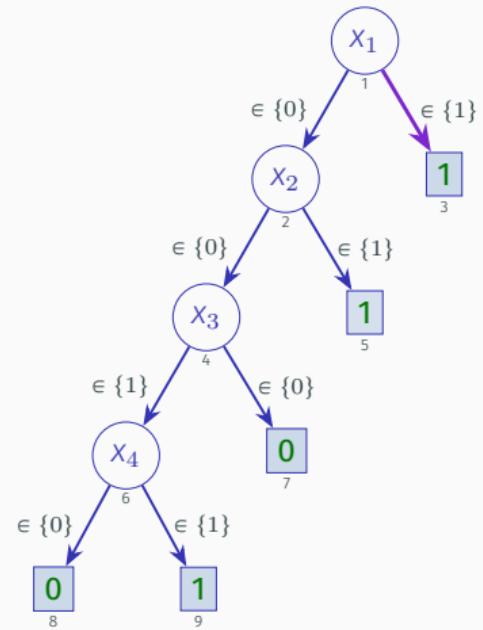
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- Is feature 3 AXp-necessary?
 - Does there exist u_3 , such that $\kappa(0, 0, u_3, 0) \neq \kappa(0, 0, 0, 0)$?
 - No!** Thus, feature 3 is **not** AXp-necessary



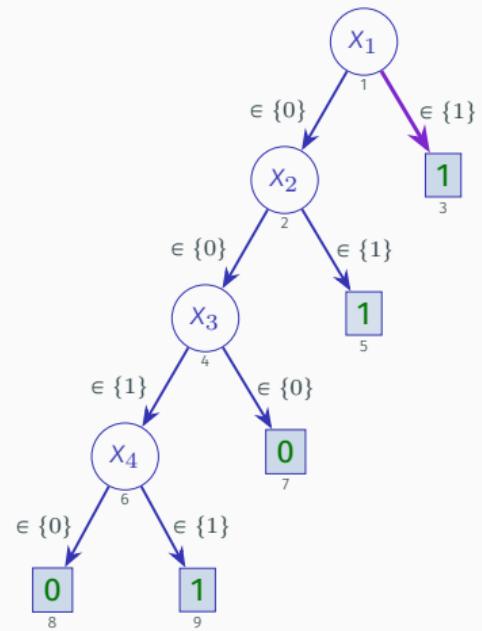
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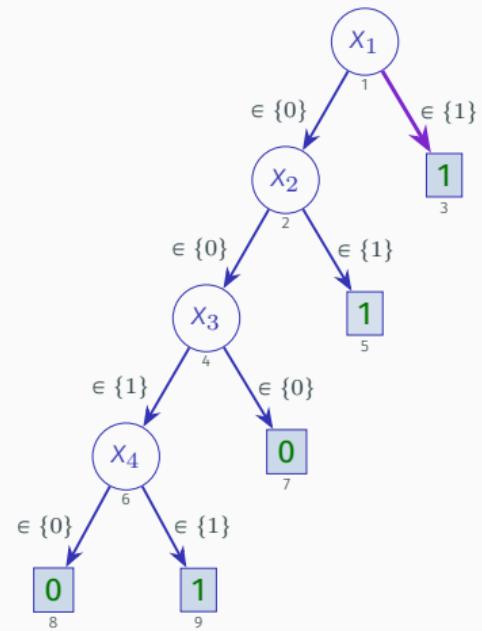
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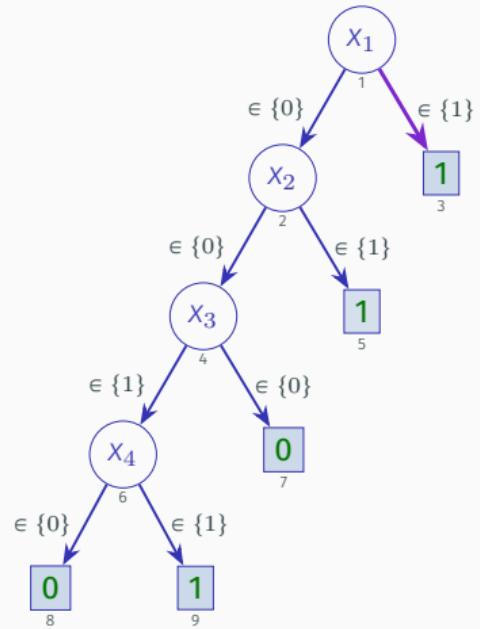
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- Confirmation:
 - CXps: $\{\{1\}, \{2\}, \{3, 4\}\}$ (2 is also AXp-necessary)
 - AXps: $\{\{1, 2, 3\}, \{1, 2, 4\}\}$



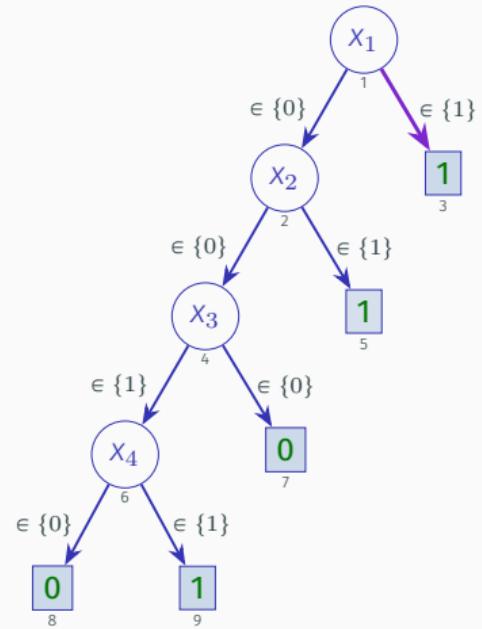
Recap example – a different instance

- Instance $(\mathbf{v}, c) = ((1, 1, 1, 1), 1)$



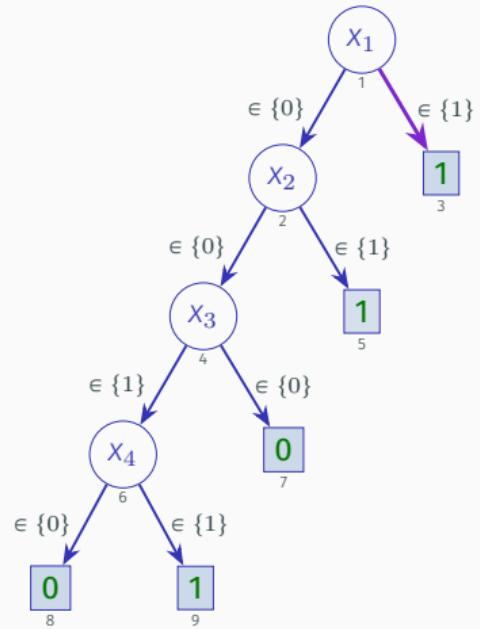
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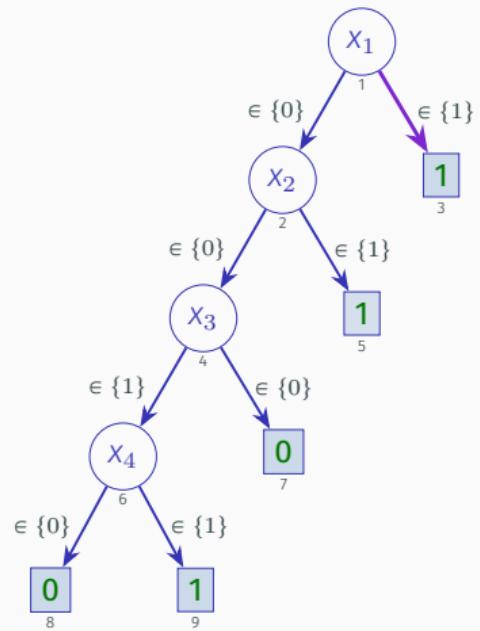
Recap example – a different instance

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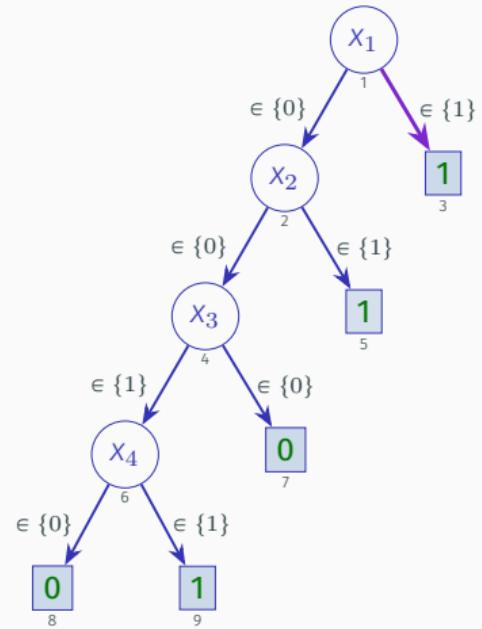
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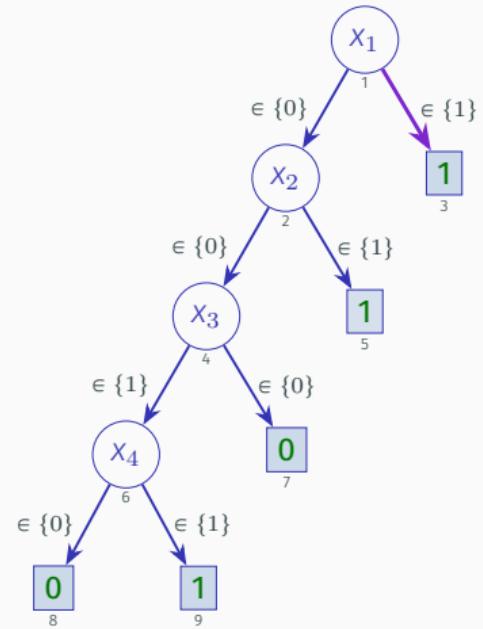
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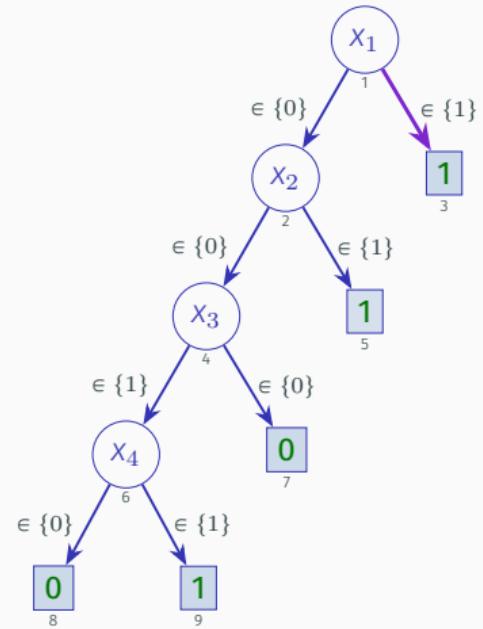
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- Are there CXp-necessary features?
 - **Yes!** Features 1 and 2 (i.e. singleton AXps)
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- Confirmation:
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Another example – feature necessity & relevancy

- Classifier: $\mathcal{F} = \{1, 2, 3, 4, 5\}$; $\mathcal{D}_i = \{0, 1\}, i = 1, \dots, 5$; $\mathcal{K} = \{0, 1\}$

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- Partially enumerate AXps/CXps, exploiting bias in enumeration

Plan for this course

- Lecture 01 – unit(s):
 - #01: Foundations
- Lecture 02 – unit(s):
 - #02: Principles of symbolic XAI – feature selection
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 – unit(s):
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 – unit(s):
 - #06: Recent, emerging & advanced topics
- Lecture 05 – unit(s):
 - #07: Principles of symbolic XAI – feature attribution (& myth of Shapley values in XAI)
 - #08: Corrected feature attribution – nuSHAP
 - #09: Conclusions & research directions

Detour: Monotonic Classification & Voting Power

Monotonically increasing boolean classifiers

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- Monotonic classifier $\mathcal{M} = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$, such that each $\mathcal{D}_i = \{0, 1\}$ and $\mathcal{K} = \{0, 1\}$ are ordered (i.e. $0 < 1$), and
 - $\kappa(\mathbf{1}) = 1$;
 - Non-constant classifier, i.e. $\kappa(\mathbf{0}) = 0$; and
 - $\kappa(\mathbf{x}_1) \leq \kappa(\mathbf{x}_2)$ when $\mathbf{x}_1 \leq \mathbf{x}_2$

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Define the explanation problems:
 - $\mathcal{E}_1 = (\mathcal{M}, (\mathbf{v}_1, 1))$
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- Then,
 - If WAXp($\mathcal{S}; \mathcal{E}_1$) holds, then WAXp($\mathcal{S}; \mathcal{E}_2$) holds; in particular:
 - $\mathbb{A}(\mathcal{E}_{\mathbf{1}})$ contains all the AXps of any instance of the form $(\mathbf{v}_r, 1)$
 - Why?
 - Pick any explanation problem \mathcal{E}_r with instance $(\mathbf{v}_r, 1)$
 - Start from $\mathbf{1} = (1, 1, \dots, 1)$
 - Remove features that take value 0 in \mathbf{v}_r ; we still have an WAXp
 - Then compute any AXp starting from features taking value 1 in \mathbf{v}_r
 - ∴ Suffices to find explanations for $\mathcal{E}_{\mathbf{1}}$ (or alternatively, the global explanations for prediction 1)

An example

- ML model $\mathcal{M} = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$:
 - Boolean classifier: $\mathcal{K} = \{0, 1\}$
 - Defined on 6 boolean features: $\mathcal{F} = \{1, 2, 3, 4, 5, 6\}$
 - I.e. $\mathcal{D}_i = \{0, 1\}, i = 1, \dots, 6$
 - With classification function:

$$\kappa(x_1, x_2, x_3, x_4, x_5, x_6) := \begin{cases} 1 & \text{IF } (4x_1 + 4x_2 + 4x_3 + 2x_4 + 2x_5 + x_6 \geq 12) \\ 0 & \text{otherwise} \end{cases}$$

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 - Feature 2: can no longer be dropped; keep

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 - Problem: find a measure of importance of each voter !
 - I.e. measure the **a priori voting power** of each voter

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Country	Acronym	# Votes
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- Perhaps surprisingly, answer is **No!**
 - In 1958, Luxembourg was a **dummy** voter/player

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which we have seen before! E.g. $\{2, 3, 4, 5\}$ is an AXp & feature 6 (L) is **irrelevant**

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[MSH24, HMS24, HM23c]

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- Homework:

- Create your own weighted voting games;
- Compute the sets of AXps and CXps; and
- Assess the importance of features and how they compare to each other

Unit #06

Advanced Topics

Outline – Unit #06

Sample-Based Explanations

Changing Assumptions (in Plain Logic-Based XAI)

Inflated Explanations

Constrained Explanations

Distance-Restricted Explanations

Probabilistic Explanations

Additional Topics

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 - From which ML models are learned!
 - Here is an idea:
 - Adopt **symbolic** (and so, rigorous) sample-based XAI

[Amg23, CA23, ACD24]

An example...

Sample:

x_1	x_2	x_3	x_4	$\kappa(\cdot)$
0	0	0	0	0
0	0	1	0	0
0	0	1	1	0
0	1	1	0	0
1	0	0	0	1
1	1	0	0	1
1	1	1	1	1

Instance: $((1, 1, 1, 1), 1)$

An example...

Sample:

x_1	x_2	x_3	x_4	$\kappa(\cdot)$
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0	0	1	0	0
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- How to explain prediction given only the sample

Instance: $((1, 1, 1, 1), 1)$

An example...

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Instance: $((1, 1, 1, 1), 1)$

- How to explain prediction given only the sample
- If $x_1 = 1$, then prediction is 1 (given the sample)

An example...

Sample:

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Instance: $((1, 1, 1, 1), 1)$

- How to explain prediction given only the sample
- If $x_1 = 1$, then prediction is 1 (given the sample)
- Sample-based AXp (sbAXp): $\{1\}$

Definitions in sample-based XAI – replace feature space with sample...

[MSLLM25]

- Let $\mathbb{S} \subseteq \mathbb{F}$ denote a **sample**, and let instance be (\mathbf{v}, c)
- Then, for $\mathcal{X} \subseteq \mathcal{F}$,

$$\text{sbWAXp}(\mathcal{X}) \coloneqq \forall (\mathbf{x} \in \mathbb{S}). \left(\bigwedge_{i \in \mathcal{X}} x_i = v_i \right) \rightarrow (\kappa(\mathbf{x}) = c)$$

- And, for $\mathcal{Y} \subseteq \mathcal{F}$,

$$\text{sbWCXp}(\mathcal{Y}) \coloneqq \exists (\mathbf{x} \in \mathbb{S}). \left(\bigwedge_{i \in \mathcal{F} \setminus \mathcal{Y}} x_i = v_i \right) \wedge (\kappa(\mathbf{x}) \neq c)$$

- sbAXps (resp. sbCXps) are the subset-minimal sets that respect the above definition for sbWAXp (resp. sbWCXp)

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- sbAXps (resp. sbCXps) are the subset-minimal sets that respect the above definition for sbWAXp (resp. sbWCXp)
 - Rigorous alternative to Anchor & variants

Approach for computing sbCXps & sbAXps

Sample:

x_1	x_2	x_3	x_4	$\kappa(\cdot)$
0	0	0	0	0
0	0	1	0	0
0	0	1	1	0
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Points \mathbf{x} w/ $\kappa(\mathbf{x}) \neq c$:

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$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

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- Set of sbCXps: $\mathbb{C} = \{\{1, 2\}, \{1, 4\}\}$

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- Set of sbCXps: $\mathbb{C} = \{\{1, 2\}, \{1, 4\}\}$
- Set of sbAXps (by MHS duality): $\mathbb{A} = \{\{1\}, \{2, 4\}\}$

- MHS duality holds for sample-based explanations:
 - $\mathcal{Y} \subseteq \mathcal{F}$ is sbCXp iff it is a MHS of set of sbAXps
 - $\mathcal{X} \subseteq \mathcal{F}$ is sbAXp iff it is a MHS of set of sbCXps
- Number of sb(W)CXps is linear on $|\mathbb{S}|$
- Number of sb(W)AXps can be exponentially large on $|\mathbb{S}|$
- Additional results:

Problem	Complexity	
	Total	Given sbCXps
All sbCXps	$\mathcal{O}(mn^2)$	—
One sbCXp	$\mathcal{O}(mn)$	$\mathcal{O}(1)$
One (smallest) sbCXp	$\mathcal{O}(mn^2)$	$\mathcal{O}(n)$
One sbAXp	$\mathcal{O}(mn)$	$\mathcal{O}(mn)$
Feature relevancy	$\mathcal{O}(mn^2)$	$\mathcal{O}(n)$
sbAXp-necessity	$\mathcal{O}(mn^2)$	$\mathcal{O}(mn)$
sbCXp-necessity	$\mathcal{O}(mn^2)$	$\mathcal{O}(n)$

- Complexity-wise:
 - Deciding the existence of an sbAXp of size no larger than k is NP-complete.
 - sbAXp enumeration corresponds to hypergraph transversal

Does sample-based XAI suffice?

- Sample-based explanations lack **coherency**:
 - There exist two instances with different predictions with AXps that cover at least one common point

[ACD24]

Does sample-based XAI suffice?

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[ACD24]

- An example:

- Sample:

Entry	x_1	x_2	$\kappa(\cdot)$
1	0	1	0
2	1	0	1
3	0	0	2

- Instance 1: $((0, 1), 0)$
 - Instance 2: $((1, 0), 1)$

$\text{AXp}(s)$ for $((0, 1), 0)$

Sample:

x_1	x_2	$\kappa(\cdot)$
0	1	0
1	0	1
0	0	2

Instance: $((0, 1), 0)$

$\text{AXp}(s)$ for $((0, 1), 0)$

Sample:

x_1	x_2	$\kappa(\cdot)$
0	1	0
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Points \mathbf{x} w/ $\kappa(\mathbf{x}) \neq c$:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

Instance: $((0, 1), 0)$

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- Set of sbCXps: $\mathbb{C} = \{\{2\}\}$
- Set of sbAXps (by MHS duality): $\mathbb{A} = \{\{2\}\}$
 - Meaning: IF $(x_2 = 1)$ THEN $\kappa(\mathbf{x}) = 0$

$\text{AXp}(s)$ for $((1, 0), 1)$

Sample:

x_1	x_2	$\kappa(\cdot)$
0	1	0
1	0	1
0	0	2

Instance: $((1, 0), 1)$

$\text{AXp}(s)$ for $((1, 0), 1)$

Sample:

x_1	x_2	$\kappa(\cdot)$
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 - Meaning: IF $(x_1 = 1)$ THEN $\kappa(\mathbf{x}) = 1$

The problem of lack of coherency

- Instance $((0, 1), 0)$ with $\text{AXp } \{2\}$, for $x_2 = 1$:
 - Points consistent with AXp : $\{(0, 1), (1, 1)\}$
 - I.e. prediction is 0 for the points $\{(0, 1), (1, 1)\}$

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- Instance $((0, 1), 0)$ with $\text{AXp } \{2\}$, for $x_2 = 1$:
 - Points consistent with AXp : $\{(0, 1), (1, 1)\}$
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- Instance $((1, 0), 1)$ with $\text{AXp } \{1\}$, for $x_1 = 1$:
 - Points consistent with AXp : $\{(1, 0), (1, 1)\}$
 - I.e. prediction is 1 for the points $\{(1, 0), (1, 1)\}$

The problem of lack of coherency

- Instance $((0, 1), 0)$ with $\text{AXp } \{2\}$, for $x_2 = 1$:
 - Points consistent with AXp : $\{(0, 1), (1, 1)\}$
 - I.e. prediction is 0 for the points $\{(0, 1), (\textcolor{red}{1}, \textcolor{red}{1})\}$
 - Instance $((1, 0), 1)$ with $\text{AXp } \{1\}$, for $x_1 = 1$:
 - Points consistent with AXp : $\{(1, 0), (1, 1)\}$
 - I.e. prediction is 1 for the points $\{(1, 0), (\textcolor{red}{1}, \textcolor{red}{1})\}$
- $\therefore (1, 1)$ assumed to have different predictions!

The problem of lack of coherency

- Instance $((0, 1), 0)$ with $\text{AXp } \{2\}$, for $x_2 = 1$:
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- $\therefore (1, 1)$ assumed to have different predictions!
- Open topic of research...

Outline – Unit #06

Sample-Based Explanations

Changing Assumptions (in Plain Logic-Based XAI)

Inflated Explanations

Constrained Explanations

Distance-Restricted Explanations

Probabilistic Explanations

Additional Topics

General definition of prediction sufficiency

- Instance (\mathbf{v}, c)
- Let $\mathcal{S} \subseteq \mathcal{F}$:
 - Recall,

$$\Upsilon(\mathcal{S}; \mathbf{v}) = \{\mathbf{x} \in \mathbb{F} \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}\}$$

- $\mathcal{S} \subseteq \mathcal{F}$ suffices for prediction c if:

$$\forall (\mathbf{x} \in \mathbb{F}). (\mathbf{x} \in \Upsilon(\mathcal{S}; \mathbf{v})) \rightarrow (\sigma(\mathbf{x}))$$

- **Obs:** a WAXp is just one possible example
- But there are other ways to study prediction sufficiency:
 - One can envision defining other sets of points Γ , parameterized by $\mathcal{E} = (\mathcal{M}, (\mathbf{v}, c))$;
 $\mathcal{S} \subseteq \mathcal{F}$ suffices for prediction c if:

$$\forall (\mathbf{x} \in \mathbb{F}). (\mathbf{x} \in \Gamma(\mathcal{S}; \mathcal{E})) \rightarrow (\sigma(\mathbf{x}))$$

- And one can also envision generalizations of σ !

Outline – Unit #06

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Constrained Explanations

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Probabilistic Explanations

Additional Topics

Towards more expressive explanations – inflated explanations

[IISM24]

- Recall:

$$\text{WAXp}(\mathcal{X}) \quad := \quad \forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (x_j = v_j) \rightarrow (\kappa(\mathbf{x}) = c)$$

- For non-boolean features, use of $=$ may convey little information, e.g. with real-valued features, having $x_1 = 1.157$ does not help in understanding what values of feature 1 are also acceptable

Towards more expressive explanations – inflated explanations

[IISM24]

- Recall:

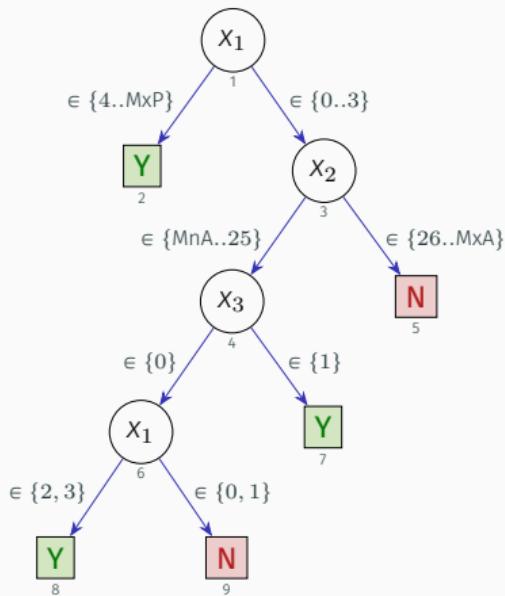
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- For non-boolean features, use of $=$ may convey little information, e.g. with real-valued features, having $x_1 = 1.157$ does not help in understanding what values of feature 1 are also acceptable
- **Inflated explanations** allow for more expressive literals, i.e. $=$ replaced with \in , and individual values replaced by ranges of values
 - Operational definition: Given an AXp, expand set of values of each feature, in some chosen order, such that the set of picked features remains unchanged

Inflated explanations – an example

[IIM22]

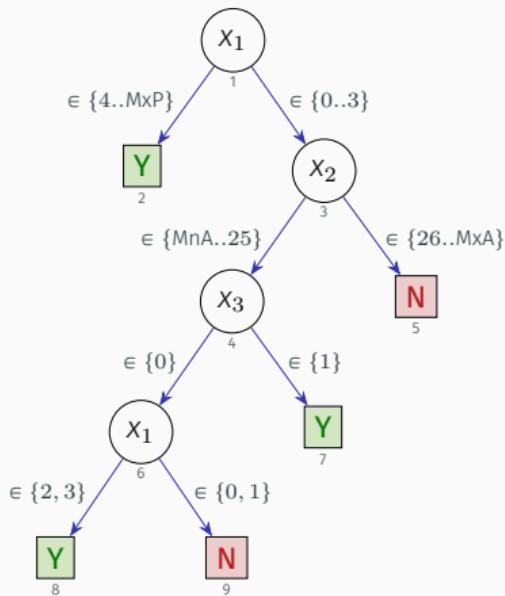
- Explanation for $((2, 20, 0), Y)?$ (Obs: MnA = 18; MxP > 4)



Inflated explanations – an example

[IIM22]

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 - AXp: {1, 2}



Inflated explanations – an example

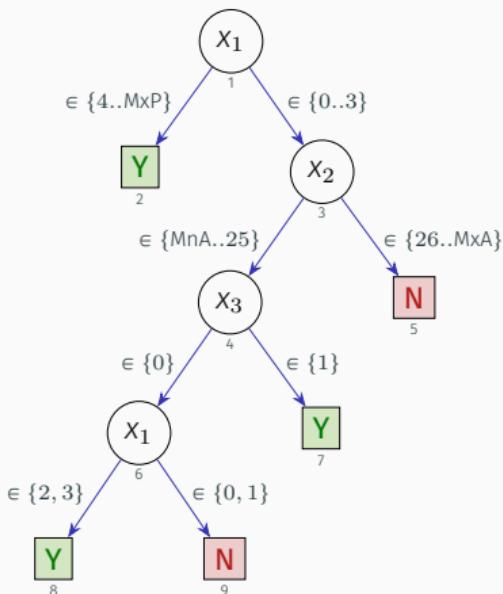
[IIM22]

- Explanation for $((2, 20, 0), Y)$? (Obs: MnA = 18; MxP > 4)

- AXp: {1, 2}

- Default interpretation:

$$\forall (\mathbf{x} \in \mathbb{F}).(x_1 = 2 \wedge x_2 = 20) \rightarrow (\kappa(\mathbf{x}) = Y)$$



Inflated explanations – an example

[IIM22]

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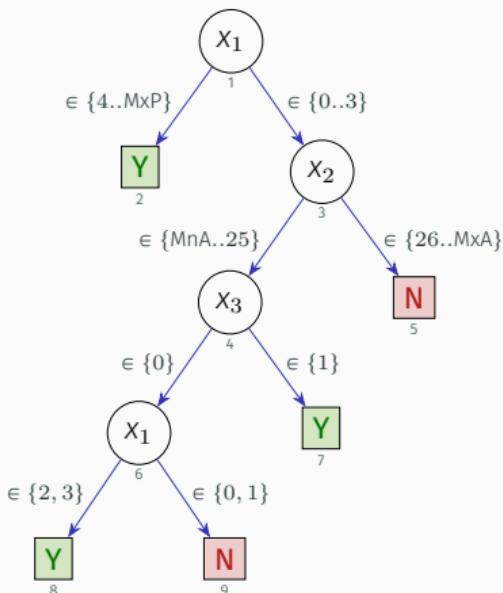
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- Corresponding rule:

$$\text{IF } (x_1 = 2 \wedge x_2 = 20) \text{ THEN } (\kappa(\mathbf{x}) = Y)$$



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[IIM22]

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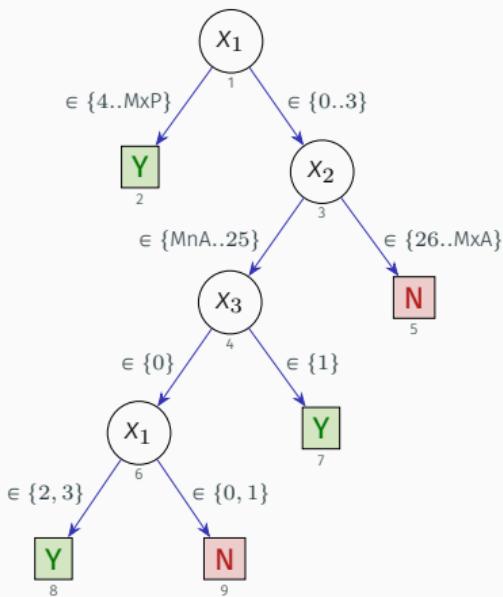
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- Corresponding rule:

$$\text{IF } (x_1 = 2 \wedge x_2 = 20) \text{ THEN } (\kappa(\mathbf{x}) = Y)$$

- With inflated explanations:

$$\forall (\mathbf{x} \in \mathbb{F}).(x_1 \in \{2..MxP\} \wedge x_2 \in \{MnA..25\}) \rightarrow (\kappa(\mathbf{x}) = Y)$$



Inflated explanations – an example

[IIM22]

- Explanation for $((2, 20, 0), Y)$? (Obs: $MnA = 18; MxP > 4$)

- A Xp : {1, 2}

- Default interpretation:

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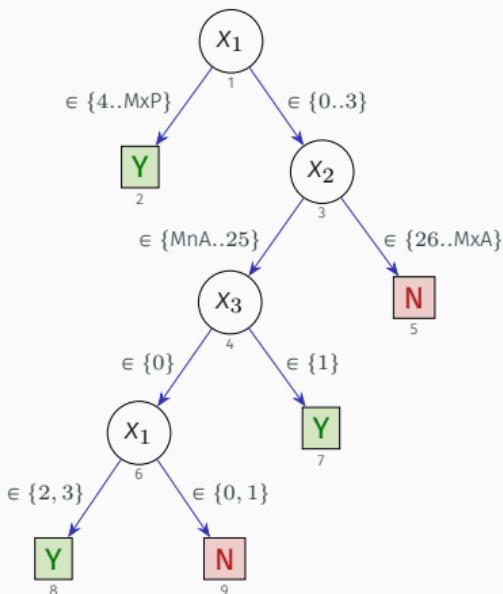
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- With inflated explanations:

$$\forall (\mathbf{x} \in \mathbb{F}).(x_1 \in \{2..MxP\} \wedge x_2 \in \{MnA..25\}) \rightarrow (\kappa(\mathbf{x}) = Y)$$

- Corresponding rule:

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Approach

- Compute Ax
- For each feature:
 - Categorical: iteratively add elements to literal
 - Ordinal:
 - Expand literal for larger values;
 - Expand literal for smaller values

Approach

- Compute $\text{AXp } \mathcal{X}$
- For each feature:
 - Categorical: iteratively add elements to literal
 - Ordinal:
 - Expand literal for larger values;
 - Expand literal for smaller values
- **Obs:** More complex alternative is to find AXp and expand domains simultaneously
 - This is conjectured to change the complexity class of finding one explanation

Another fun example (from 2019) – (inflated) AXp?

[CdPA⁺19]

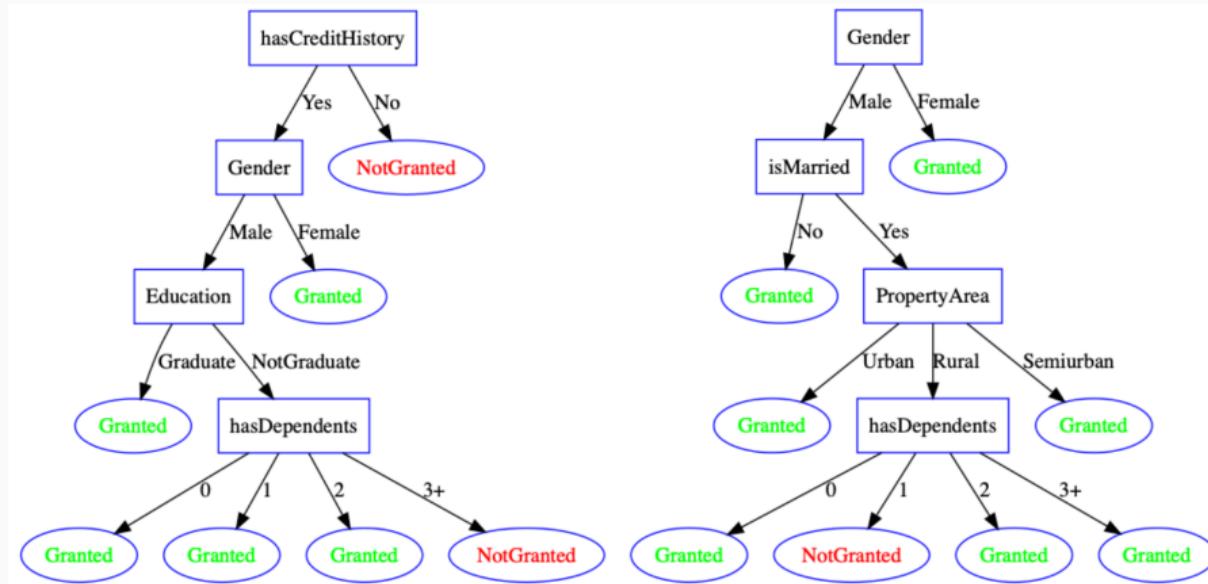


Fig. 2: Decision trees of size ‘small’ in the loan domain, extracted without (left) and with (right) a domain ontology. As it can be seen the features used in the creation of the conditions in the split nodes are different.

Instance: `Gender=Male, Education=NotGraduate, hasCreditHistory=Yes, isMarried=Yes, PropertyArea=Rural, isSelfEmployed>No, hasDependents=2`

Another fun example (now from 2020/21) – (inflated) AXp?

[CWBdPM21]

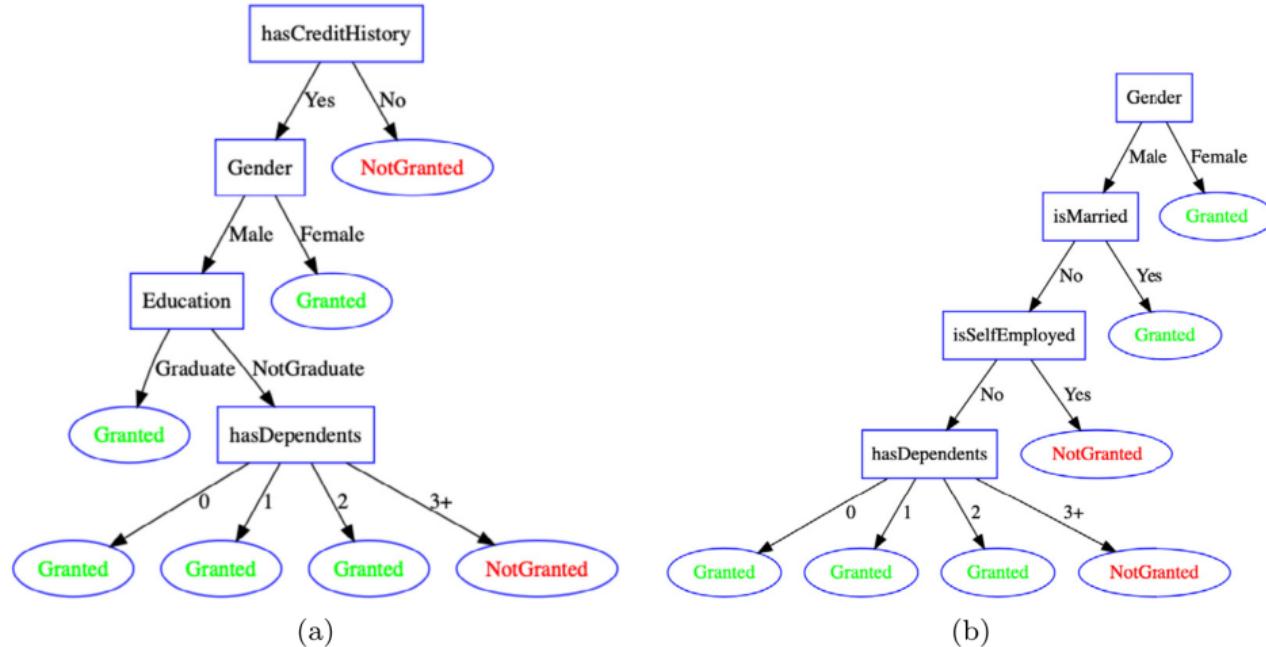


Fig. 2. Decision trees of size ‘small’ in the loan domain, extracted without (a) and with (b) a domain ontology. It can be seen that the use of an ontology leads to different features appearing in the split nodes. For instance, in the ontology used to build tree (b) the concept `Gender` is more abstract than `isMarried` and `isSelfEmployed` has thus a lower information content according to Definition 3.1. Concepts with lower information content are favoured as conditions for split nodes in the tree according to Definition 3.2, which leads to `Gender` being used first by TREPAN-Reloaded when it generated the split nodes of tree (b). Furthermore, the ontology does not include concepts associated to `hasCreditHistory` and `Education`, which are therefore not considered in the construction of tree (b).

Outline – Unit #06

Sample-Based Explanations

Changing Assumptions (in Plain Logic-Based XAI)

Inflated Explanations

Constrained Explanations

Distance-Restricted Explanations

Probabilistic Explanations

Additional Topics

Not all inputs may be possible – input constraints

[GR22, YIS⁺23]

- The (implicit) assumption that all inputs are possible is often unrealistic
 - I.e. it may be impossible for some points in feature space to be observed

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 - Learn simple rules relating inputs
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$$\forall (\mathbf{x} \in \mathbb{F}). \left[\bigwedge_{j \in \mathcal{X}} (x_j = v_j) \wedge \mathcal{C}(\mathbf{x}) \right] \rightarrow (\kappa(\mathbf{x}) = c)$$

$$\exists (\mathbf{x} \in \mathbb{F}). \left[\bigwedge_{j \in \mathcal{X}} (x_j = v_j) \wedge \mathcal{C}(\mathbf{x}) \right] \wedge (\kappa(\mathbf{x}) \neq c)$$

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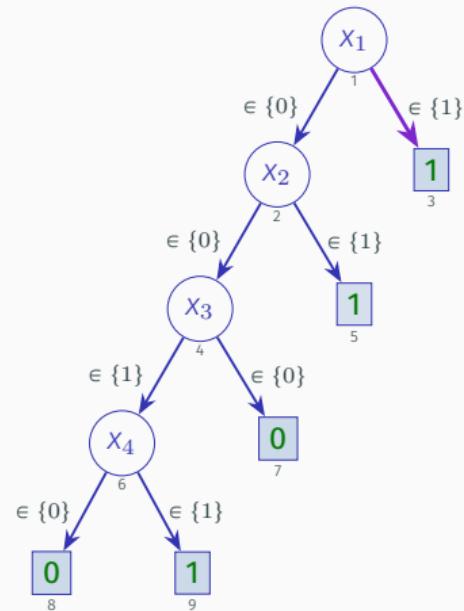
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- Compute AXps/CXps given new definitions
- Constrained AXps/CXps find other applications!

An example

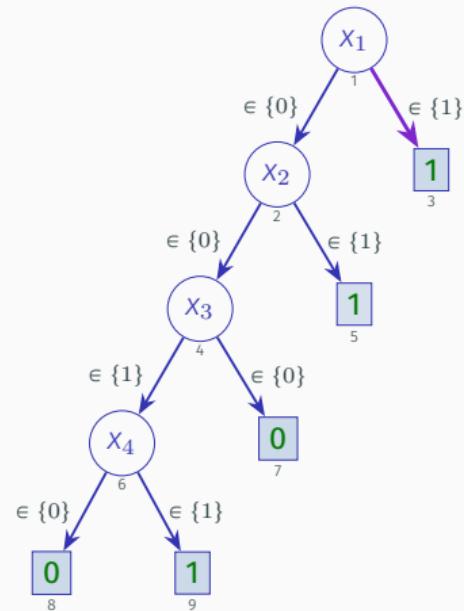
- Instance: $((1, 1, 1, 1), 1)$
- Unconstrained AXps:



- Constraint: $\{(x_3 \rightarrow x_4), (x_4 \rightarrow x_3)\}$

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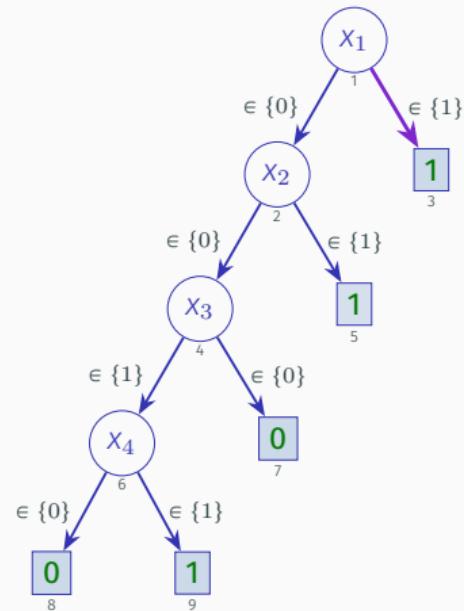
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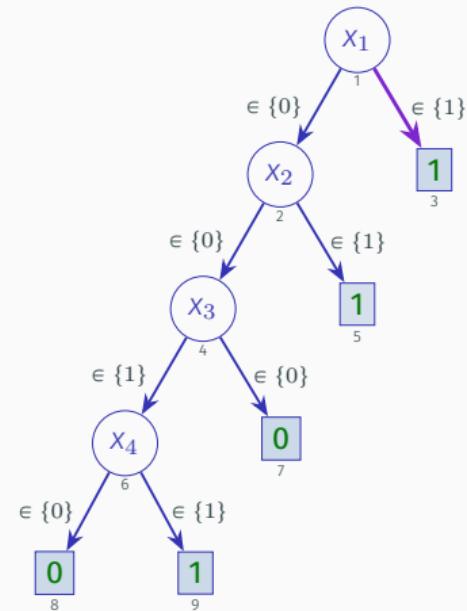
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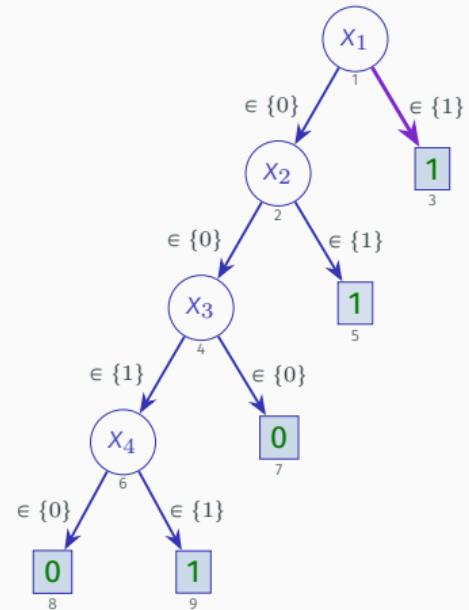
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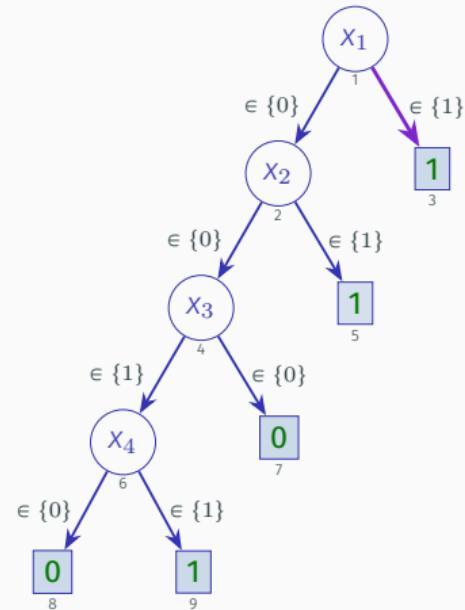
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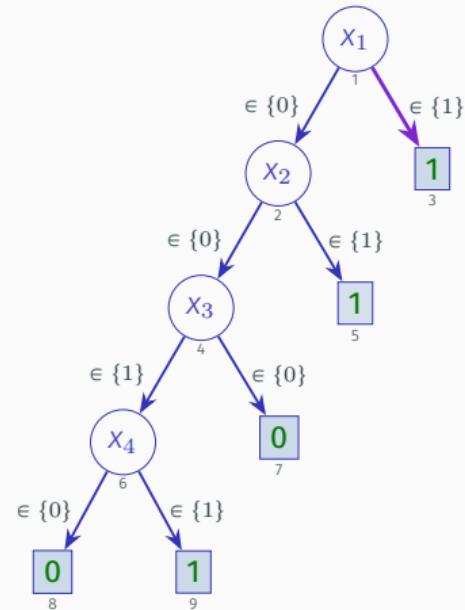
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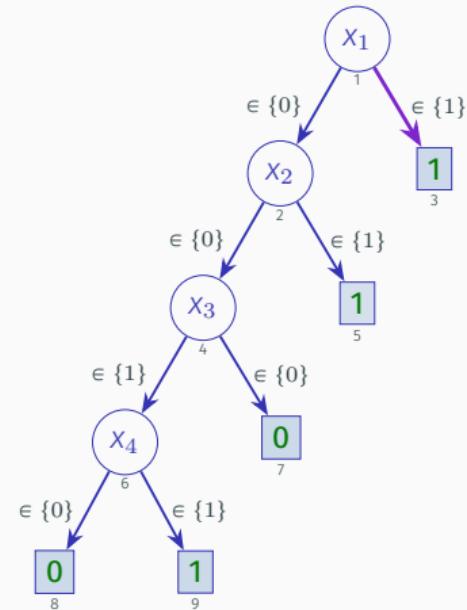
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How to tackle poor performance on NNs?

- For NNs, computation of plain AXps scales to a few tens of neurons

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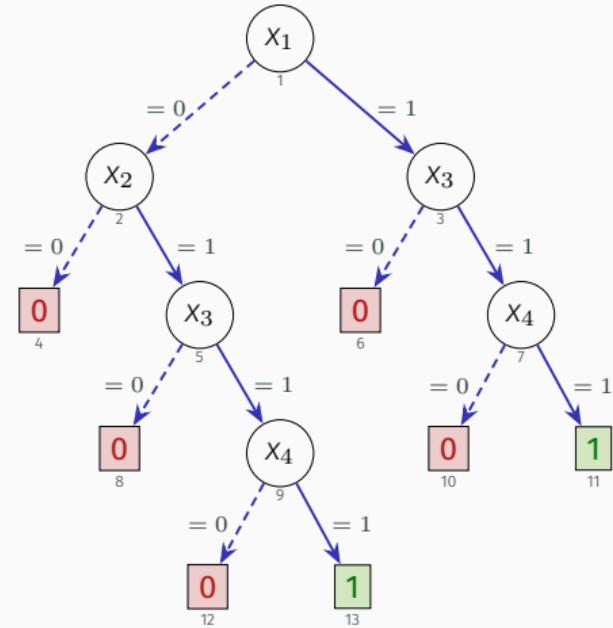
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- Change definition of WAXp/WCXp to account for l_p distance to \mathbf{v} :

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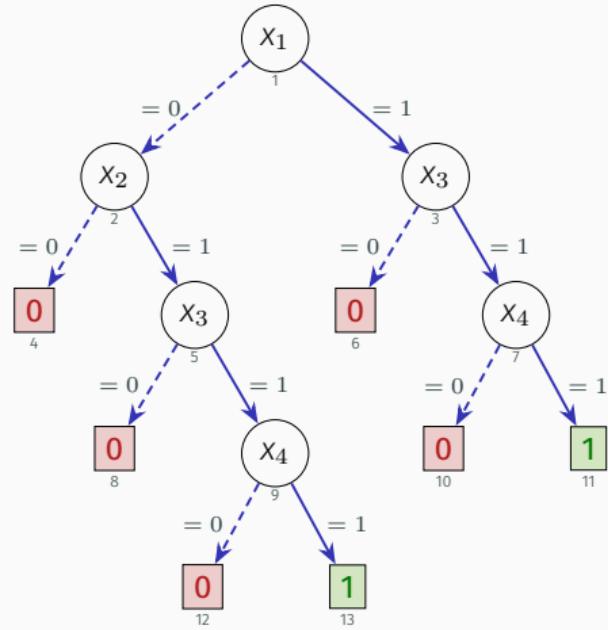
- Norm l_p is arbitrary, e.g. Hamming, Manhattan, Euclidean, etc.
- **Distance-restricted explanations:** $\partial \text{AXp} / \partial \text{CXp}$

An example – DT & instance $((1, 1, 1, 1), 1)$



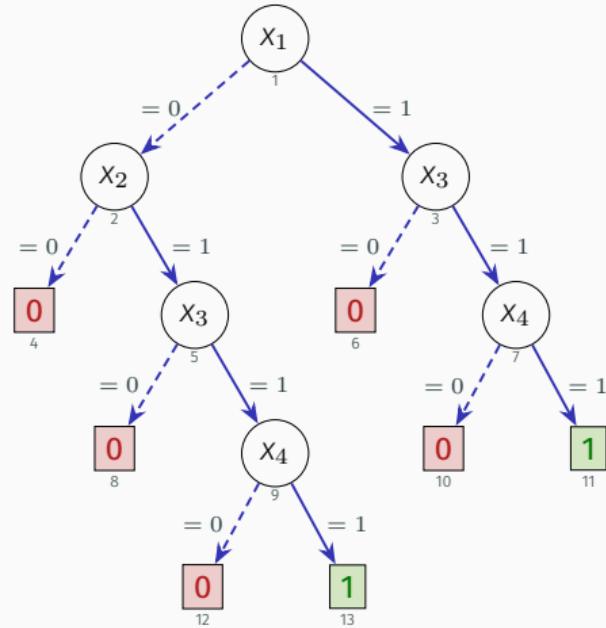
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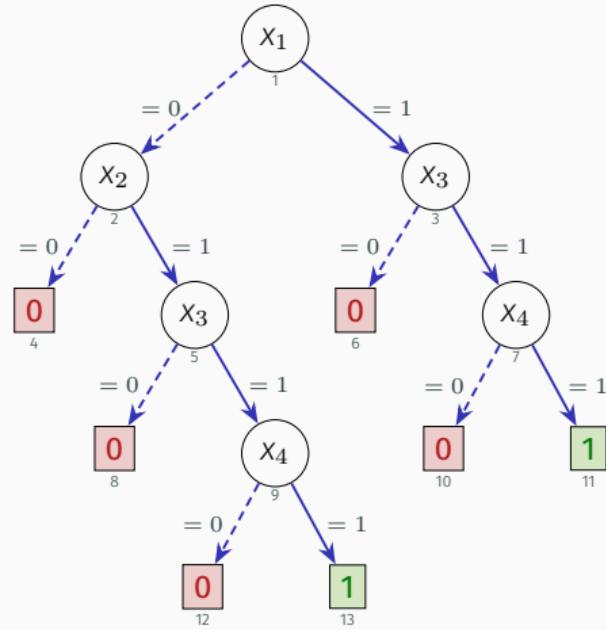
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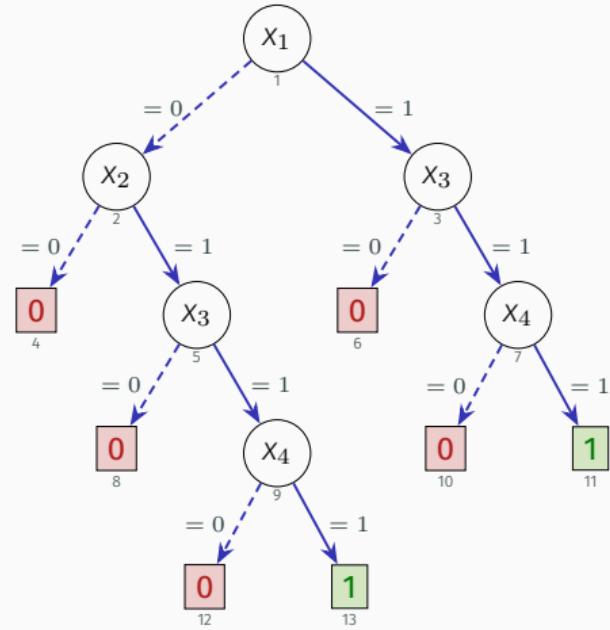
- AXps? $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
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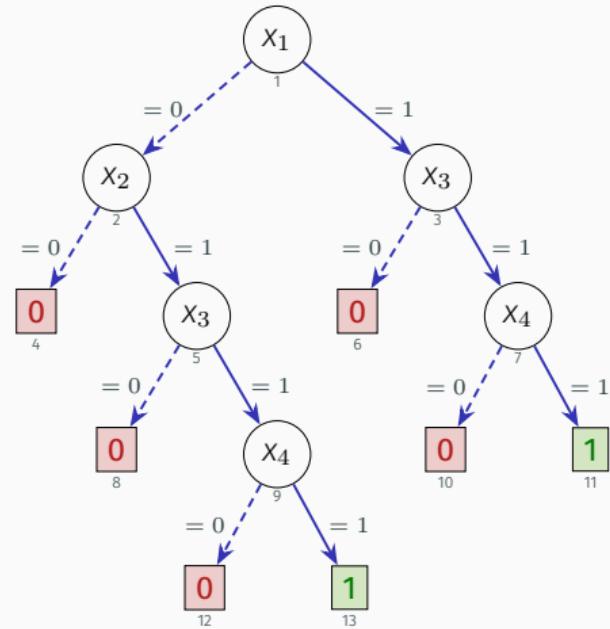
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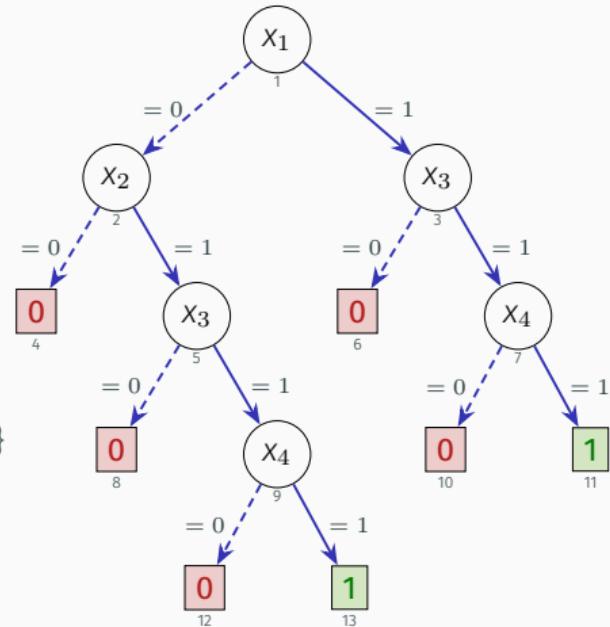
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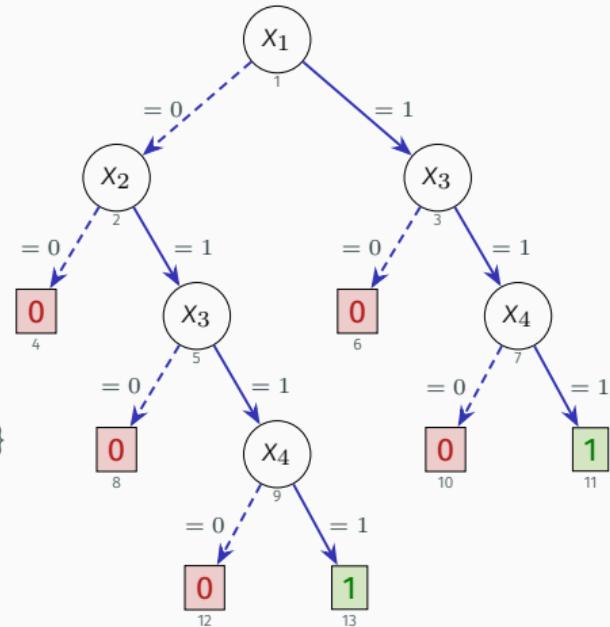
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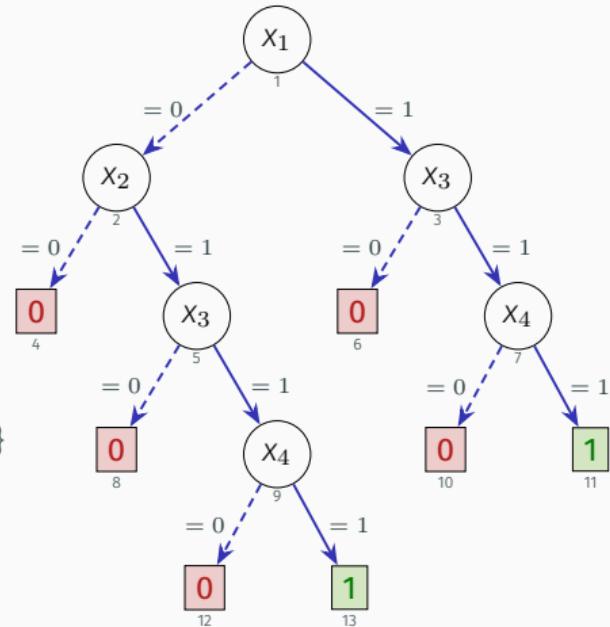
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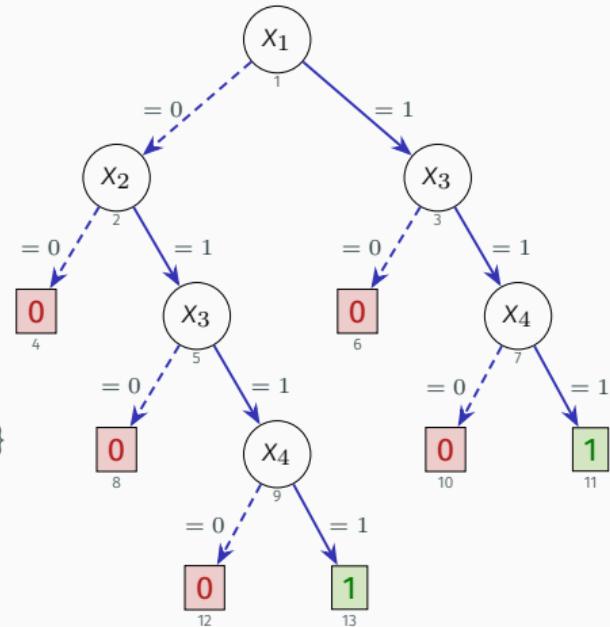
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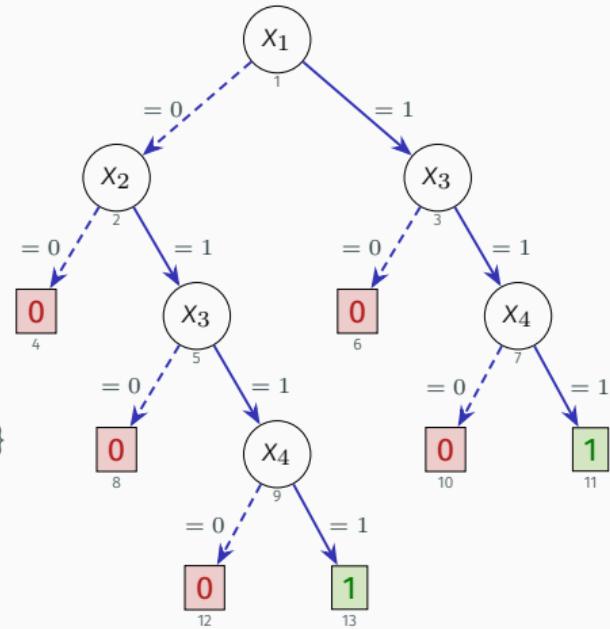
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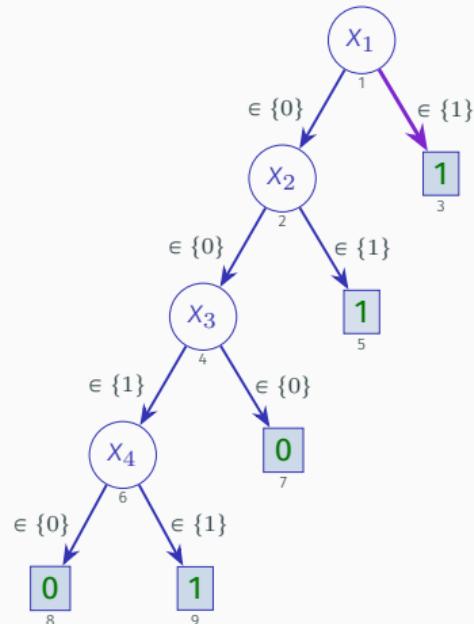


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- Given ϵ , larger adversarial examples are excluded

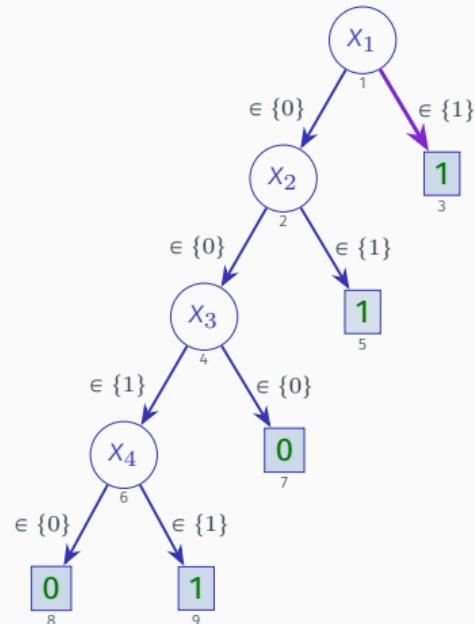


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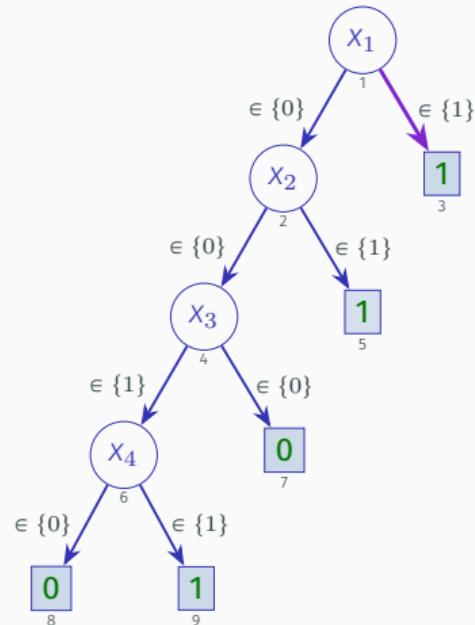
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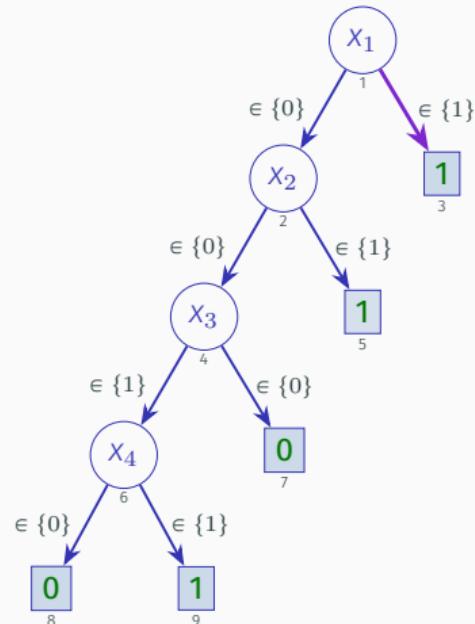
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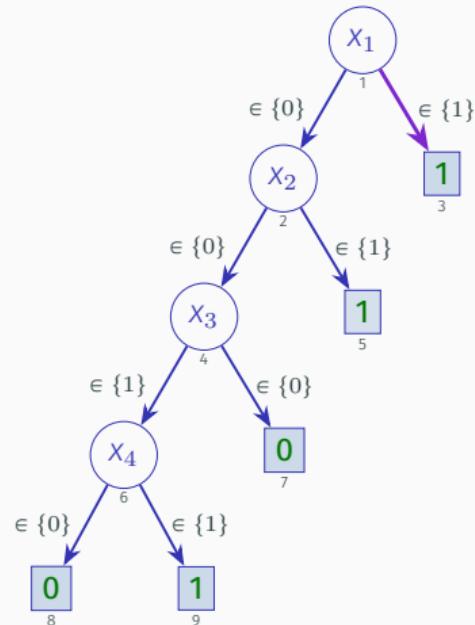
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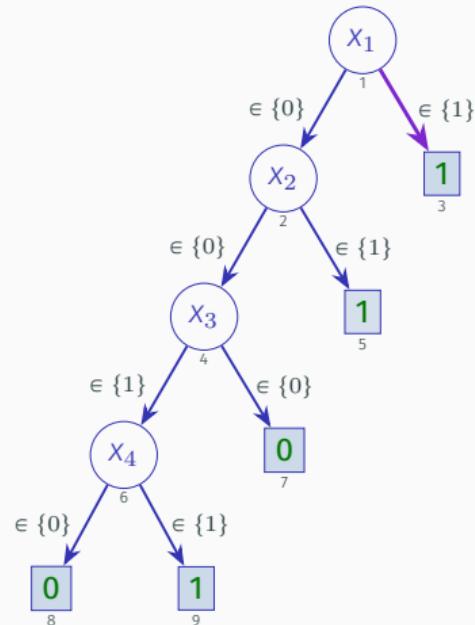
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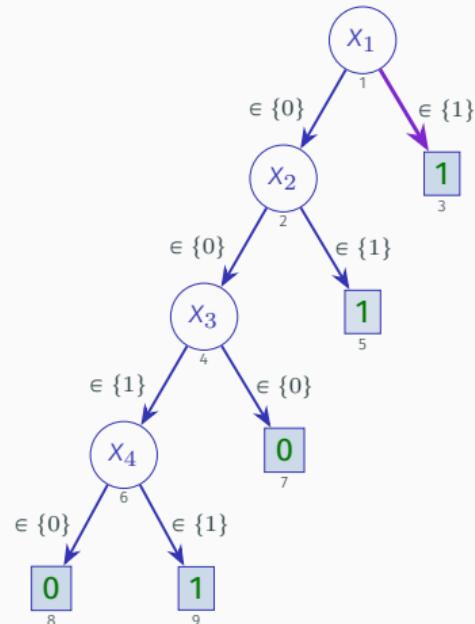
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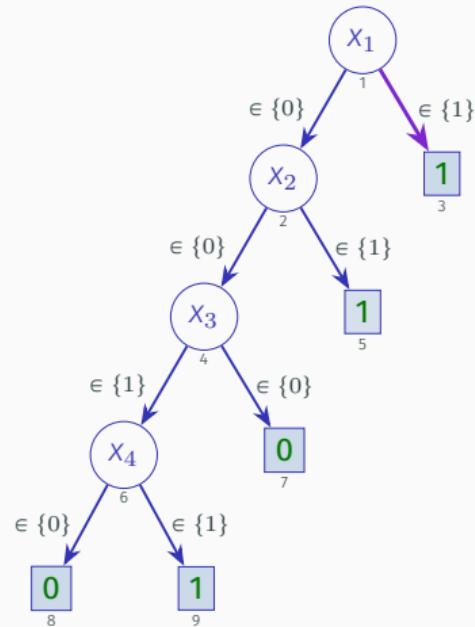
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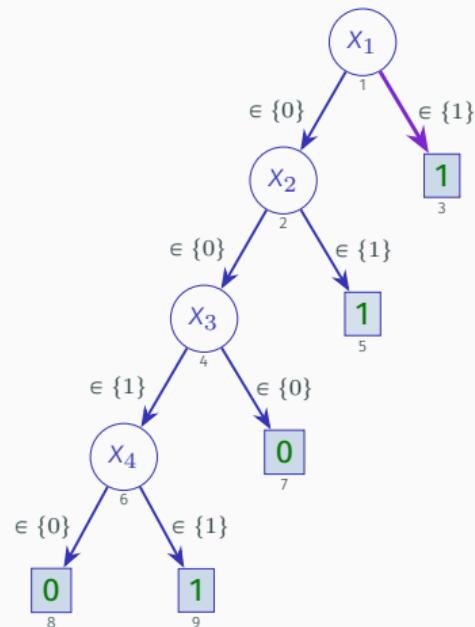
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Relating explanations with adversarial examples

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- Efficiency of distance-restricted explanations correlates with efficiency of finding adversarial examples
 - One can use most complete robustness tools, e.g. VNN-COMP [BMB⁺23]
- Clear scalability improvements for explaining NNs (see next) [HM23b, WWB23, IHM⁺24a, IHM⁺24b]

Input: Arguments: ϵ ; Parameters: \mathcal{E}, p

Output: One $\text{dAXp } \mathcal{S}$

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1: function FindAXpDel( $\epsilon; \mathcal{E}, p$ )
2:    $\mathcal{S} \leftarrow \mathcal{F}$                                  $\triangleright$  Initially, no feature is allowed to change
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- **Obs:** Efficiency of logic-based XAI tracks efficiency of robustness tools
- **Limitation:** Running time grows with number of features

Results for NNs in 2023 (using Marabou [KHI⁺19])

[HM23b]

DNN	points	AXp	#Calls	Time	#TO	AXp	#Calls	Time	#TO
$\epsilon = 0.1$					$\epsilon = 0.05$				
ACASXU_1_5	#1	3	5	185.9	0	2	5	113.8	0
	#2	2	5	273.8	0	1	5	33.2	0
	#3	0	5	714.2	0	0	5	4.3	0
ACASXU_3_1	#1	0	5	2219.3	0	0	5	14.2	0
	#2	2	5	4263.5	1	0	5	1853.1	0
	#3	1	5	581.8	0	0	5	355.9	0
ACASXU_3_2	#1	3	5	13739.3	2	1	5	6890.1	1
	#2	3	5	226.4	0	2	5	125.1	0
	#3	2	5	1740.6	0	2	5	173.6	0
ACASXU_3_5	#1	4	5	43.6	0	2	5	59.4	0
	#2	3	5	5039.4	0	2	5	4303.8	1
	#3	2	5	5574.9	1	2	5	2660.3	0
ACASXU_3_6	#1	1	5	6225.0	1	0	5	51.0	0
	#2	3	5	4957.2	1	2	5	1897.3	0
	#3	1	5	196.1	0	1	5	919.2	0
ACASXU_3_7	#1	3	5	6256.2	0	4	5	26.9	0
	#2	4	5	311.3	0	1	5	6958.6	1
	#3	2	5	7756.5	1	1	5	7807.6	1
ACASXU_4_1	#1	2	5	12413.0	2	1	5	5090.5	1
	#2	1	5	5035.1	1	0	5	2335.6	0
	#3	4	5	1237.3	0	4	5	1143.4	0
ACASXU_4_2	#1	4	5	15.9	0	4	5	12.1	0
	#2	3	5	1507.6	0	1	5	111.3	0
	#3	2	5	5641.6	2	0	5	1639.1	0

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Scales to a few hundred neurons

Recent improvements

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- To drop features from $\mathcal{S} \subseteq \mathcal{F}$, it is open whether parallelization might be applicable
 - Algorithm FindAXpDel is mostly sequential (see above)
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 - Algorithm FindAXpDel is mostly sequential (see above)
 - Exploit parallelization for other algorithms, e.g. [dichotomic search](#) [IHM+ 24b]
- However, to decide whether \mathcal{S} is an AXp, we can exploit parallelization:
 - Recall: $\text{AXp}(\mathcal{X}) := \text{WAXp}(\mathcal{X}) \wedge \forall(t \in \mathcal{X}). \neg \text{WAXp}(\mathcal{X} \setminus \{t\})$
 - Each $\neg \text{WAXp}(\cdot)$ (and also $\text{WAXp}(\cdot)$) check can be run in parallel!
 - Do this opportunistically, i.e. when set \mathcal{S} is expected to be AXp [IHM+ 24b]

More recent results (from 2024)...

[IHM⁺ 24a, IHM⁺ 24b]

Model	Deletion							SwiftXplain						
	avgC	nCalls	Len	Mn	Mx	avg	TO	avgC	nCalls	Len	FD%	Mn	Mx	avg
gtsrb-dense	0.06	1024	448	52.0	76.3	63.1	0	0.23	54	447	77.4	10.8	14.0	12.2
gtsrb-convSmall	0.06	1024	309	59.2	82.6	65.1	0	0.22	74	313	39.7	15.1	19.5	16.2
gtsrb-conv	—	—	—	—	—	—	100	96.49	45	174	33.2	3858.7	6427.7	4449.4
mnist-denseSmall	0.28	784	177	190.9	420.3	220.4	0	0.77	111	180	15.5	77.6	104.4	85.1
mnist-dense	0.19	784	231	138.1	179.9	150.6	0	0.75	183	229	11.5	130.1	145.5	136.8
mnist-convSmall	—	—	—	—	—	—	100	98.56	52	116	21.3	4115.2	6858.3	5132.8

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Largest for MNIST: 10142 neurons
Largest for GSTRB: 94308 neurons

Outline – Unit #06

Sample-Based Explanations

Changing Assumptions (in Plain Logic-Based XAI)

Inflated Explanations

Constrained Explanations

Distance-Restricted Explanations

Probabilistic Explanations

Additional Topics

Probabilistic (formal) explanations

[WMHK21, IIN⁺22, IH⁺22, ABOS22, IH⁺23, IMM24]

- Explanation size is critical for human understanding [Mil56]
- Probabilistic explanations provide smaller explanations, by trading off rigor of explanation by explanation size

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- Explanation size is critical for human understanding [Mil56]
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- Definition of weak probabilistic AXp $\mathcal{X} \subseteq \mathcal{F}$:

$$\text{WPAXp}(\mathcal{X}) \quad := \quad \Pr(\kappa(\mathbf{x}) = c \mid \mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}}) \geq \delta$$

- Obs: $\mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}}$ requires points $\mathbf{x} \in \mathbb{F}$ to match the values of \mathbf{v} for the features dictated by \mathcal{X}
- Obs: for $\delta = 1$ we obtain a WAXp

Definitions

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- Weak probabilistic AXp (WPAXp):

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– definition is non-monotonic

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– may differ from PAXp due to non-monotonicity

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 - Recent dedicated algorithms for simple ML models [IHI⁺23]
 - Recent approximate algorithms for complex ML models [IMM24]

Results for decision trees

Dataset	MinPAXp										LmPAXp							Anchor												
	DT		Path			δ	Length			Prec		Time		Length			Prec		m_{\leq}		Time		D	Length			Prec		Time	
	N	A	M	m	avg		M	m	avg	avg	avg	avg	M	m	avg	avg	avg	avg	avg	avg	avg	M	m	avg	F_{\#P}	avg	avg			
adult	1241 89 14 3 10.7						100	11	3	6.8	100	2.34	11	3	6.9	100	100	0.00	d	12	2	7.0	26.8	76.8	0.96					
	95	11	3	6.2	98.4		5.36	11	3	6.3	98.6	99.0	0.01	u	12	3	10.0	29.4	93.7	2.20										
	90	11	2	5.6	94.6		4.64	11	2	5.8	95.2	96.4	0.01																	
dermatology	71 100 13 1 5.1						100	12	1	4.4	100	0.35	12	1	4.4	100	100	0.00	d	31	1	4.8	58.1	32.9	3.10					
	95	12	1	4.1	99.7		0.37	12	1	4.1	99.7	99.3	0.00	u	34	1	13.1	43.2	87.2	25.13										
	90	11	1	4.0	98.8		0.35	11	1	4.0	98.8	100	0.00																	
kr-vs-kp	231 100 14 3 6.6						100	12	2	4.8	100	0.93	12	2	4.9	100	100	0.00	d	36	2	7.9	44.8	69.4	1.94					
	95	11	2	3.9	98.1		0.97	11	2	4.0	98.1	100	0.00	u	12	2	3.6	16.6	97.3	1.81										
	90	10	2	3.2	95.4		0.92	10	2	3.3	95.4	99.0	0.00																	
letter	3261 93 14 4 11.8						100	12	4	8.2	100	16.06	11	4	8.2	100	100	0.00	d	16	3	13.2	43.1	71.3	12.22					
	95	12	4	8.0	99.6		18.28	11	4	8.0	99.5	100	0.00	u	16	3	13.7	47.3	66.3	10.15										
	90	12	4	7.7	97.7		16.35	10	4	7.8	97.8	100	0.00																	
soybean	219 100 16 3 7.3						100	14	3	6.4	100	0.92	14	3	6.5	100	100	0.00	d	35	2	8.6	55.4	33.6	5.43					
	95	14	3	6.4	99.8		0.95	14	3	6.4	99.8	100	0.00	u	35	3	19.2	66.0	75.0	38.96										
	90	14	3	6.1	98.1		0.94	14	3	6.1	98.2	98.5	0.00																	
spambase	141 99 14 3 8.5						0	12	3	7.4	100	1.23	12	3	7.5	100	100	0.01	d	38	2	6.3	65.3	63.3	24.12					
	95	9	1	3.7	96.1		2.16	9	1	3.8	96.5	100	0.01	u	57	3	28.0	86.2	65.3	834.70										
	90	6	1	2.4	92.4		2.15	8	1	2.4	92.2	100	0.01																	

Results for naive Bayes classifiers

Dataset	(#F #I)	NBC	AXp	LmPAXp ≤ 9						LmPAXp ≤ 7						LmPAXp ≤ 4					
		A%	Length	δ	Length	Precision	W%	Time	Length	Precision	W%	Time	Length	Precision	W%	Time	Length	Precision	W%	Time	
adult	(13 200)	81.37	6.8 \pm 1.2	98	6.8 \pm 1.1	100 \pm 0.0	100	0.003	6.3 \pm 0.9	99.61 \pm 0.6	96	0.023	4.8 \pm 1.3	98.73 \pm 0.5	48	0.059					
				95	6.8 \pm 1.1	99.99 \pm 0.2	100	0.074	5.9 \pm 1.0	98.87 \pm 1.8	99	0.058	3.9 \pm 1.0	96.93 \pm 1.1	80	0.071					
				93	6.8 \pm 1.1	99.97 \pm 0.4	100	0.104	5.7 \pm 1.3	98.34 \pm 2.6	100	0.086	3.4 \pm 0.9	95.21 \pm 1.6	90	0.093					
				90	6.8 \pm 1.1	99.95 \pm 0.6	100	0.164	5.5 \pm 1.4	97.86 \pm 3.4	100	0.100	3.0 \pm 0.8	93.46 \pm 1.5	94	0.103					
agaricus	(23 200)	95.41	10.3 \pm 2.5	98	7.7 \pm 2.7	99.12 \pm 0.8	92	0.593	6.4 \pm 3.0	98.75 \pm 0.6	87	0.763	6.0 \pm 3.1	98.67 \pm 0.5	29	0.870					
				95	6.9 \pm 3.1	97.62 \pm 2.1	95	0.954	5.3 \pm 3.2	96.59 \pm 1.6	92	1.273	4.8 \pm 3.3	96.24 \pm 1.2	55	1.217					
				93	6.5 \pm 3.1	96.65 \pm 2.8	95	1.112	4.8 \pm 3.1	95.38 \pm 1.9	93	1.309	4.3 \pm 3.1	94.92 \pm 1.3	64	1.390					
				90	5.9 \pm 3.3	94.95 \pm 4.1	96	1.332	4.0 \pm 3.0	92.60 \pm 2.8	95	1.598	3.6 \pm 2.8	92.08 \pm 1.7	76	1.830					
chess	(37 200)	88.34	12.1 \pm 3.7	98	8.1 \pm 4.1	99.27 \pm 0.6	64	0.383	5.9 \pm 4.9	98.70 \pm 0.4	64	0.454	5.7 \pm 5.0	98.65 \pm 0.4	46	0.457					
				95	7.7 \pm 3.8	98.51 \pm 1.4	68	0.404	5.5 \pm 4.4	97.90 \pm 0.9	64	0.483	5.3 \pm 4.5	97.85 \pm 0.8	46	0.478					
				93	7.3 \pm 3.5	97.56 \pm 2.4	68	0.419	5.0 \pm 4.1	96.26 \pm 2.2	64	0.485	4.8 \pm 4.1	96.21 \pm 2.1	64	0.493					
				90	7.3 \pm 3.5	97.29 \pm 2.9	70	0.413	4.9 \pm 4.0	95.99 \pm 2.6	64	0.483	4.8 \pm 4.0	95.93 \pm 2.5	64	0.543					
vote	(17 81)	89.66	5.3 \pm 1.4	98	5.3 \pm 1.4	100 \pm 0.0	100	0.000	5.3 \pm 1.3	99.95 \pm 0.2	100	0.007	4.6 \pm 1.1	99.60 \pm 0.4	64	0.014					
				95	5.3 \pm 1.4	100 \pm 0.0	100	0.000	5.3 \pm 1.3	99.93 \pm 0.3	100	0.008	4.1 \pm 1.0	98.25 \pm 1.7	64	0.018					
				93	5.3 \pm 1.4	100 \pm 0.0	100	0.000	5.2 \pm 1.3	99.78 \pm 1.1	100	0.012	4.1 \pm 0.9	98.10 \pm 1.9	64	0.018					
				90	5.3 \pm 1.4	100 \pm 0.0	100	0.000	5.2 \pm 1.3	99.78 \pm 1.1	100	0.012	4.0 \pm 1.2	97.24 \pm 3.1	64	0.022					
kr-vs-kp	(37 200)	88.07	12.2 \pm 3.9	98	7.8 \pm 4.2	99.19 \pm 0.5	64	0.387	6.5 \pm 4.7	98.99 \pm 0.4	64	0.427	6.1 \pm 4.9	98.88 \pm 0.3	43	0.457					
				95	7.3 \pm 3.9	98.29 \pm 1.4	64	0.416	6.0 \pm 4.3	97.89 \pm 1.1	64	0.453	5.5 \pm 4.5	97.79 \pm 0.9	43	0.462					
				93	6.9 \pm 3.5	97.21 \pm 2.5	69	0.422	5.6 \pm 3.8	96.82 \pm 2.2	64	0.448	5.2 \pm 4.0	96.71 \pm 2.1	43	0.468					
				90	6.8 \pm 3.5	96.65 \pm 3.1	69	0.418	5.4 \pm 3.8	95.69 \pm 3.0	64	0.468	5.0 \pm 4.0	95.59 \pm 2.8	61	0.487					
mushroom	(23 200)	95.51	10.7 \pm 2.3	98	7.5 \pm 2.4	98.99 \pm 0.7	90	0.641	6.5 \pm 2.6	98.74 \pm 0.5	83	0.751	6.3 \pm 2.7	98.70 \pm 0.4	18	0.828					
				95	6.5 \pm 2.6	97.35 \pm 1.8	96	1.011	5.1 \pm 2.5	96.52 \pm 1.0	90	1.130	5.0 \pm 2.5	96.39 \pm 0.8	54	1.113					
				93	5.8 \pm 2.8	95.77 \pm 2.7	96	1.257	4.4 \pm 2.5	94.67 \pm 1.6	94	1.297	4.2 \pm 2.4	94.48 \pm 1.3	65	1.324 _{186 / 238}					

Results for decision diagrams

Dataset	#I	#F	OMDD		δ	MinPAXp						LmPAXp					
						Length			Prec	Time	Length			Prec	m_{\subseteq}	Time	
			#N	A%		M	m	avg	avg	avg	M	m	avg	avg	avg	avg	
lending	100	9	1103	81.7	100	9	6	8.0	100	24.24	9	6	7.9	100	100	1.57	
					95	9	5	7.8	99.7	21.48	9	6	7.8	99.8	100	100	1.49
					90	9	4	7.2	96	24.65	9	5	7.4	97.0	100	100	1.48
monk2	100	6	70	79.3	100	6	4	5.1	100	0.10	6	4	5.1	100	100	0.03	
					95	6	4	5.1	100	0.09	6	4	5.1	100	100	0.03	
					90	6	3	4.8	98.1	0.09	6	3	4.8	98.1	100	100	0.03
postoperative	74	8	109	80	100	8	4	6.1	100	0.26	8	4	6.2	100	100	0.04	
					95	8	2	6.0	99.3	0.25	8	2	6.0	99.3	100	100	0.04
					90	8	2	5.3	95.9	0.23	8	2	5.4	96.6	94.6	100	0.04
tic_tac_toe	100	9	424	70.3	100	9	5	7.7	100	3.60	9	5	7.8	100	100	0.38	
					95	9	5	7.5	99.5	3.24	9	5	7.7	99.6	99.0	100	0.38
					90	9	3	7.3	98.3	4.06	9	3	7.5	98.6	98.0	100	0.38
xd6	100	9	76	83.1	100	9	4	4.6	100	0.10	9	4	4.6	100	100	0.03	
					95	9	3	3.8	97	0.09	9	3	3.8	97.0	99.0	100	0.03
					90	9	3	3.3	94.8	0.10	9	3	3.4	94.6	100	100	0.03

Remarks on LmPAXps

[IHI⁺23]

- LmPAXps ignore non-monotonicity, and so overapproximate PAXps
 - Theoretical guarantees, but may be reducible
- For DTs, computation of LmPAXps is in P
- Experimental results confirm LmPAXps match PAXps in most cases
- Recent results on approximating LmPAXps for RFs

[IMM24]

Outline – Unit #06

Sample-Based Explanations

Changing Assumptions (in Plain Logic-Based XAI)

Inflated Explanations

Constrained Explanations

Distance-Restricted Explanations

Probabilistic Explanations

Additional Topics

Surrogate models in logic-based XAI

[BAMT21]

- Motivation:
 - Logic-based XAI does not yet scale for highly complex ML models
 - Surrogate models find many uses in ML, for approximating complex models

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 - Compute rigorous explanation: plain AXp, probabilistic AXp,
- Report computed explanation as explanation for the complex ML model

Certified explainer (for monotonic classification)

[HM23f]

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Plan for this course – light at the end of the tunnel...

- Lecture 01 – unit(s):
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Questions?

Lecture 05

Recapitulate fourth lecture

- Monotonic classifiers vs. weighted voting games
- Advanced topics:
 - Sample-based explanations
 - Inflated explanations
 - Probabilistic explanations
 - Constrained explanations
 - Distance-restricted explanations
 - Explanations using surrogate models
 - Certified explainability

- Every WVG \mathcal{G} , described by $[q; n_1, \dots, n_m]$, can be represented as a monotonically increasing boolean classifier $\mathcal{M} = (\mathcal{F}, \{0, 1\}^m, \{0, 1\}, \kappa)$, such that:
 - Each voter i is mapped to a boolean feature i , such that feature i takes value 1 if voter i votes Yes; otherwise it takes value 0;
 - The classification function $\kappa : \mathbb{F} \rightarrow \{0, 1\}$ is defined by:

$$\kappa(\mathbf{x}) = \begin{cases} 1 & \text{if } \sum_{i=1}^m n_i x_i \geq q \\ 0 & \text{otherwise} \end{cases}$$

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∴ WVGs can be analyzed by studying the AXps/CXps of monotonically increasing boolean classifiers

Another WVG

- WVG: [25; 10, 9, 7, 1, 1, 1, 1, 1, 1]

Another WVG

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- Computing the AXps:
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- Q: How should features be ranked in terms of importance?

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Unit #07

Principles of Symbolic XAI – Feature Attribution

Outline – Unit #07

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

A Correct New SHAP – nuSHAP

Voting Power & Power Indices

Feature Importance Scores

Detour: Standard SHAP Intro (from another course...)

What are Shapley values?

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 - Measures the contribution of each player to a cooperative game

[Sha53]

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[Sha53]

[LC01, SK10, SK14, DSZ16, LL17, ABBM21, VLSS21, VLSS22, ABBM23]

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- Shapley values are becoming ubiquitous in XAI... – E.g. see slides from other XAI course...

[LC01, SK10, SK14, DSZ16, LL17, ABBM21, VLSS21, VLSS22, ABBM23]

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🛡️ 🔍 https://en.wikipedia.org/wiki/Shapley_value

📋 ⭐

Accessed 2023/06/14

In machine learning [edit]

The Shapley value provides a principled way to explain the predictions of nonlinear models common in the field of [machine learning](#). By interpreting a model trained on a set of features as a value function on a coalition of players, Shapley values provide a natural way to compute which features contribute to a prediction.^[17] This unifies several other methods including Locally Interpretable Model-Agnostic Explanations (LIME),^[18] DeepLIFT,^[19] and Layer-Wise Relevance Propagation.^[20]

17. ^ Lundberg, Scott M.; Lee, Su-In (2017). "A Unified Approach to Interpreting Model Predictions". *Advances in Neural Information Processing Systems*. 30: 4765–4774. arXiv:1705.07874. Retrieved 2021-01-30.

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- **Q:** Do Shapley values for XAI **really** provide a rigorous measure of feature importance?

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[ABBM21, ABBM23]

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- $\phi: 2^{\mathcal{F}} \rightarrow \mathbb{R}$ defined by,

$$\phi(\mathcal{S}) = 1/2^{|\mathcal{F} \setminus \mathcal{S}|} \sum_{\mathbf{x} \in \Upsilon(\mathcal{S})} \kappa(\mathbf{x}) = v_e(\mathcal{S})$$

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$$\text{Sc}(i) = \sum_{\mathcal{S} \subseteq (\mathcal{F} \setminus \{i\})} \frac{|\mathcal{S}|!(|\mathcal{F}| - |\mathcal{S}| - 1)!}{|\mathcal{F}|!} \times (\phi(\mathcal{S} \cup \{i\}) - \phi(\mathcal{S}))$$

For all subsets of features, excluding i , compute the expected value of the classifier, with and without i fixed, weighted by $\frac{1}{n} \binom{n}{|\mathcal{S}|}^{-1}$

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Marginal contribution
(in SHAP lingo)!

[ABBM21, ABBM23]

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How are Shapley values computed in practice?

- Exact evaluation is computationally (very) hard [VLSS21, ABBM21, VLSS22, ABBM23, HMS24]
- SHAP proposes a sample-based approach; with **no** guarantees of rigor [LL17]
 - Recent experiments revealed little to **no** correlation between Shapley values and SHAP's results [HM23c]

How are Shapley values computed in practice?

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- SHAP proposes a sample-based approach; with **no** guarantees of rigor [LL17]
 - Recent experiments revealed little to **no** correlation between Shapley values and SHAP's results [HM23c]
- **Polynomial-time** algorithm for deterministic decomposable boolean circuits [ABBM21]
- **Polynomial-time** algorithm for boolean functions represented with a truth-table [HM23c]

What do Shapley values tell in terms of feature importance?

- [SK10] reads:

“According to the 2nd axiom, if two features values have an identical influence on the prediction they are assigned contributions of equal size. The 3rd axiom says that if a feature has no influence on the prediction it is assigned a contribution of 0.”

(Obs: the axioms refer to the axiomatic characterization of Shapley values.)

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- Obs: Shapley values are defined **axiomatically**, i.e. **no** immediate relationship with AXp's/CXp's or with feature (ir)relevancy
 - Qs: can we have **irrelevant** features with a non-zero Shapley value, and/or **relevant** features with a Shapley of zero?
 - Recall: **relevant** features occur in some AXp/CXp; **irrelevant** features do **not** occur in **any** AXp/CXp

Outline – Unit #07

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

A Correct New SHAP – nuSHAP

Voting Power & Power Indices

Feature Importance Scores

- Boolean classifier, instance (\mathbf{v}, c) , and some $i, i_1, i_2 \in \mathcal{F}$:

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Shapley values vs. feature (ir)relevancy – identified issues

[HM23c, HM23d, HM23e, MH23, HMS24, MSH24]

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$$[\text{Irrelevant}(i_1) \wedge (\text{Sv}(i_1) \neq 0)] \wedge [\text{Relevant}(i_2) \wedge (\text{Sv}(i_2) = 0)]$$

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- Issue I3 occurs if,

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Any of these issues is a cause
of (serious) concern per se!

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Some stats – all boolean functions with 4 variables

[HM23c, HM23d, HM23e, MH23, HMS24, MSH24]

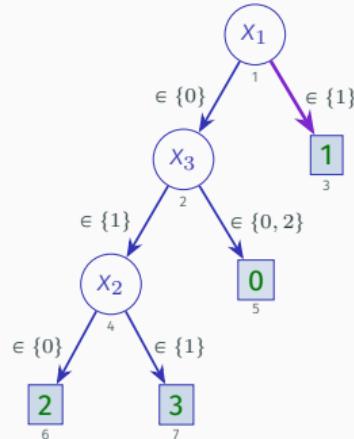
Issue-related metric	Value	Recap issue
# of functions	65536	
# number of instances	1048576	
# of I1 issues	781696	
# of functions with I1 issues	65320	
% I1 issues / function	99.67	$[\text{Irrelevant}(i) \wedge (\text{Sv}(i) \neq 0)]$
# of I2 issues	105184	
# of functions with I2 issues	40448	
% I2 issues / function	61.72	$[\text{Irrelevant}(i_1) \wedge \text{Relevant}(i_2) \wedge (\text{Sv}(i_1) > \text{Sv}(i_2))]$
# of I3 issues	43008	
# of functions with I3 issues	7800	
% I3 issues / function	11.90	$[\text{Relevant}(i) \wedge (\text{Sv}(i) = 0)]$
# of I4 issues	5728	
# of functions with I4 issues	2592	
% I4 issues / function	3.96	$[\text{Irrelevant}(i_1) \wedge (\text{Sv}(i_1) \neq 0)] \wedge [\text{Relevant}(i_2) \wedge (\text{Sv}(i_2) = 0)]$
# of I5 issues	1664	
# of functions with I5 issues	1248	
% I5 issues / function	1.90	$[\text{Irrelevant}(i) \wedge \forall_{1 \leq j \leq m, j \neq i} (\text{Sv}(j) < \text{Sv}(i))]$

Previous results do matter! Let's go non-boolean...

row #	x_1	x_2	x_3	$\kappa_1(\mathbf{x})$	$\kappa_2(\mathbf{x})$
1	0	0	0	0	0
2	0	0	1	4	2
3	0	0	2	0	0
4	0	1	0	0	0
5	0	1	1	7	3
6	0	1	2	0	0
7	1	0	0	1	1
8	1	0	1	1	1
9	1	0	2	1	1
10	1	1	0	1	1
11	1	1	1	1	1
12	1	1	2	1	1

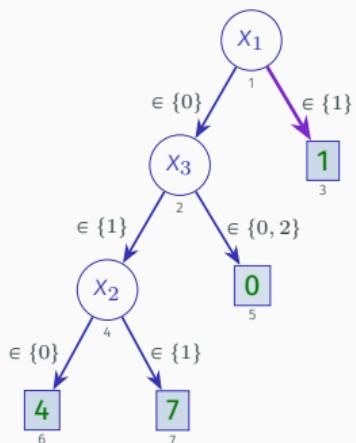
DT1

Tabular representations



DT2

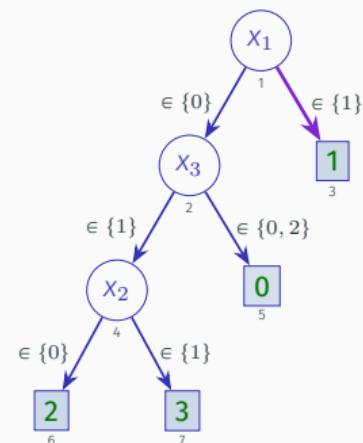
Instance $((1, 1, 2), 1)$ – which feature matters the most for prediction 1?



DT1

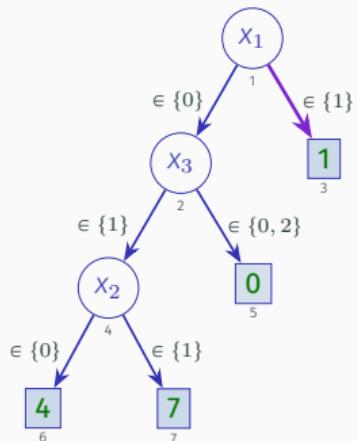
row #	x_1	x_2	x_3	$\kappa_1(\mathbf{x})$	$\kappa_2(\mathbf{x})$
1	0	0	0	0	0
2	0	0	1	4	2
3	0	0	2	0	0
4	0	1	0	0	0
5	0	1	1	7	3
6	0	1	2	0	0
7	1	0	0	1	1
8	1	0	1	1	1
9	1	0	2	1	1
10	1	1	0	1	1
11	1	1	1	1	1
12	1	1	2	1	1

Tabular representations



DT2

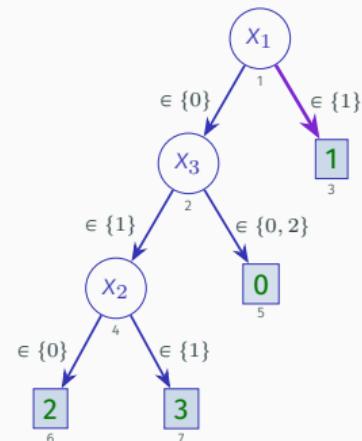
Computing XPs – make sense...



DT1

row #	x_1	x_2	x_3	$\kappa_1(\mathbf{x})$	$\kappa_2(\mathbf{x})$
1	0	0	0	0	0
2	0	0	1	4	2
3	0	0	2	0	0
4	0	1	0	0	0
5	0	1	1	7	3
6	0	1	2	0	0
7	1	0	0	1	1
8	1	0	1	1	1
9	1	0	2	1	1
10	1	1	0	1	1
11	1	1	1	1	1
12	1	1	2	1	1

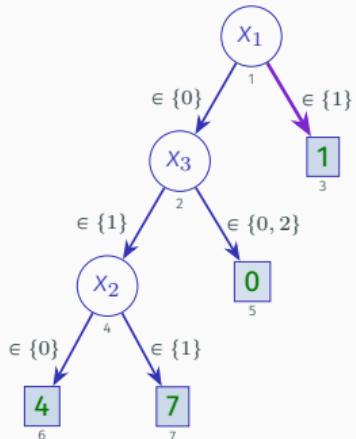
Tabular representations



DT2

XPs: AXps/CXps		
DT	AXps	CXps
DT1	{1}	{1}
DT2	{1}	{1}

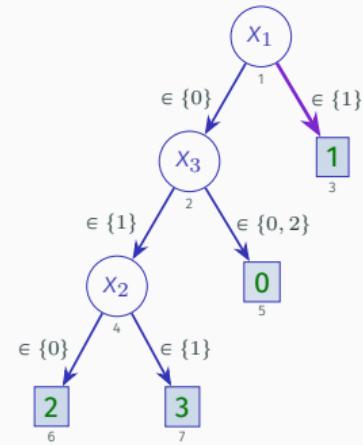
Computing XPs, AEs – also make sense...



DT1

row #	x_1	x_2	x_3	$\kappa_1(\mathbf{x})$	$\kappa_2(\mathbf{x})$
1	0	0	0	0	0
2	0	0	1	4	2
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Tabular representations

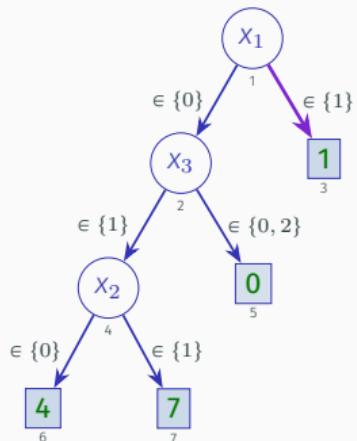


DT2

XPs: AXps/CXps		
DT	AXps	CXps
DT1	{1}	{1}
DT2	{1}	{1}

Adversarial Examples	
DT	l_0 -minimal AEs
DT1	{1}
DT2	{1}

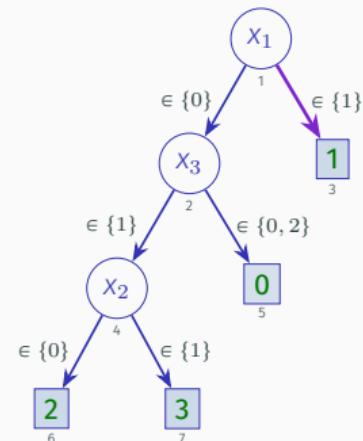
Computing XPs, AEs & Svs



DT1

row #	x_1	x_2	x_3	$\kappa_1(\mathbf{x})$	$\kappa_2(\mathbf{x})$
1	0	0	0	0	0
2	0	0	1	4	2
3	0	0	2	0	0
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Tabular representations



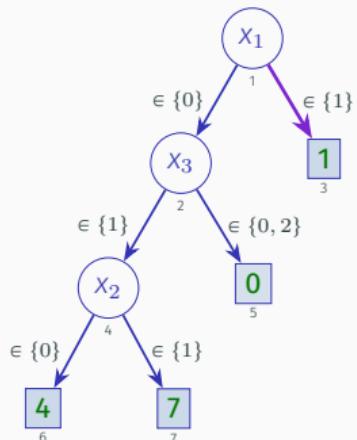
DT2

XPs: AXps/CXps		
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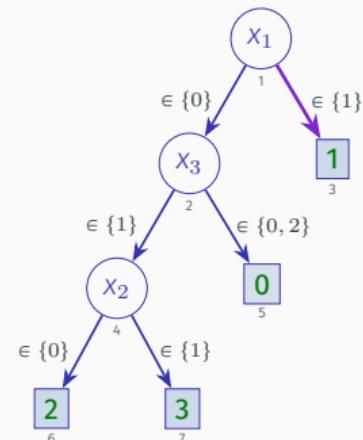
Shapley values			
DT	Sc(1)	Sc(2)	Sc(3)
DT1	0.000	0.083	-0.500
DT2	0.278	0.028	-0.222

Computing XPs, AEs & Svs – what???



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1	0	0	0	0	0
2	0	0	1	4	2
3	0	0	2	0	0
4	0	1	0	0	0
5	0	1	1	7	3
6	0	1	2	0	0
7	1	0	0	1	1
8	1	0	1	1	1
9	1	0	2	1	1
10	1	1	0	1	1
11	1	1	1	1	1
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DT2

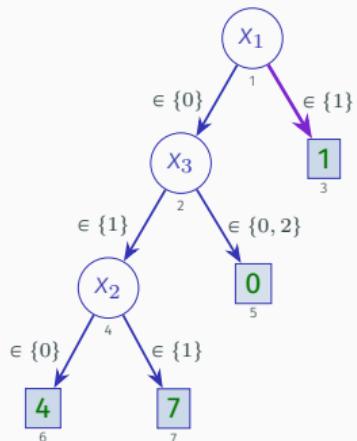
Tabular representations

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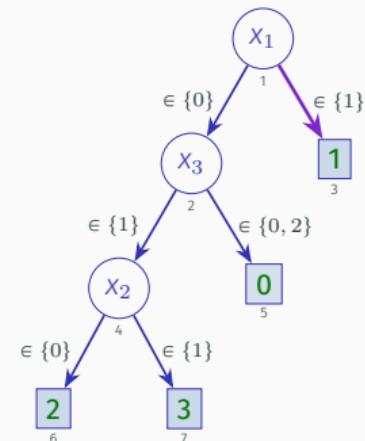
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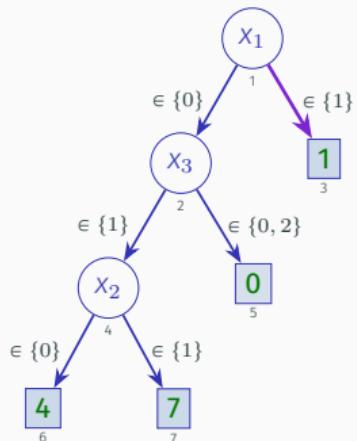
DT2

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DT2	{1}	{1}

Adversarial Examples	
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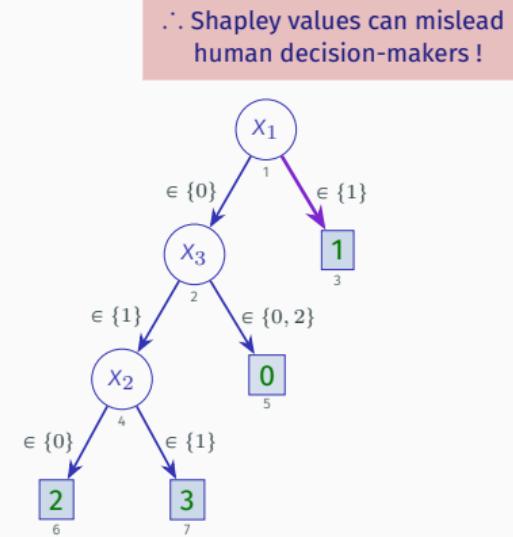
Computing XPs, AEs & Svs – what???



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10	1	1	0	1	1
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Tabular representations



DT2

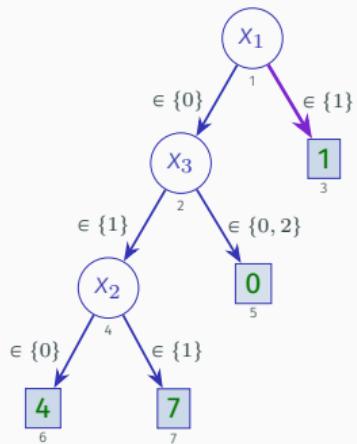
XPs: AXps/CXps		
DT	AXps	CXps
DT1	{1}	{1}
DT2	{1}	{1}

Adversarial Examples	
DT	l_0 -minimal AEs
DT1	{1}
DT2	{1}

Shapley values				
DT	Sc(1)	Sc(2)	Sc(3)	
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. . . Shapley values can mislead human decision-makers !

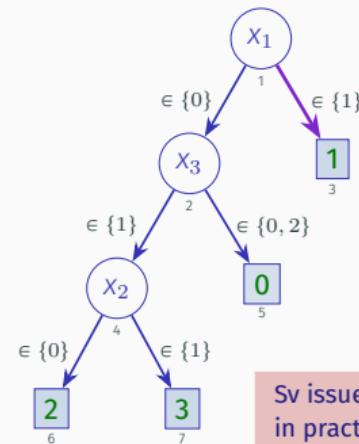
Computing XPs, AEs & Svs – what???



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8	1	0	1	1	1
9	1	0	2	1	1
10	1	1	0	1	1
11	1	1	1	1	1
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Tabular representations



DT2

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Sv issues also occur in practice [HM23e]

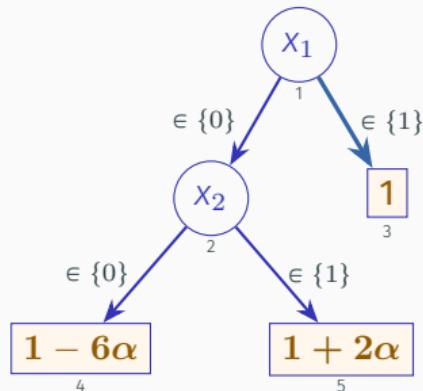
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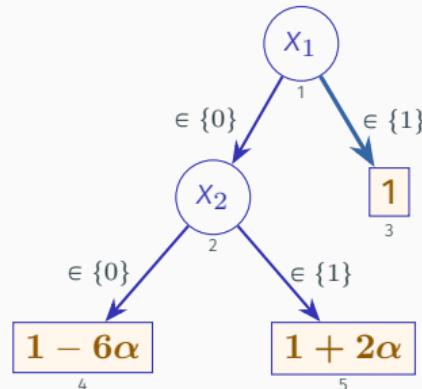
Another example – arbitrary mistakes!

[LHAMS24]



Another example – arbitrary mistakes!

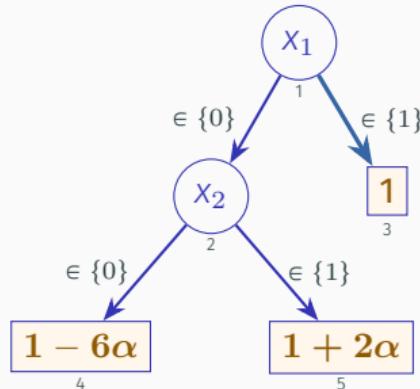
[LHAMS24]



- Instance: $((1, 1), 1)$
- Obs: $\alpha \neq 0$

Another example – arbitrary mistakes!

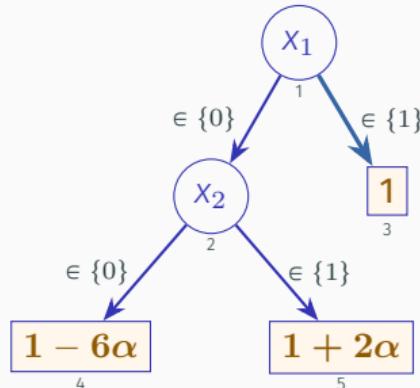
[LHAMS24]



- Instance: $((1, 1), 1)$
- Obs: $\alpha \neq 0$
- $\text{Sc}(1) = 0$
- $\text{Sc}(2) = \alpha$

Another example – arbitrary mistakes!

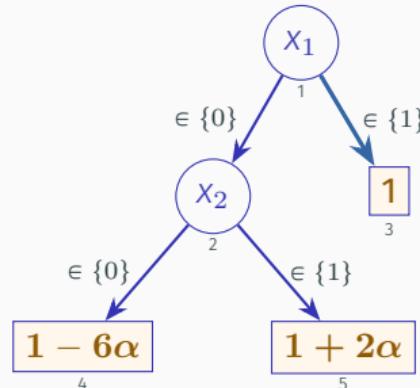
[LHAMS24]



- Instance: $((1, 1), 1)$
- Obs: $\alpha \neq 0$
- $\text{Sc}(1) = 0$
- $\text{Sc}(2) = \alpha$ (you can pick the α ...)

Another example – arbitrary mistakes!

[LHAMS24]

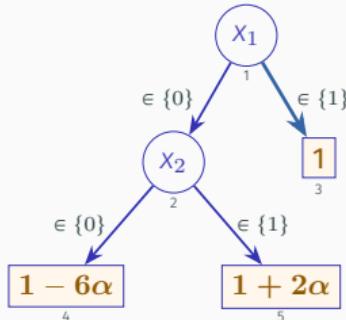


- Instance: $((1, 1), 1)$
- Obs: $\alpha \neq 0$
- $\text{Sc}(1) = 0$
- $\text{Sc}(2) = \alpha$ (you can pick the α ...)

Example devised by O. Letoffe, PhD student at IRIT

More detail

row	x_1	x_2	$\rho(\mathbf{x})$	$\rho_a(\mathbf{x})$ $\alpha = 1/2$	$\rho_b(\mathbf{x})$ $\alpha = 1/4$
1	0	0	$1 - 6\alpha$	-2	$-1/2$
2	0	1	$1 + 2\alpha$	2	$3/2$
3	1	0	1	1	1
4	1	1	1	1	1



\mathcal{S}	$\text{rows}(\mathcal{S})$	$v_e(\mathcal{S})$
\emptyset	1, 2, 3, 4	$1 - \alpha$
$\{x_1\}$	3, 4	1
$\{x_2\}$	2, 4	$1 + \alpha$
$\{x_1, x_2\}$	4	1

$i = 1$					
\mathcal{S}	$v_e(\mathcal{S})$	$v_e(\mathcal{S} \cup \{1\})$	$\Delta_1(\mathcal{S})$	$\varsigma(\mathcal{S})$	$\varsigma(\mathcal{S}) \times \Delta_1(\mathcal{S})$
\emptyset	$1 - \alpha$	1	α	$1/2$	$\alpha/2$
$\{2\}$	$1 + \alpha$	1	$-\alpha$	$1/2$	$-\alpha/2$
$\text{Sc}_E(1) =$				0	
$i = 2$					
\mathcal{S}	$v_e(\mathcal{S})$	$v_e(\mathcal{S} \cup \{2\})$	$\Delta_2(\mathcal{S})$	$\varsigma(\mathcal{S})$	$\varsigma(\mathcal{S}) \times \Delta_2(\mathcal{S})$
\emptyset	$1 - \alpha$	$1 + \alpha$	2α	$1/2$	α
$\{1\}$	1	1	0	$1/2$	0
$\text{Sc}_E(2) =$				α	

SHAP scores also fail with regression models

[LHM24]

- Let $\mathcal{F} = \{1, 2\}$, $\mathbb{D}_1 = \mathbb{D}_2 = \mathbb{D} = [-1/2, 3/2]$, $\mathbb{F} = \mathbb{D} \times \mathbb{D}$
 - Also, let $\mathbb{D}^+ = [1/2, 3/2]$ and $\mathbb{D}^- = \mathbb{D} \setminus \mathbb{D}^+$
- Regression model maps to real values, i.e. $\mathbb{K} = \mathbb{R}$:

$$\rho_2(x_1, x_2) = \begin{cases} x_1 & \text{if } x_1 \in \mathbb{D}^+ \\ x_2 - 2 & \text{if } x_1 \notin \mathbb{D}^+ \wedge x_2 \notin \mathbb{D}^+ \\ x_2 + 1 & \text{if } x_1 \notin \mathbb{D}^+ \wedge x_2 \in \mathbb{D}^+ \end{cases}$$

- Average values unchanged (wrt previous example), and so $Sc(1) = 0$ and $Sc(2) = \alpha$

SHAP scores even fail when Lipschitz continuity holds!

$$\rho_3(x_1, x_2) = \begin{cases} x_1 & \text{if } x_2 \leq 1 \wedge \alpha x_1 \leq \alpha \\ (1 + 4|\alpha|)x_1 - 4|\alpha| & \text{if } x_2 \leq 1 \wedge \alpha x_1 \geq \alpha \\ 28|\alpha|x_1x_2 + (1 - 28|\alpha|)x_1 - 28|\alpha|x_2 + 28|\alpha| & \text{if } x_2 \geq 1 \wedge \alpha x_1 \leq \alpha \\ -4|\alpha|x_1x_2 + (1 + 8|\alpha|)x_1 + 4|\alpha|x_2 - 8|\alpha| & \text{if } x_2 \geq 1 \wedge \alpha x_1 \geq \alpha \end{cases}$$

[LHM24]

- As before, average values unchanged, and so $\text{Sc}(1) = 0$ and $\text{Sc}(2) = \alpha$

Outline – Unit #07

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

A Correct New SHAP – nuSHAP

Voting Power & Power Indices

Feature Importance Scores

Corrected SHAP scores & feature importance scores

[LHMS24, LHAMS24]

- Is the theory of Shapley values **incorrect?**

Corrected SHAP scores & feature importance scores

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 - In XAI: characteristic function uses the **expected value**
 - This defines the *marginal contribution* in SHAP lingo...

[SK10, SK14, LL17]

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 - Resulting scores are (**still**) Shapley values & identified issues no longer observed

[LHMS24]

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 - **Feature importance scores** (more later):
 - Generalize recent axiomatic aggregations
 - Adapt best known power indices
 - Devise new scores for XAI

[SK10, SK14, LL17]

[LHMS24]

[LHAMS24]

[BIL⁺24]

An initial compromise

[LHAMS24]

- Replace the characteristic function used for SHAP scores:

$$v_e(\mathcal{S}) := \mathbf{E}[\tau(\mathbf{x}) \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}]$$

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$$\sigma(\mathbf{x}) = \begin{cases} 1 & \text{if } (\kappa(\mathbf{x}) = \kappa(\mathbf{v})) \\ 0 & \text{otherwise} \end{cases}$$

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- Developed SSHAP prototype using SHAP's code base

[LHMS24]

Fixing the known issues of SHAP scores

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$$v_a(\mathcal{S}) := \begin{cases} 1 & \text{if } \mathbf{E}[\sigma(\mathbf{x}) \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}] = 1 \\ 0 & \text{otherwise} \end{cases}$$

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- Known issues of SHAP scores guaranteed **not** to occur
- **Corrected** SHAP scores reveal tight connection between XAI by feature selection (i.e. WAXps) and feature attribution

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A glimpse of NuSHAP

- Shapley values estimated with well-known algorithm – CGT
 - Strong theoretical guarantees on approximation of Shapley values
 - With enough sampling, given by ϵ and α :

[CGT09]

$$\text{Prob}[|\hat{Sc}(i) - Sc(i)| \leq \epsilon] \geq 1 - \alpha$$

- E.g. we used $\epsilon = 0.0015$ and $\alpha = 0.015$

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- E.g. we used $\epsilon = 0.0015$ and $\alpha = 0.015$
- Replace expected value with novel characteristic function: test for WAXp
 - New approach for computing symbolic explanations, targeting scalability for complex models
 - Replace WAXp check with sbWAXp check, i.e. polynomial-time check
 - Flexibility in the sample chosen, e.g. training data

NuSHAP vs. *SHAP

- Compute SHAP scores with NuSHAP and SHAP
- Compare features' rankings using Rank-Biased Overlap (RBO) [WMZ10]
 - Give weight to differences in first k elements of ranking
 - E.g. $\text{RBO}([0, 1, 2, 3, 4, 5, 6, 7, 8, 9], [0, 1, 2, 3, 4, 5, 6, 7, 8, 9], k = 5) = 1.0$
- Results for different datasets and ML models (using scikit, XGBoost):
 - LR: (adult, corral); DT: (iris, mux6); KNN: (connect_4, spambase, spectf);
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[WMZ10]

		adult	corral	iris	mux6	connect_4	spambase	spectf	clean1	coil2000	dna	MNIST
Min	nuSHAP vs. SHAP	0.08	0.17	0.31	0.32	0.0	0.01	0.0	0.0	0.0	0.0	0.0
	nuSHAP vs. SHAP	0.05	0.12	0.27	0.32	0.0	0.05	0.0	0.0	0.0	0.03	0.0
Max	nuSHAP vs. SHAP	0.96	0.96	0.94	0.97	0.9	0.94	0.91	0.69	0.69	0.88	0.06
	nuSHAP vs. SHAP	0.88	0.97	0.94	0.95	0.77	0.94	0.91	0.88	0.69	0.88	0.06
Mean	nuSHAP vs. SHAP	0.37	0.53	0.84	0.7	0.21	0.41	0.2	0.12	0.05	0.17	0.0
	nuSHAP vs. SHAP	0.31	0.5	0.84	0.69	0.19	0.42	0.19	0.17	0.08	0.43	0.0

NuSHAP vs. *SHAP – run times

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Tool SHAP produces results of very poor quality!

NuSHAP vs. *SHAP – run times

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	adult	corral	iris	mux6	connect_4	spambase	spectf	clean1	coil2000	dna	MNIST
SHAP	3.4	0.1	0.0	0.0	21.7	0.5	0.7	6.8	28.2	23.0	281.3
nuSHAP	1.9	1.5	1.5	1.5	4.5	2.7	2.9	2.7	1.7	4.5	48.9
#Samples	68045.5	63.7	955.4	63.9	9202.5	13654.1	36459.5	3929.6	2960.8	2756.8	2929.9

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Recap: weighted voting games

- General set up of weighted voting games:
 - Assembly \mathcal{A} of voters, with $m = |\mathcal{A}|$
 - Each voter $i \in \mathcal{A}$ votes **Yes** with n_i votes; otherwise no votes are counted (and he/she votes **No**)
 - A coalition is a subset of voters, $\mathcal{C} \subseteq \mathcal{A}$
 - Quota q is the sum of votes required for a proposal to be approved
 - Coalitions leading to sums not less than q are **winning** coalitions
 - A **weighted voting game (WVG)** is a tuple $[q; n_1, \dots, n_m]$
 - Example: $[12; 4, 4, 4, 2, 2, 1]$
 - Problem: find a measure of importance of each voter !
 - I.e. measure the **a priori voting power** of each voter

What are power indices?

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- **Power indices** assign a measure of importance to each voter
- Many power indices proposed over the years:

- Penrose [Pen46]
- Shapley-Shubik [SS54]
- Banzhaf [Bil65]
- Coleman [Col71]
- Johnston [Joh78]
- Deegan-Packel [DP78]
- Holler-Packel [HP83]
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- Responsability* [CH04, BIL⁺24]
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 - ...
- What characterizes power indices?
 - Account for the cases when voter is *critical* for a winning coalition
 - E.g. in previous example, Luxembourg is never critical for a winning coalition
 - Account for whether coalition is subset-minimal or cardinality-minimal

Towards defining power indices

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 - This means that a voter i is **critical** when:
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- Understanding (subset-)minimal winning coalitions:
 - A winning coalition is subset-minimal if removing any single voter results in a losing coalition
 - A winning coalition is cardinality-minimal if it has the smallest cardinality among subset-minimal winning coalitions
 - Recall that minimal winning coalitions can be obtained by computing the AXps of a monotonically increasing boolean classifier

Example power indices I

[LHAMS24]

- Necessary definitions (using formal XAI notation...):

$$\mathbb{W}\mathbb{A}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \mid \text{WAXp}(\mathcal{S}; \mathcal{E}) \wedge i \in \mathcal{S}\}$$

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- Definitions of $\mathbb{W}\mathbb{A}$, $\mathbb{W}\mathbb{C}$, \mathbb{A} , and \mathbb{C} mimic the ones above, but without specifying a voter
- Power indices of Holler-Packel and Deegan-Packel:

[HP83, DP78]

$$\text{Sc}_H(i; \mathcal{E}) = \sum_{\mathcal{S} \in \mathbb{A}_i(\mathcal{E})} (1/|\mathbb{A}(\mathcal{E})|)$$

$$\text{Sc}_D(i; \mathcal{E}) = \sum_{\mathcal{S} \in \mathbb{A}_i(\mathcal{E})} (1/(|\mathcal{S}| \times |\mathbb{A}(\mathcal{E})|))$$

Example power indices I

[LHAMS24]

- Necessary definitions (using formal XAI notation...):

$$\mathbb{W}\mathbb{A}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \mid \text{WAXp}(\mathcal{S}; \mathcal{E}) \wedge i \in \mathcal{S}\}$$

$$\mathbb{W}\mathbb{C}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \mid \text{WCXp}(\mathcal{S}; \mathcal{E}) \wedge i \in \mathcal{S}\}$$

$$\mathbb{A}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \mid \text{AXp}(\mathcal{S}; \mathcal{E}) \wedge i \in \mathcal{S}\}$$

$$\mathbb{C}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \mid \text{CXp}(\mathcal{S}; \mathcal{E}) \wedge i \in \mathcal{S}\}$$

- Definitions of $\mathbb{W}\mathbb{A}$, $\mathbb{W}\mathbb{C}$, \mathbb{A} , and \mathbb{C} mimic the ones above, but without specifying a voter
- Power indices of Holler-Packel and Deegan-Packel:

[HP83, DP78]

$$\text{Sc}_H(i; \mathcal{E}) = \sum_{\mathcal{S} \in \mathbb{A}_i(\mathcal{E})} (1/|\mathbb{A}(\mathcal{E})|)$$

$$\text{Sc}_D(i; \mathcal{E}) = \sum_{\mathcal{S} \in \mathbb{A}_i(\mathcal{E})} (1/(|\mathcal{S}| \times |\mathbb{A}(\mathcal{E})|))$$

- **Obs:** One *only* needs the **AXps**

Example power indices II

- Additional definitions:

$$\text{Crit}(i, \mathcal{S}; \mathcal{E}) := \text{WAXp}(\mathcal{S}; \mathcal{E}) \wedge \neg \text{WAXp}(\mathcal{S} \setminus \{i\}; \mathcal{E})$$

Example power indices II

- Additional definitions:

$$\text{Crit}(i, \mathcal{S}; \mathcal{E}) := \text{WAXp}(\mathcal{S}; \mathcal{E}) \wedge \neg \text{WAXp}(\mathcal{S} \setminus \{i\}; \mathcal{E})$$

- Power indices of Shapley-Shubik, Banzhaf and Johnston:

[SS54, BI65, Joh78]

$$Sc_S(i; \mathcal{E}) = \sum_{\mathcal{S} \subseteq \mathcal{F} \wedge \text{Crit}(i, \mathcal{S}; \mathcal{E})} \left(1 / \binom{|\mathcal{F}| - 1}{|\mathcal{S}| - 1} \right)$$

$$Sc_B(i; \mathcal{E}) = \sum_{\mathcal{S} \subseteq \mathcal{F} \wedge \text{Crit}(i, \mathcal{S}; \mathcal{E})} \left(1 / 2^{|\mathcal{F}| - 1} \right)$$

$$Sc_J(i; \mathcal{E}) = \sum_{\mathcal{S} \subseteq \mathcal{F} \wedge \text{Crit}(i, \mathcal{S}; \mathcal{E})} \left(1 / \Delta(\mathcal{S}) \right)$$

Example power indices II

- Additional definitions:

$$\text{Crit}(i, \mathcal{S}; \mathcal{E}) := \text{WAXp}(\mathcal{S}; \mathcal{E}) \wedge \neg \text{WAXp}(\mathcal{S} \setminus \{i\}; \mathcal{E})$$

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$$Sc_J(i; \mathcal{E}) = \sum_{\mathcal{S} \subseteq \mathcal{F} \wedge \text{Crit}(i, \mathcal{S}; \mathcal{E})} \left(1 / \Delta(\mathcal{S}) \right)$$

- One needs the **WAXps** to find critical voters...

Example #01

- WVG: [9; 9, 2, 2, 2, 2, 1, 1]

Example #01

- WVG: [9; 9, 2, 2, 2, 2, 1, 1]
- AXps:

1					
2	3	4	5	6	
2	3	4	5	7	

Example #01

- WVG: [9; 9, 2, 2, 2, 2, 1, 1]
- AXps:

1					
2	3	4	5	6	
2	3	4	5	7	

- Holler-Packel scores: $\langle 0.333, 0.667, 0.667, 0.667, 0.667, 0.333, 0.333 \rangle$
- Banzhaf scores (normalized): $\langle 0.813, 0.040, 0.040, 0.040, 0.040, 0.013, 0.013 \rangle$
- Shapley-Shubik scores: $\langle 0.810, 0.043, 0.043, 0.043, 0.043, 0.010, 0.010 \rangle$
- Different relative orders of voter importance... which ones seem more realistic?

Example #02

- WVG: [16; 10, 6, 4, 2, 2]

Example #02

- WVG: [16; 10, 6, 4, 2, 2]
- AXps:

1	2	
1	3	4
1	3	5

Example #02

- WVG: [16; 10, 6, 4, 2, 2]
- AXps:

1	2	
1	3	4
1	3	5

- Deegan-Packel scores: $\langle 0.389, 0.167, 0.222, 0.111, 0.111 \rangle$
- Banzhaf scores (normalized): $\langle 0.524, 0.238, 0.143, 0.048, 0.048 \rangle$
- Shapley-Shubik scores: $\langle 0.617, 0.200, 0.117, 0.033, 0.033 \rangle$
- Different relative orders of voter importance... which ones seem more realistic?

Example #03

- WVG: [6; 4, 2, 1, 1, 1, 1]

Example #03

- WVG: [6; 4, 2, 1, 1, 1, 1]
- AXps:

2	3	4	5	6
1	3	4		
1	4	5		
1	4	6		
1	3	6		
1	5	6		
1	2			
1	3	5		

Example #03

- WVG: [6; 4, 2, 1, 1, 1, 1]
- AXps:

2	3	4	5	6
1	3	4		
1	4	5		
1	4	6		
1	3	6		
1	5	6		
1	2			
1	3	5		

- Deegan-Packel scores: $\langle 0.312, 0.087, 0.150, 0.150, 0.150, 0.150 \rangle$
- Banzhaf scores (normalized): $\langle 0.542, 0.125, 0.083, 0.083, 0.083, 0.083 \rangle$
- Shapley-Shubik scores: $\langle 0.533, 0.133, 0.083, 0.083, 0.083, 0.083 \rangle$
- Different relative orders of voter importance... which ones seem more realistic?

Example #04

- WVG: [21; 12, 9, 4, 4, 1, 1, 1]

Example #04

- WVG: [21; 12, 9, 4, 4, 1, 1, 1]
- AXps:

1	2		
1	3	4	5
1	3	4	6
1	3	4	7

Example #04

- WVG: [21; 12, 9, 4, 4, 1, 1, 1]
- AXps:

1	2		
1	3	4	5
1	3	4	6
1	3	4	7

- Deegan-Packel scores: $\langle 0.312, 0.125, 0.188, 0.188, 0.062, 0.062, 0.062 \rangle$
- Banzhaf scores (normalized): $\langle 0.481, 0.309, 0.086, 0.086, 0.012, 0.012, 0.012 \rangle$
- Shapley-Shubik scores: $\langle 0.574, 0.257, 0.074, 0.074, 0.007, 0.007, 0.007 \rangle$
- Different relative orders of voter importance... which ones seem more realistic?

Outline – Unit #07

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

A Correct New SHAP – nuSHAP

Voting Power & Power Indices

Feature Importance Scores

From power indices to feature importance scores

- A **Feature Importance Score** (FIS) is a measure of feature importance in XAI, parameterizable on an **explanation problem** and a chosen **characteristic function**
 - Explanation problem: $(\mathcal{M}, (\mathbf{v}, q))$
 - Define characteristic function using explanation problem (more next slide)
- Obs: Can adapt (generalized) power indices as templates for feature importance scores
- Obs: Can devise new templates and/or new FISs

Some examples (1 of 2)

- More notation:

$$\Delta_i(\mathcal{S}; \mathcal{E}, v) = v(\mathcal{S}; \mathcal{E}) - v(\mathcal{S} \setminus \{i\}; \mathcal{E})$$

- Can use **any** characteristic function, including those presented earlier in this lecture

Some examples (1 of 2)

- More notation:

$$\Delta_i(\mathcal{S}; \mathcal{E}, v) = v(\mathcal{S}; \mathcal{E}) - v(\mathcal{S} \setminus \{i\}; \mathcal{E})$$

- Can use **any** characteristic function, including those presented earlier in this lecture

- Some templates:

- Shapley-Shubik:

$$\text{TSc}_S(i; \mathcal{E}, v) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v)}{|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1}} \right)$$

- Banzhaf:

$$\text{TSc}_B(i; \mathcal{E}, v) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v)}{2^{|\mathcal{F}|-1}} \right)$$

Some examples (1 of 2)

- More notation:

$$\Delta_i(\mathcal{S}; \mathcal{E}, v) = v(\mathcal{S}; \mathcal{E}) - v(\mathcal{S} \setminus \{i\}; \mathcal{E})$$

- Can use **any** characteristic function, including those presented earlier in this lecture

- Some templates:

- Shapley-Shubik:

$$\text{TSc}_S(i; \mathcal{E}, v) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v)}{|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1}} \right)$$

- Banzhaf:

$$\text{TSc}_B(i; \mathcal{E}, v) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v)}{2^{|\mathcal{F}|-1}} \right)$$

- Can use other templates

Some examples (1 of 2)

- More notation:

$$\Delta_i(\mathcal{S}; \mathcal{E}, v) = v(\mathcal{S}; \mathcal{E}) - v(\mathcal{S} \setminus \{i\}; \mathcal{E})$$

- Can use **any** characteristic function, including those presented earlier in this lecture

- Some templates:

- Shapley-Shubik:

$$TSc_S(i; \mathcal{E}, v) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v)}{|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1}} \right)$$

- Banzhaf:

$$TSc_B(i; \mathcal{E}, v) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v)}{2^{|\mathcal{F}|-1}} \right)$$

- Can use other templates

- Can devise FISs without exploiting existing templates

Some examples (2 of 2)

- Recall WAXp-based characteristic function:

$$v_a(\mathcal{S}) := \begin{cases} 1 & \text{if } \mathbf{E}[\sigma(\mathbf{x}) \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}] = 1 \\ 0 & \text{otherwise} \end{cases}$$

Some examples (2 of 2)

- Recall WAXp-based characteristic function:

$$v_a(\mathcal{S}) := \begin{cases} 1 & \text{if } \mathbf{E}[\sigma(\mathbf{x}) \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}] = 1 \\ 0 & \text{otherwise} \end{cases}$$

- Some FISs:

- Shapley-Shubik:

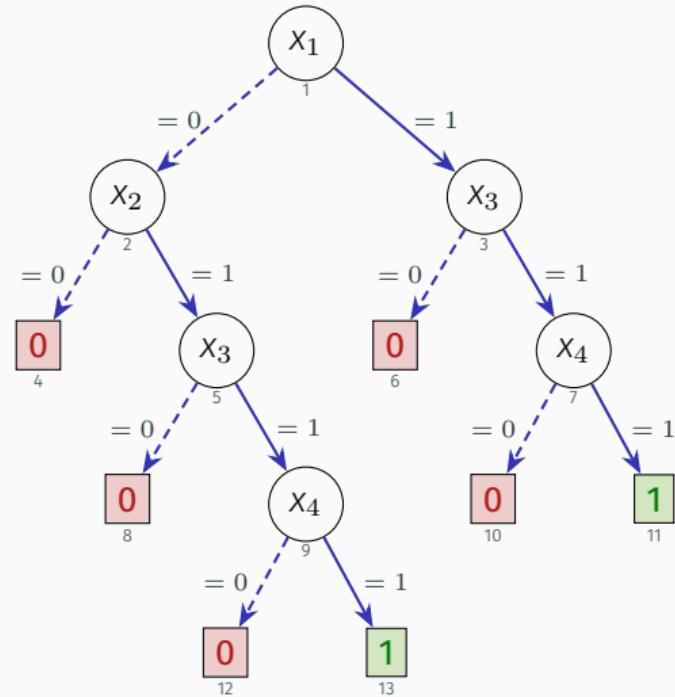
$$\text{Sc}_S(i; \mathcal{E}) := \text{TSc}_S(i; \mathcal{E}, v_a) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v_a)}{|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1}} \right)$$

- Banzhaf:

$$\text{Sc}_B(i; \mathcal{E}) := \text{TSc}_B(i; \mathcal{E}, v_a) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S}; \mathcal{E}, v_a)}{2^{|\mathcal{F}|-1}} \right)$$

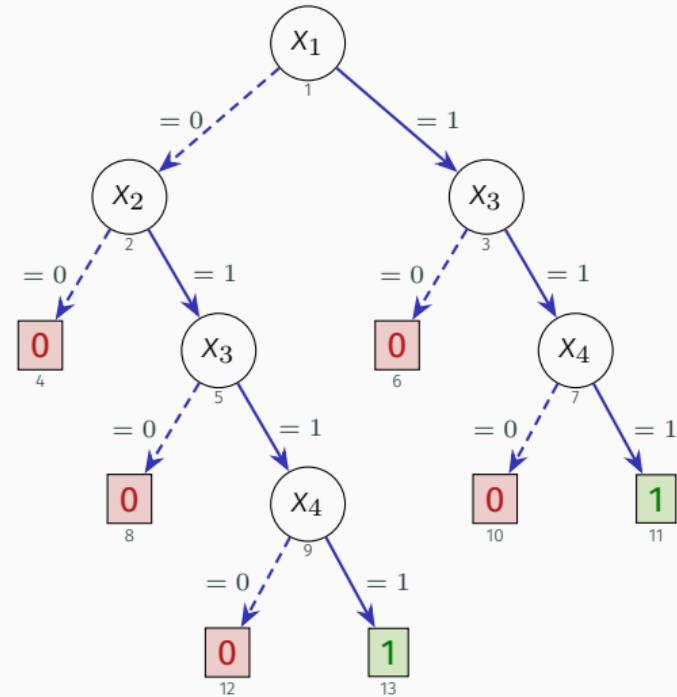
A concrete example

- AXps: $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
- Feature attribution:



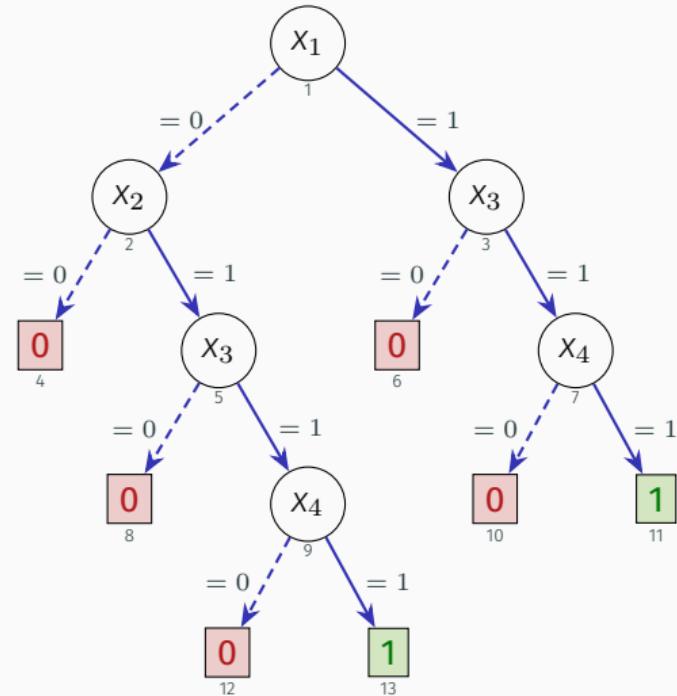
A concrete example

- AXps: $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
- Feature attribution:
 - SS: $\langle 0.083, 0.083, 0.417, 0.417 \rangle$



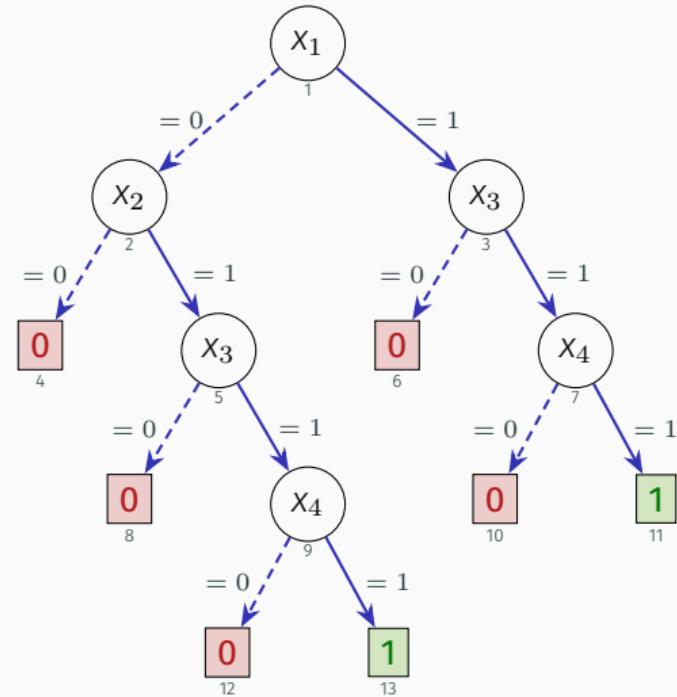
A concrete example

- AXps: $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
- Feature attribution:
 - SS: $\langle 0.083, 0.083, 0.417, 0.417 \rangle$
 - B (norm.): $\langle 0.125, 0.125, 0.375, 0.375 \rangle$



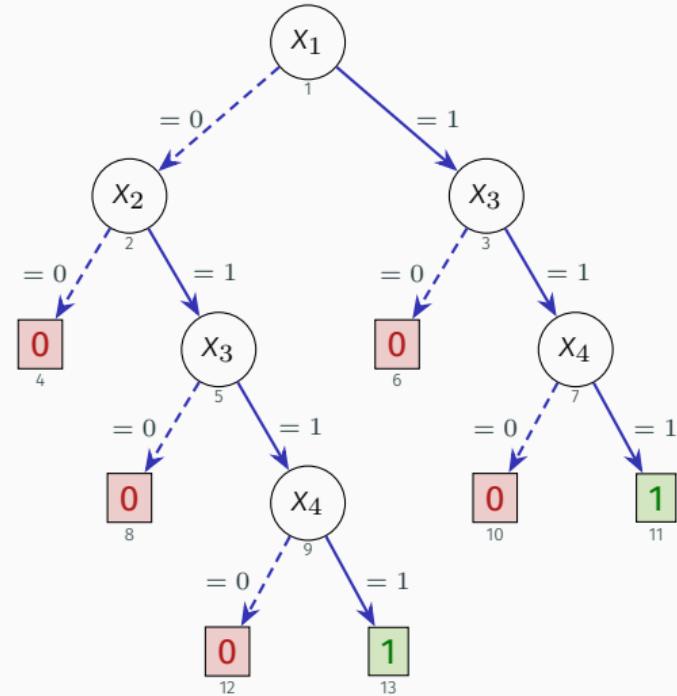
A concrete example

- AXps: $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
- Feature attribution:
 - SS: $\langle 0.083, 0.083, 0.417, 0.417 \rangle$
 - B (norm.): $\langle 0.125, 0.125, 0.375, 0.375 \rangle$
 - J (norm.): $\langle 0.111, 0.111, 0.389, 0.389 \rangle$



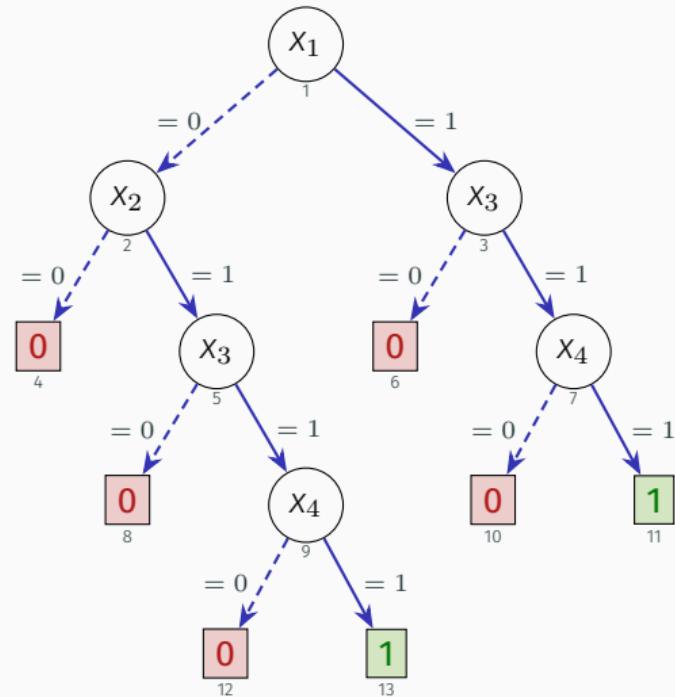
A concrete example

- AXps: $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
- Feature attribution:
 - SS: $\langle 0.083, 0.083, 0.417, 0.417 \rangle$
 - B (norm.): $\langle 0.125, 0.125, 0.375, 0.375 \rangle$
 - J (norm.): $\langle 0.111, 0.111, 0.389, 0.389 \rangle$
 - HP: $\langle 0.167, 0.167, 0.333, 0.333 \rangle$



A concrete example

- AXps: $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
- Feature attribution:
 - SS: $\langle 0.083, 0.083, 0.417, 0.417 \rangle$
 - B (norm.): $\langle 0.125, 0.125, 0.375, 0.375 \rangle$
 - J (norm.): $\langle 0.111, 0.111, 0.389, 0.389 \rangle$
 - HP: $\langle 0.167, 0.167, 0.333, 0.333 \rangle$
 - DP: $\langle 0.167, 0.167, 0.333, 0.333 \rangle$



Questions?

Unit #08

Conclusions & Research Directions

Outline – Unit #08

Some Words of Concern

Conclusions & Research Directions

Can non-symbolic XAI's myths be stopped?

SHAP on 2023/05/31:

The screenshot shows a Google Scholar search results page. The search query is "A unified approach to interpreting model predictions". The top result is a paper by SM Lundberg and SI Lee, titled "A unified approach to interpreting model predictions". The abstract discusses the tension between accuracy and interpretability in complex models. The page includes filters for time (Any time, Since 2023, Since 2022, Since 2019, Custom range...), sorting options (Sort by relevance, Sort by date), and other search parameters (Any type, Review articles, include patents, include citations). A sidebar on the left shows a list of filters and sorting options.

A unified approach to interpreting model predictions

SM Lundberg, SI Lee - Advances in neural information ..., 2017 - proceedings.neurips.cc

Understanding why a model makes a certain prediction can be as crucial as the prediction's accuracy in many applications. However, the highest accuracy for large modern datasets is often achieved by complex models that even experts struggle to interpret, such as ensemble or deep learning models, creating a tension between accuracy and interpretability. In response, various methods have recently been proposed to help users interpret the predictions of complex models, but it is often unclear how these methods are related and ...

☆ Save 99 Cite Cited by 13080 Related articles All 17 versions

Any time

Since 2023

Since 2022

Since 2019

Custom range...

Sort by relevance

Sort by date

Any type

Review articles

include patents

include citations

[PDF] neurips.cc

Can non-symbolic XAI's myths be stopped?

SHAP on 2024/09/15:

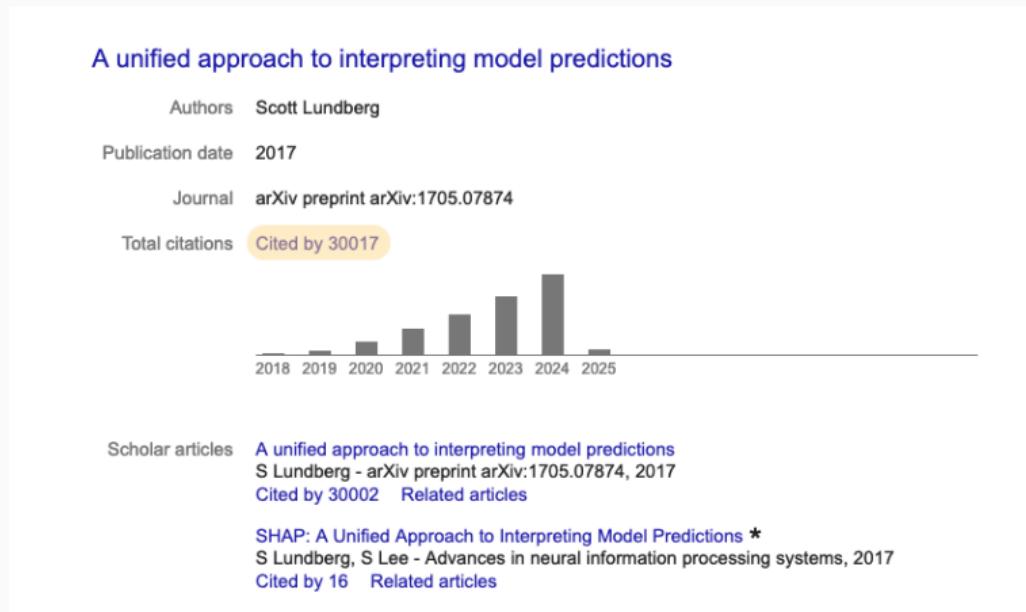
The screenshot shows a Google Scholar search results page. The search query is "A unified approach to interpreting model predictions". The results list two papers:

- [CITATION] A unified approach to interpreting model predictions**
S Lundberg - arXiv preprint arXiv:1705.07874, 2017
☆ Save ⚡ Cite Cited by 25778 Related articles
- [CITATION] A unified approach to interpreting model predictions**
M Scott, L Su-In - Advances in neural information ..., 2017 - Curran Associates, Inc
☆ Save ⚡ Cite Cited by 108 Related articles

On the left sidebar, there are filters for time (Any time, Since 2024, Since 2023, Since 2020, Custom range...), sorting options (Sort by relevance, Sort by date), and type (Any type, Review articles). At the bottom, there are checkboxes for "include patents" (unchecked) and "include citations" (checked).

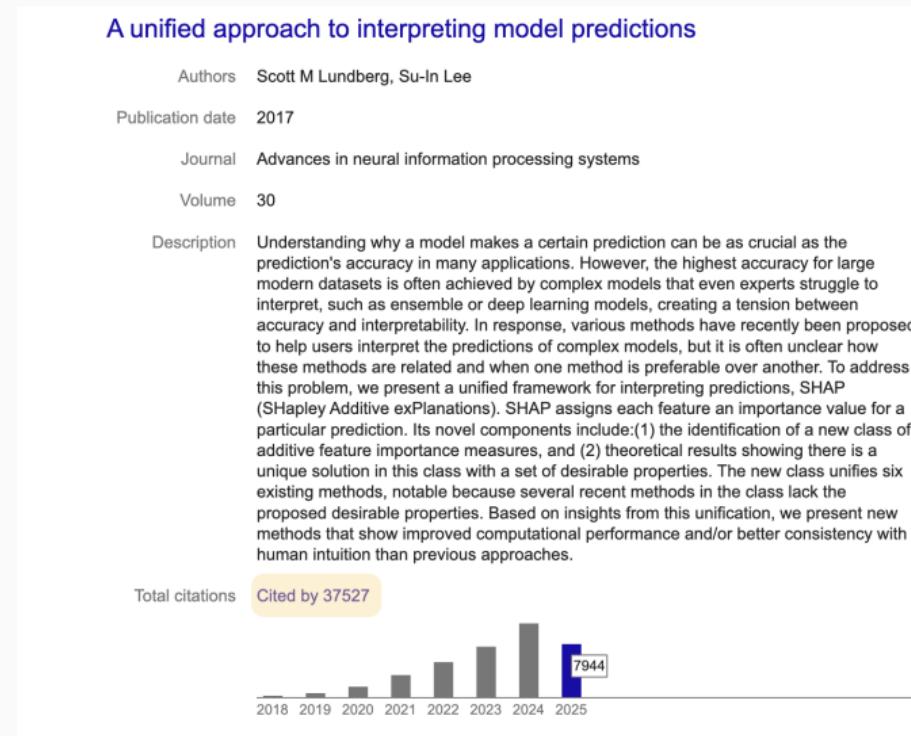
Can non-symbolic XAI's myths be stopped?

SHAP on 2025/01/12:



Can non-symbolic XAI's myths be stopped?

SHAP on 2025/07/14:



Can non-symbolic XAI's myths be stopped?

SHAP on 2025/07/14:

A unified approach to interpreting model predictions

Authors Scott M Lundberg, Su-In Lee

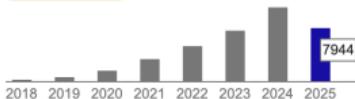
Publication date 2017

Journal Advances in neural information processing systems

Volume 30

Description Understanding why a model makes a certain prediction can be as crucial as the prediction's accuracy in many applications. However, the highest accuracy for large modern datasets is often achieved by complex models that even experts struggle to interpret, such as ensemble or deep learning models, creating a tension between accuracy and interpretability. In response, various methods have recently been proposed to help users interpret the predictions of complex models, but it is often unclear how these methods are related and when one method is preferable over another. To address this problem, we present a unified framework for interpreting predictions, SHAP (SHapley Additive exPlanations). SHAP assigns each feature an importance value for a particular prediction. Its novel components include:(1) the identification of a new class of additive feature importance measures, and (2) theoretical results showing there is a unique solution in this class with a set of desirable properties. The new class unifies six existing methods, notable because several recent methods in the class lack the proposed desirable properties. Based on insights from this unification, we present new methods that show improved computational performance and/or better consistency with human intuition than previous approaches.

Total citations Cited by 37527



But,

Theoretical SHAP scores can mislead;
& results of tool SHAP of poor quality!

Many, many high-risk uses of SHAP & clones

He et al. *Journal of Translational Medicine* (2024) 22:686
https://doi.org/10.1186/s12967-024-05417-y

Journal of Translational
Medicine

RESEARCH

Open Access



Predictive models for personalized precision medical intervention in spontaneous regression stages of cervical precancerous lesions

XGBoost-SHAP-based interpretable diagnostic framework for alzheimer's disease

Hypothesis-free discovery of novel cancer predictors using machine learning

Explainable AI-based Deep-SHAP for mapping the multivariate relationships between regional neuroimaging biomarkers and cognition

npj Digital Medicine

Interpretable prediction of 30-day mortality in patients with acute pancreatitis based on machine learning and SHAP

scientific reports

scientific reports

OPEN

An explainable machine learning framework for lung cancer hospital length of stay prediction

© J. Marques-Silva

PLOS ONE

RESEARCH ARTICLE

Combining explainable machine learning, demographic and multi-omic data to inform precision medicine strategies for inflammatory bowel disease

scientific reports

OPEN

Explanatory predictive model for COVID-19 severity risk employing machine learning, shapley addition, and LIME



ARTICLE OPEN

Comparing machine learning algorithms for predicting ICU admission and mortality in COVID-19



scientific reports

OPEN

The importance of interpreting machine learning models for blood glucose prediction in diabetes: an analysis using SHAP



OPEN SHAP based predictive modeling for 1 year all-cause readmission risk in elderly heart failure patients: feature selection and model interpretation



230 / 238

What next?

What next? Massive retraction (of tens of thousands) of papers??



thanks to ChatGPT...

What next? Massive retraction (of tens of thousands) of papers??



& beware of high-risk uses of SHAP! 😞

thanks to ChatGPT...

What's the bottom line?

What's the bottom line?

- Non-symbolic XAI research experiences a persistent “*Don’t Look Up*” moment...



What's the bottom line?

- Non-symbolic XAI research experiences a persistent “*Don’t Look Up*” moment...



BTW, there are a multitude of proposed uses of LIME/Shap in medicine... ⚠️

Some unsettling works...

- For DTs:
 - One AXp in polynomial-time [IIM20, HIIM21, IIM22]
 - All CXps in polynomial-time [HIIM21, IIM22]

Some unsettling works...

- For DTs:
 - One AXp in polynomial-time [IIM20, HIIM21, IIM22]
 - All CXps in polynomial-time [HIIM21, IIM22]

Declarative Reasoning on Explanations Using Constraint Logic Programming

Abstract. Explaining opaque Machine Learning (ML) models is an increasingly relevant problem. Current explanation in AI (XAI) methods suffer several shortcomings, among others an insufficient incorporation of background knowledge, and a lack of abstraction and interactivity with the user. We propose REASONX, an explanation method based on Constraint Logic Programming (CLP). REASONX can provide declarative, interactive explanations for decision trees, which can be the ML models under analysis or global/local surrogate models of any black-box model. Users can express background or common sense knowledge using linear constraints and MILP optimization over features of factual and contrastive instances, and interact with the answer constraints at different levels of abstraction through constraint projection. We present here the architecture of REASONX, which consists of a Python layer, closer to the user, and a CLP layer. REASONX's core execution engine is a Prolog meta-program with declarative semantics in terms of logic theories.

arXiv:2309.00422v1 [cs.AI] 1 Sep 2023

Some unsettling works...

- For DTs:
 - One AXp in polynomial-time
 - All CXps in polynomial-time

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]

HHAI 2024: Hybrid Human AI Systems for the Social Good
F. Lorig et al. (Eds.)
© 2024 The Authors.

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of the Creative Commons Attribution Non-Commercial License 4.0 (CC BY-NC 4.0).
doi:10.3233/FAIA240183*

Exploring Large Language Models Capabilities to Explain Decision Trees

Some unsettling works...

- For DTs:
 - One AXp in polynomial-time
 - All CXps in polynomial-time

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]

Explainable Artificial Intelligence for Academic Performance Prediction. An Experimental Study on the Impact of Accuracy and Simplicity of Decision Trees on Causability and Fairness Perceptions

FAccT '24, June 03–06, 2024, Rio de Janeiro, Brazil
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ACM ISBN 979-8-4007-0450-5/24/06
<https://doi.org/10.1145/3630106.3658953>

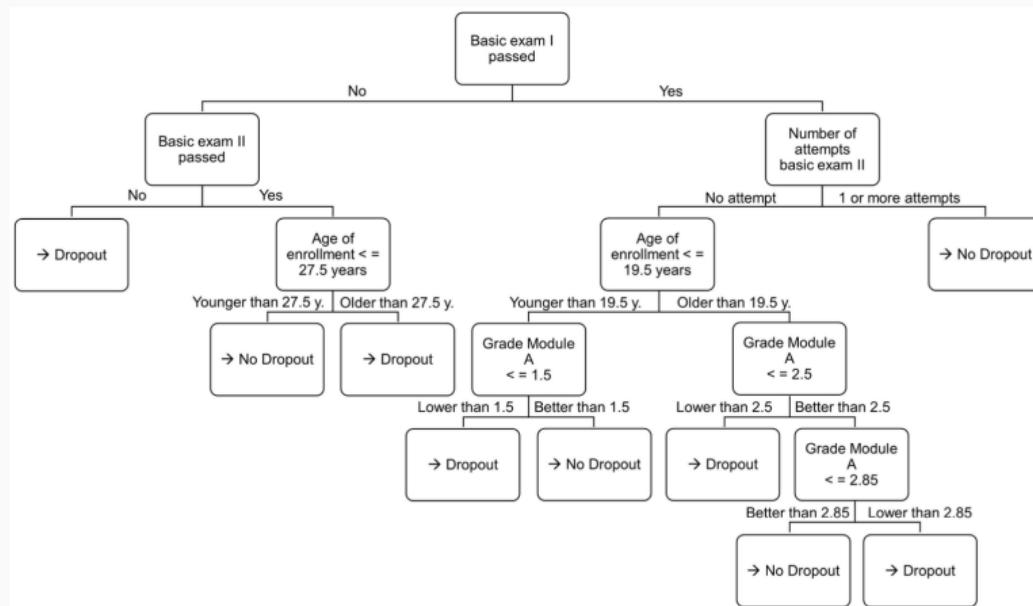
Some unsettling works...

- For DTs:

- One AXp in polynomial-time
- All CXps in polynomial-time

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]



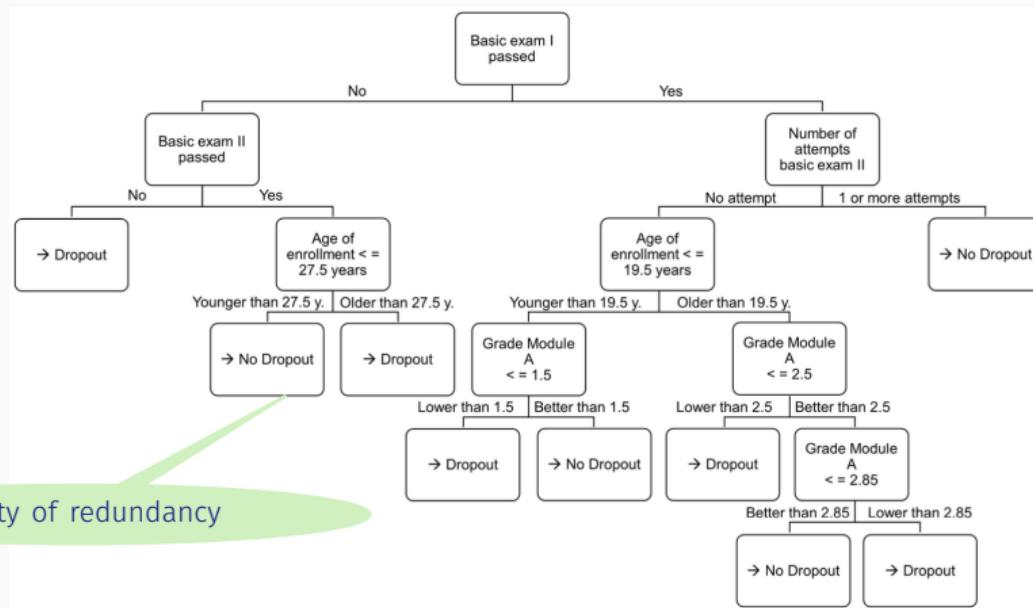
Some unsettling works...

- For DTs:

- One AXp in polynomial-time
- All CXps in polynomial-time

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]



Outline – Unit #08

Some Words of Concern

Conclusions & Research Directions

Conclusions

- Covered logic-based (aka symbolic, aka formal) XAI & its recent progress:
 - Abductive & contrastive explanations
 - Reviewed their computation in practice
 - Duality & enumeration
 - Other explainability queries – feature necessity & relevancy

Conclusions

- Covered logic-based (aka symbolic, aka formal) XAI & its recent progress:
 - Abductive & contrastive explanations
 - Reviewed their computation in practice
 - Duality & enumeration
 - Other explainability queries – feature necessity & relevancy
- Showed that formal XAI **disproves** some myths of (heuristic) XAI:
 - Explainability using intrinsic interpretability is a **myth**
 - The rigor of model-agnostic explanations is a **myth**
 - The rigor of SHAP scores as a measure of relative feature importance is a **myth**

Conclusions

- Covered logic-based (aka symbolic, aka formal) XAI & its recent progress:
 - Abductive & contrastive explanations
 - Reviewed their computation in practice
 - Duality & enumeration
 - Other explainability queries – feature necessity & relevancy
- Showed that formal XAI **disproves** some myths of (heuristic) XAI:
 - Explainability using intrinsic interpretability is a **myth**
 - The rigor of model-agnostic explanations is a **myth**
 - The rigor of SHAP scores as a measure of relative feature importance is a **myth**
- Demonstrated tight connection between (rigorous) feature selection and (rigorous) feature attribution in XAI

Conclusions

- Covered logic-based (aka symbolic, aka formal) XAI & its recent progress:
 - Abductive & contrastive explanations
 - Reviewed their computation in practice
 - Duality & enumeration
 - Other explainability queries – feature necessity & relevancy
- Showed that formal XAI **disproves** some myths of (heuristic) XAI:
 - Explainability using intrinsic interpretability is a **myth**
 - The rigor of model-agnostic explanations is a **myth**
 - The rigor of SHAP scores as a measure of relative feature importance is a **myth**
- Demonstrated tight connection between (rigorous) feature selection and (rigorous) feature attribution in XAI
- Symbolic XAI exhibits links with many fields of research:
machine learning, artificial intelligence, formal methods, automated reasoning, optimization, computational social choice (& game theory), etc.

Research directions

Research directions

- Scalability, scalability, and scalability

Research directions

- Scalability, scalability, and scalability
- Sample-based explanations & coherency

Research directions

- Scalability, scalability, and scalability
- Sample-based explanations & coherency
- Rigorous feature attribution

Research directions

- Scalability, scalability, and scalability
- Sample-based explanations & coherency
- Rigorous feature attribution
- Checking & certification of XAI tools

Research directions

- Scalability, scalability, and scalability
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- Open complexity results

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- Open complexity results
- Preferred explanations

Research directions

- Scalability, scalability, and scalability
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- Preferred explanations
- Distance-restricted explanations

Research directions

- Scalability, scalability, and scalability
- Sample-based explanations & coherency
- Rigorous feature attribution
- Checking & certification of XAI tools
- Open complexity results
- Preferred explanations
- Distance-restricted explanations
- Probabilistic explanations

Research directions

- Scalability, scalability, and scalability
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- Rigorous feature attribution
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- Open complexity results
- Preferred explanations
- Distance-restricted explanations
- Probabilistic explanations
- Any ideas from you?

Research directions

- Scalability, scalability, and scalability
- Sample-based explanations & coherency
- Rigorous feature attribution
- Checking & certification of XAI tools
- Open complexity results
- Preferred explanations
- Distance-restricted explanations
- Probabilistic explanations
- Any ideas from you?
- ... And trying to curb the **massive** momentum of (heuristic) XAI **myths!**

What this course covered

- Lecture 01 – unit(s):
 - #01: Foundations
- Lecture 02 – unit(s):
 - #02: Principles of symbolic XAI – feature selection
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 – unit(s):
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 – unit(s):
 - #06: Recent, emerging & advanced topics
- Lecture 05 – unit(s):
 - #07: Principles of symbolic XAI – feature attribution (& myth of Shapley values in XAI)
 - #08: Corrected feature attribution – nuSHAP
 - #09: Conclusions & research directions

Some food for thought...

"All truths are easy to understand once they are discovered; the point is to discover them."

(G. Galilei)

"Beware of false knowledge; it is more dangerous than ignorance."

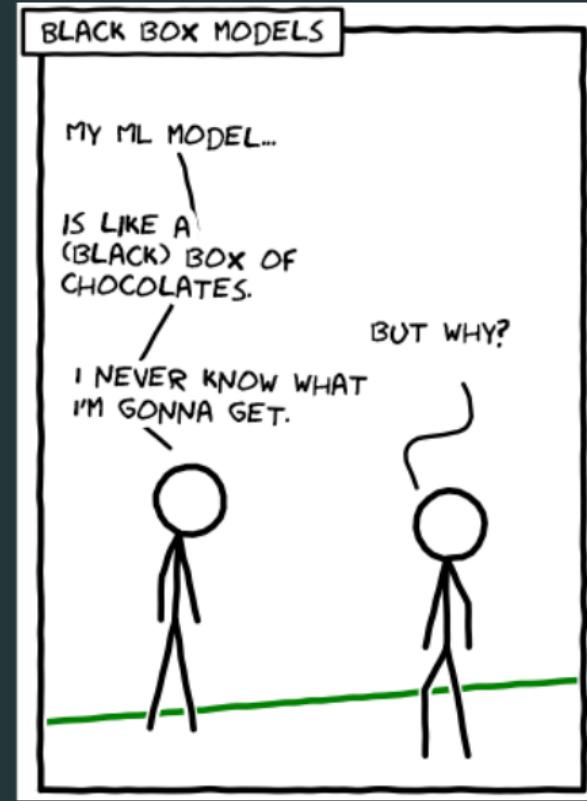
(G. B. Shaw)

"He who loves practice without theory is like the sailor who boards ship without a rudder and compass and never knows where he may cast."

(L. da Vinci)

Q & A

Acknowledgment: joint work with X. Huang, Y. Izza, O. Létoffé, A. Ignatiev, N. Narodytska, M. Cooper, N. Asher, A. Morgado, J. Planes, et al.



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